DIONEX

PeakNet 6 Tutorial and User's Guide

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SCIENTIFIC

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A

AAA-Direct™ Amino Acid Analysis System
AAES™
Acrodisk® (Gelman Sciences, Inc.)
Advanced Computer Interface (ACI)
Advanced Gradient Pump (AGP)
AES™ Atlas Electrolytic Suppressor
AD20 UV/VIS Absorbance Detector
AminoPac® Columns
AminoTrap™ Columns
AMMS®-ICE, AMMS-ICE II Anion MicroMembrane Suppressor
AppliCard™
Aroclor™ (Monsanto Corp.)
AS40 Automated Sampler
AS3500 Autosampler
ASE® 200 or 300 Accelerated Solvent Extractor or Solvent Controller
ASI-100™ or ASI-100T™ Automated Sample Injector
ASRN™ Anion Self-Regenerating Neutralizer
ASRS®, ASRS®-II, or ASRS®-ULTRA Anion Self-Regenerating Suppressor
Atlas™
Auto OnGuard™ (but OnGuard®)
AutoASE® Software
Autoion®
AutoNeutralization™ System or Technology
AutoRegen® System
AutoSelect™
AutoSuppression® Technology
Anion Self-Regenerating Suppressor®

B

BioLC® System
BioPlus™ Columns
BioSelect™ (The Separations Group)
BorateTrap™ Column

C

CA Carbamate Analyzer
CAES™
CarboPac™ MA1, PA1, PA10, PA-100 Columns
Cation Atlas™ Electrolytic Suppressor
Cation MicroMembrane Suppressor®
Cation Self-Regenerating Suppressor®
CD Builder™ (AppletWare Inc.)
ChromatoCritters™
CH-2 Column Heater
CHX650 Column Temperature Controller
CHROMELEON™
CMD™ Carbohydrate Membrane Desalter
CMMS® Cation MicroMembrane Suppressor
CSRN™ Cation Self-Regenerating Neutralizer
CSRS®, CSRS®-II, CSRS®-ULTRA Cation Self-Regenerating Suppressor
CD20 Conductivity Detector
CMMS®-II Cation MicroMembrane Suppressor®

D

DataDetective™ (AppletWare, Inc.)
dBASE® (Borland International, Inc.)
Dequest® (Monsanto Corporation)
Dionex®
DNAPac® Column (for NucleoPac)
DNAPhor™ SB1.5 kB Sieving Buffer Kit (for NucleoPhor)
Dowex® (Dow Chemical Company)
DX-80 Ion Analyzer
DX-120 Ion Chromatograph
DX-500 HPLC System
DX-500 Ion Chromatography (IC) System
DX-800 Process Analyzer
DX-LAN™ Instrument Interface
DXSil™

E

ED40 Electrochemical Detector
EluGen®
Eluent Gradient Mixers (GM-2, GM-3, GM-4)
EO1 Eluent/Solvent Organizer

F

Flarefit®
FPLC® (Pharmacia LKB)
Freon® (E.I. du Pont de Nemours & Co.)

G

GP40 Gradient Pump
GP50 Gradient Pump

H

HPIC® (mostly replaced by IonPac®)
HPICE® (mostly replaced by IonPac® ICE)
Hydromatrix™ (Varian Associates, Inc.)

I

ICE (ion-exclusion columns, e.g., ICE-AS6)
InkJet (Hewlett-Packard)
IonPac® Columns
IonPhor™ Electrolyte Buffers
IonSep® Reagents
IP20 Isocratic Pump
Irganox® (Ciba)

K

Kalrez® (E.I. du Pont de Nemours & Co.)
KEL-F® (3M Corporation)

L

LANtastic® (Artisoft, Inc.)
LaserJet® (Hewlett-Packard Corporation)
LC5 Injection Module
LC10 Chromatography Organizer
LC20 Chromatography Enclosure
LC25 Chromatography Oven
LC30 Chromatography Oven

M

MetPac™ Reagents
MFC-1 (Metal-Free Column)
MICRO® (International Products Corp.)
MicroBead™MicroInjection Valve
MicroMembrane™ Suppressors
MMS™ MicroMembrane Suppressor
Mono Q® (Pharmacia LKB)
MonoStandard®
MPIC® (Mobile Phase IC)
MS-DOS® (Microsoft Corporation)

N

N-EVAP® (Organomation Associates, Inc.)
NovaPak® (Waters Corp.)
NucleoPac (now DNAPac®)
NucleoPhor (now DNAPhor™)

O

OligoStandards™
OmniPac® Columns
OnGuard®, OnGuard®-II Sample Prep Station
(but Auto OnGuard™)
Optima™ (Fisher Scientific)
ORBO™ (Supelco, Inc.)

P

PaintJet® (Hewlett-Packard)
PC10 Postcolumn Pneumatic Controller
PC10 Reagent Delivery Module
PD40 Diode Array Detector
PeakNet® Chromatography Workstation
Pentium® (Intel)
Pico-Buffer®
PolyVial™
PowerPoint® (Microsoft)
Process 450 (data system for 8200 series)
ProPac® Columns

S

SelectaPore™ Columns (The Separations Group)
Self-Regenerating Suppressor®
Series 600 SFC and SFC/GC Systems
SFE-723 Supercritical Fluid Extractor
SP10 AutoNeutralization™ System
SpeedVac™ (Savant Corp.)
SRC SRS Controller)
SRN™ Self-Regenerating Neutralizer
SRS® Self-Regenerating Suppressor
Summit™ HPLC System (initial capped only)
SUPELCOSIL™, Supelguard™ (Supelco, Inc.)
Superose® (Pharmacia LKB)
SupraPur® (EM Industries, Inc.)

T

TAC-1 (Trace Anion Concentrator)
TCC-1 (Trace Cation Concentrator)
Teflon®, Tefzel® (E.I. du Pont de Nemours & Co.)
ThermoFlare™
Triton® X-100 (Rohm & Haas)
TurboVap® (Zymark Corporation)

U

UI20 Universal Interface
Ultrex® (J.T. Baker)

V

Vespel® (E.I. du Pont de Nemours & Co.)
VHP™ (The Separations Group, Inc.)
Vydac® Columns (The Separations Group, Inc.)

W

Windows® 98 (Microsoft Corporation - Windows is ® only if used together with 98, etc. not when used alone)
Windows NT®
Windows™ (Microsoft Corporation)
Wonderware® (Wonderware Corporation)
Wonderware InTouch® (Wonderware Corporation)
WordPerfect® (WordPerfect Corporation)

X, Y, and Z

Zitex® (Norton Chemplast)
Zorbax® (E.I. du Pont de Nemours & Co.)

Numbers

201HS™ (The Separations Group, Inc.)
201TP™ (The Separations Group, Inc.)
202TP™ (The Separations Group, Inc.)
208HS™ (The Separations Group, Inc.)
208TP™ (The Separations Group, Inc.)
214TP™ (The Separations Group, Inc.)
218MR™ (The Separations Group, Inc.)
218TP™ (The Separations Group, Inc.)
219TP™ (The Separations Group, Inc.)
228TP™ (The Separations Group, Inc.)
259VHP™ (The Separations Group, Inc.)
300VHP™ (The Separations Group, Inc.)
301VHP™ (The Separations Group, Inc.)
302IC4.6™ (The Separations Group, Inc.)
400VHP™ (The Separations Group, Inc.)

PeakNet 6 Tutorial

PeakNet 6 Tutorial Contents

The Dionex Chromatography Management System - Tutorial

Welcome to the Dionex CMS, the innovative chromatography management system!

This tutorial will help you to learn how to use the Dionex Chromatography Management System step by step:

- **Starting the program**
- **Performing an analysis**
- **Reprocessing data**

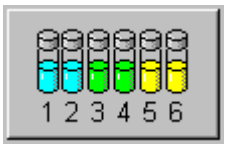
☞ ***Tip:*** The following arrow ➔ marks references within the Tutorial. The arrow is given in front of the title to which the reference relates: *(**e.g.** ➔Contents Overview).*

Contents Overview

I.

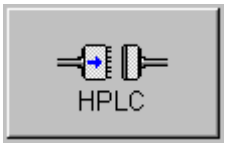
➔*Starting the Dionex Chromatography Management System*: As soon as your computer and one of the operating systems Windows 98 or Windows NT/Windows 2000 are running, the Dionex Chromatography Management System can be started via the Windows Start button on the task bar.

II.



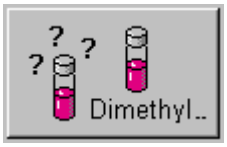
Managing Data: The Dionex Chromatography Management System allows you to manage data in folders and directories similar to Microsoft Windows. The tool that helps you to handle your chromatography data is the ➔*Browser*.

III.



Controlling your HPLC system: Ensure that your chromatography, HPLC, GC, or CE instruments are correctly connected to the PC via a serial port. Using the ➔*Control Panel* allows you to operate the pump, autosampler, detector, etc. from your PC. In addition, you can create a ➔*Control File (PGM File)* to control your system automatically.

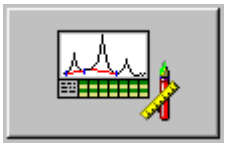
IV.



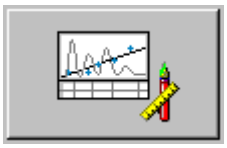
Analyzing Samples: Are your instruments controllable via the PC? Then, you can start your first analysis. Create a ➔*Sample List (= Sequence)* to use all capabilities the Dionex Chromatography Management System offers.
Use the ➔*Sequence Wizard* to include the samples to be processed in the sample list. The Wizard allows you to define the order of sample processing, the injection volumes, the sample type (analysis or standard), and where the Dionex Chromatography Management System finds information on how to perform the analysis.

The latter is by entering a program and a method name, and by creating the corresponding files (PGM file, QNT file, see below).

As soon as you have created the sample list, you can start the ➔*Analysis*. The resulting data is automatically saved.

V. 

Reprocessing Data: The analysis result can be viewed and edited on the screen. ➔*Data Reprocessing* allows you to manually change integration limits directly in the chromatogram or to evaluate samples again ("offline") based on new parameters.

VI. 

Quantifying: Using a ➔*Quantification Method (QNT File)* allows you to minimize the reprocessing effort for individual chromatograms. The QNT Method defines the detection parameters, the peak identification, and the calibration of the substances in the sequence.

VII. 

Printing Results: Analysis data can be ➔*printed* at any time. For perfect adjustment to your personal requirements, you can create your own report templates in the ➔*Printer Layout*, define your own result variables, or embed your company logo.

VIII. 

Online Help: This Tutorial can only deal with selected aspects of the Dionex Chromatography Management System. For further information, please see the detailed descriptions in the ➔*Online Help* or in the User Manual.

I. Starting the Dionex Chromatography Management System

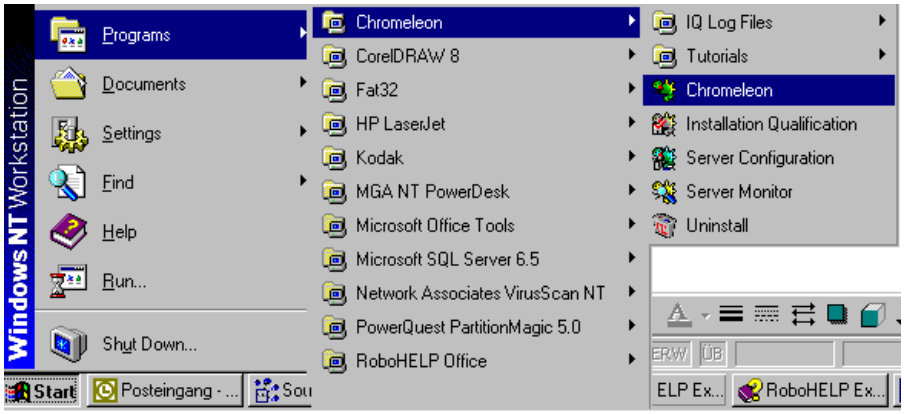
The Dionex Chromatography Management System can be used both, under Windows 98 and Windows NT/Windows 2000. It has been designed as client/server program to allow operation in a network.

The main characteristic of client/server systems is: Certain processes are performed on the client, while others run on the server. The correct cooperation between the client and the server is crucial to the full functionality of the program. The client and the server are not required to be located on the same computer. Communication via a network or a modem will be sufficient. Since the client and the ➔*Server* are independent programs, they have to be started separately.

- Click the **Start** button to open the **Start** menu. Move the mouse cursor to **Programs** to display the submenus.
- Move the mouse cursor to the submenu of your Dionex Chromatography Management System, e.g. **CHROMELEON**. Again, several submenus are shown.

Starting the Client Program

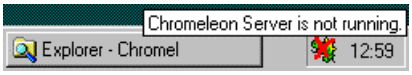
- Click **CHROMELEON** to start the chromatography management system.
- If User Management was enabled during the installation, a logon dialog box appears. In this case, enter your user ID and your personal password.



Starting the Server Program

If you do not only want to view data but control an entire chromatography system and perform your own analyses, you need to start the server program (Server Monitor). The server controls all connected instruments and allows direct instrument operation and control via the PC.

- Choose **Server Monitor** to start the **Chromeleon Server Monitor** program. The CHROMELEON icon appears on the Windows task bar next to the Windows system clock.



☞ ***Tip:*** When being installed, the Dionex Chromatography Management System creates a link in the Autostart group and the corresponding icon will be displayed. You can also configure the program to start whenever the computer is started.

- Move the mouse cursor over the icon. You will see the quick info message: **CHROMELEON Server is not running**.
- Open the context menu (right mouse button) and choose **Start Server** (or double-click the icon and press **Start**). The icon goes through different color phases. Gray coloring indicates that the server is running idle.

- Both, the client program and the server program are active now. The client control panel allows direct access to all instruments connected to the server.

Note: The instruments of a system are combined in a common ➔*Timebase*. Installing and configuring instruments and timebases are via the installation program (= Server Configuration). The Dionex Service normally performs this during the installation.

II. The Browser

The Browser window is loaded automatically whenever the Dionex Chromatography Management System is started.

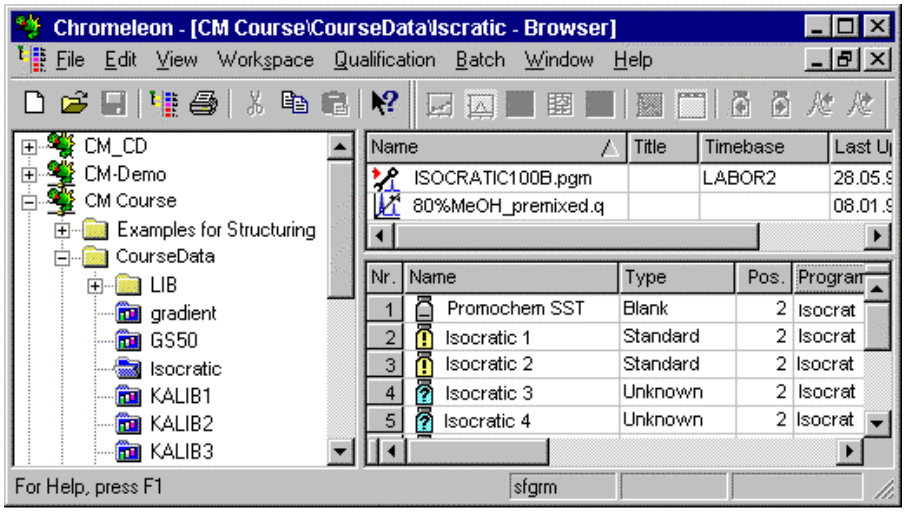
Opening the Browser

- Click the Browser icon to open the Browser window or to display it on top.

1. Browser Appearance and Functions

Caution: The Browser window is similar to the Windows Explorer. However, do not confuse the Browser window with the Windows Explorer! Do not use the Windows Explorer for operations within the datasources of the Dionex Chromatography Management System!

The left window section consists of a tree structure with different levels. The right window section shows detailed information on the currently selected item.



The ➔*Datasources* (e.g. <ComputerName_local>) are the top level of the structure and serve to store data and results. The icon next to the datasource name indicates its type (CHROMELEON, GynkoSoft etc.).

- Click the **+** or **-** symbol next to a datasource to expand or collapse the corresponding directory structure (yellow folders).

The lowest levels contain the ➔*Sequences* (blue folders) created by the user. The easiest case is that one sequence is created per timebase when the Dionex Chromatography Management System is installed. This sequence is called **Manual** and is located in a separate directory of the local datasource. The directory has the name of the local timebase.

- Select a **directory** to display its subdirectories in the right window section.
- Select a **sequence** to view files and samples contained in the sequence.

The upper window section shows different file types,

Symbol	File Extension	File Type
	*.pgm	Control file or PGM file
	*.qnt	Quantification method
	*.rdf	Report template or report definition

while the lower window section shows the individual samples of the sequence in the sample list. The different icons stand for the different sample types:

Symbol	Name	Sample Type
	Unknown	Unknown sample
	Blank Run	Blank
	Validation	Validation sample
	Standard	Standard sample
	Matrix	Matrix blank sample

Opening Files

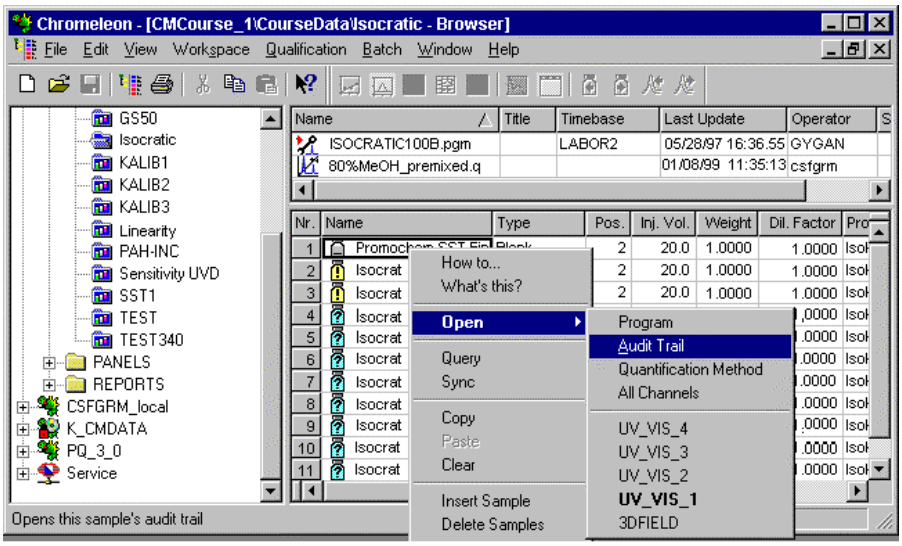
Open a file by double-clicking its name in the Browser window. Depending on the file type, the Dionex Chromatography Management System will load the appropriate chromatographic environment.

- Double-clicking a control file (PGM file) opens the PGM editor.
- Double-clicking a quantification method (QNT file) opens the QNT editor.
- Double-clicking a PAN file opens a control panel.
- Double-clicking a report template (report definition file = RDF) opens the Printer Layout.

Opening Samples

When opening samples, consider the following (independent of the file type):

- If for a processed sample (**Status = finished**) raw data exist for several channels, double-clicking the sample opens one channel only.
- Select a sample (here **sample1**) and open the context menu via the right mouse button. Choose the channel to be opened. In the submenu of the **Open** command, the Dionex Chromatography Management System lists all channels that exist for one sample.



If four different channels of a sample are recorded with a diode array detector during sample processing, as is in this example, a separate chromatogram will be available for each channel (here: **3DFIELD** and **UV_VIS-1** to **UV_VIS-3**).

- Select the channel or the chromatogram you wish to view.

The highlighted channel (here: **UV_VIS-1**) is used as the "preferred channel". The preferred channel is automatically opened when double-clicking a sample. The channel to be used by the Dionex Chromatography Management System as preferred channel is set in the **File** menu under **Preferences**.

Moving and Copying Items

- Use the mouse cursor to select the subdirectory, the sequence, or the file you wish to move or copy. Within a datasource, dragging and dropping an object will move the item. However, when you drag an item from one datasource to another, it will be copied, not moved.
- Simultaneously holding the CTRL key copies the item instead of moving it and moves it instead of copying it, respectively.
- *Exception*: For security reasons, samples can only be copied and deleted afterwards. They cannot be moved directly!

2. Installing Datasources

Datasources

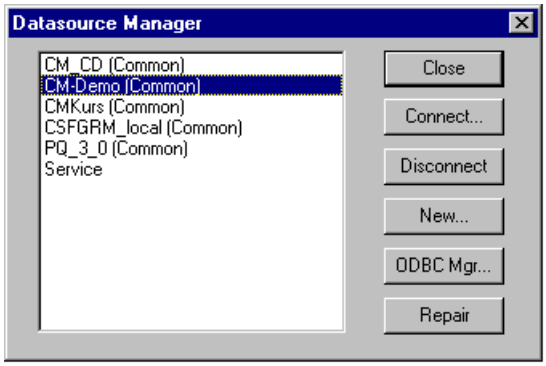
Datasources represent the top level in the Browser. Each user can access at least one datasource, the default datasource created during the installation (<PC-NAME_LOCAL>).

Creating additional datasources or accessing datasources on other computer in the network is often useful. Therefore, these options are supported as well. The section below describes how to create links to other datasources (Note: for a detailed description of how to create a new datasource, refer to the section **How to ...: Actions in the Browser / Setting up a Datasource** in the User Manual and the Online Help).

All steps required for setting up datasources start via the **Datasources** command in the **File** menu.

- Open the Browser and choose the **Datasources** command.

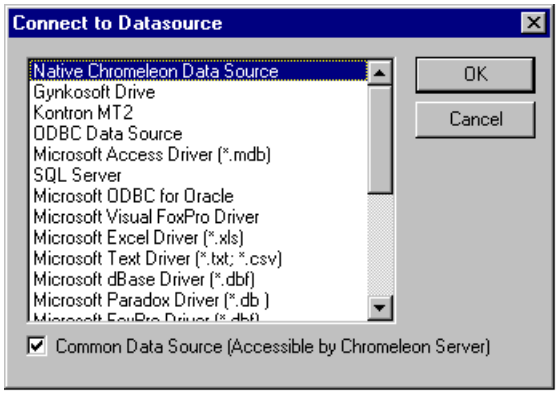
The **Datasource Manager** shows all datasources that the client can currently access.



Connecting an Existing Datasource ("Connect")

If the user knows the directory in which the other datasource is located, he can connect to this datasource.

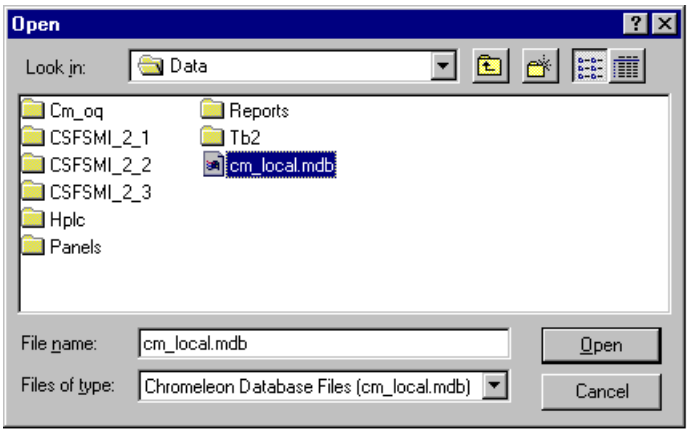
- Press the **Connect** button of the Datasource Manager to establish the connection.
- Choose the **format** of the underlying database.



Usually, you will select datasources of the Dionex Chromatography Management System (**Native Chromeleon Data Source**) or "old" directories of the GynkoSoft chromatography data system (= "GynkoSoft Drives" from version 5.xx). Other formats that are supported include default Microsoft Access databases (**mdb container**), SQL server, and Oracle databases.

- Choose the appropriate datasource type and press **OK**.

- Via the following dialog box, navigate to the network folder that houses the datasource.

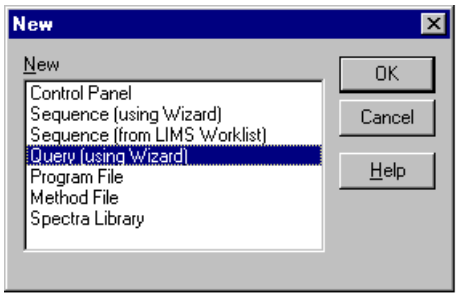


- Select the folder and press **OK**.

Caution: If the folder and the datasource are located on a remote computer, the user of the computer must share the corresponding folder (Windows 98 command: "Shared as")! If he does, the connection to the selected datasource will be established. The name and the type icon of the datasource will appear in the Browser.

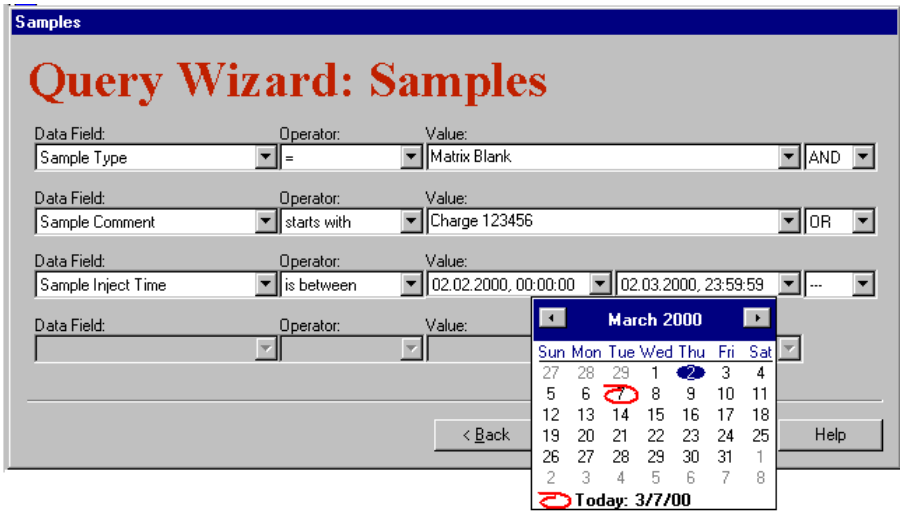
3. Finding Samples (Query)

Often, you will have to find samples according to defined problems. Instead of endlessly poring over old folders, you can use the query function of the Browser to do so easily, fast, and purposefully. Select **New** in the **File** menu to start the Query Wizard:



On the first query page, define whether to perform the query in the selected datasource or in a fixed one. Also, define whether to search for sequence properties, sample properties, or any other properties of samples.

On the next pages, define the variable whose properties you want to find in the **Data Field**. Select an operator and define the value. The combo box to the right of the respective line allows you to enter a logical connective with another query property. Only after having entered **AND** or **OR** you can enter another property:

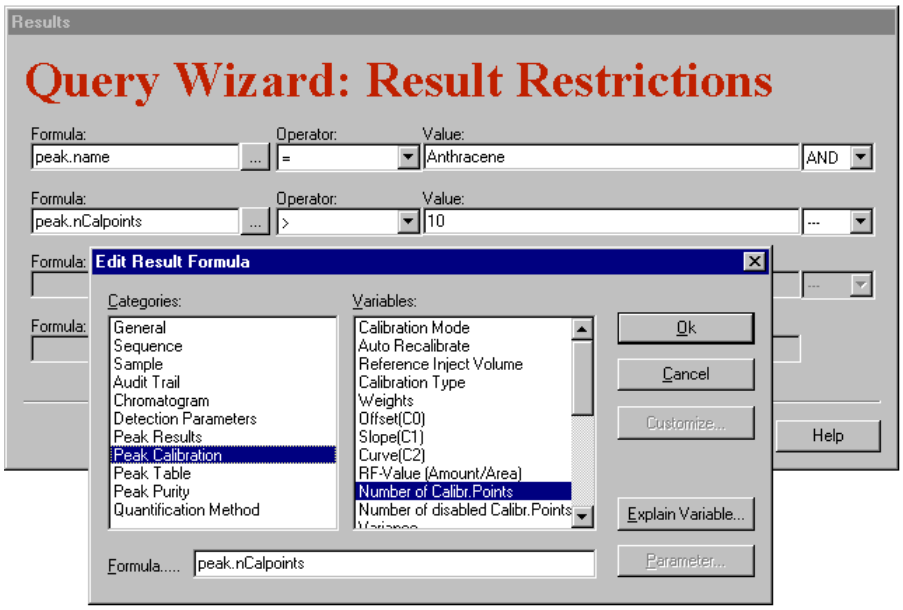


The following query searches for all samples with

- sample type = **Matrix Blank** and
- whose comments start with **Charge 123456** or
- an injection date between 2/2/2000 and 2/3/2000

On the next page, enter the following settings in order to restrict the query to samples

- containing an Anthracene peak or
- containing more than 10 calibration points.

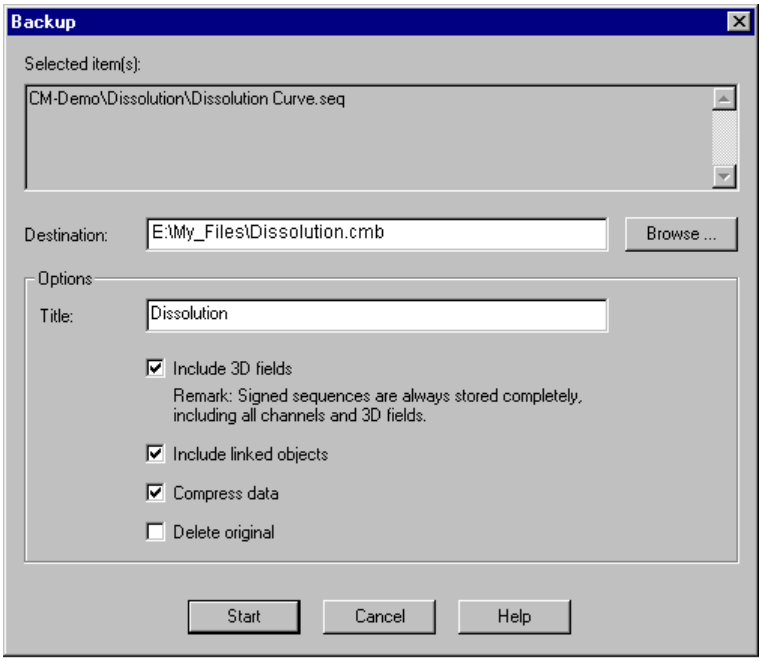


4. Saving / Exchanging Data (Backup/Restore)

In the course of time, large amounts of data will result, especially when PDA detectors are used, but also when a great number of sequences is recorded. To ensure that you can continue to store data on your hard disc, you have to delete some of your data from time to time. However, these data must not be destroyed permanently. They still have to be available for future use. Of course, you can save the respective sequences and datasource on your network as well.

However, the Dionex Chromatography Management System offers the possibility to backup sequences, directories, or entire datasources and save these backup files (which can also be compressed) e.g. on CD. Proceed as follows:

- Select the object to be saved.
- Use **Backup** of **Export/Backup** command in the **File** menu.
- Indicate where to save the backup file and define all further backup options:



- Start the Backup to create the backup file. The extension of the backup file is **cmb**.

Data that were saved in this way can be used again later via the **Restore** function. Use **Restore** of **Import/Restore** command in the **File** menu. Find the respective backup file and indicate where to restore it.

The Backup and Restore functions are an easy way to save large amounts of data in such a way that they can be quickly accessed later. Structure and cross-references remain intact. In addition, these functions facilitate exchanging data via E-mail.

5. Electronic Signature

Electronic Signature allows you to sign the results from your ➔*Raw Data*, which is an important function within the scope of quality assurance and GLP. Thus, you can sign and save ➔*Sequence* reports that have been accepted as correct so that the results can be checked and understood to the last detail.

Electronic Signature includes three steps:

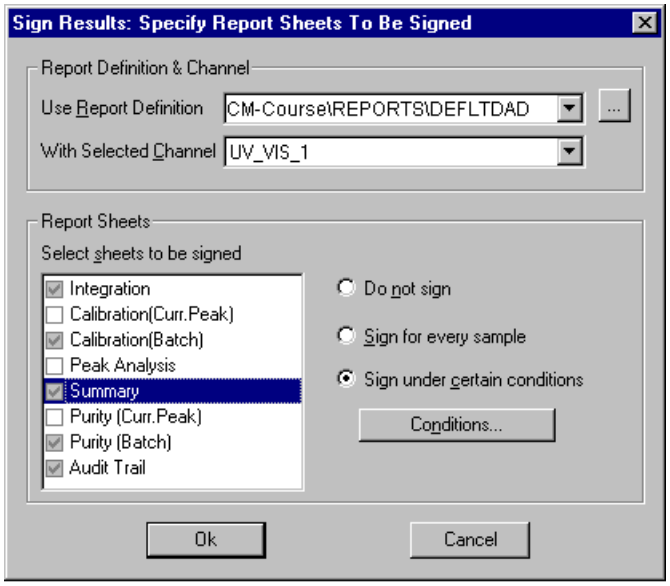
- Submit
- Review
- Approve

Typically, the report is signed and **submitted** by the user who created it. Having **reviewed** the report, the laboratory manager will sign it. Finally, the quality assurance manager will approve the results.

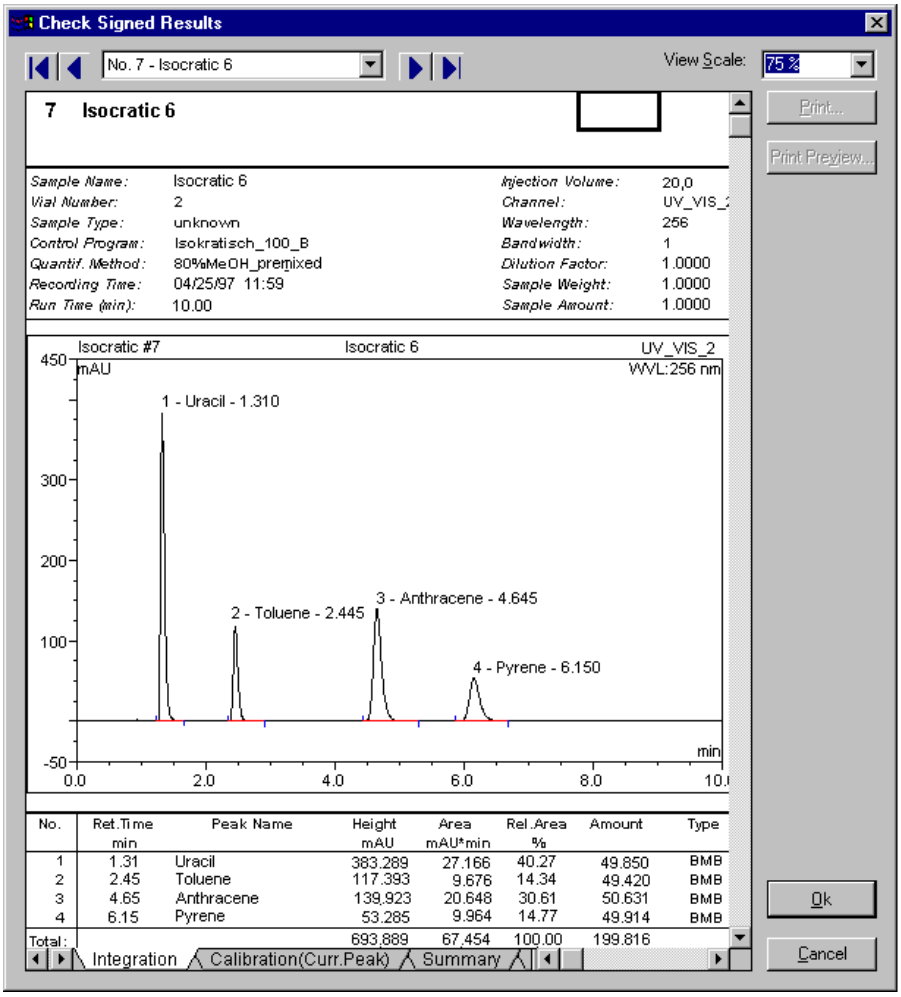
Note: Electronic Signature is available only for activated user databases that have been created with version 6.10 (or a higher version) of the CmUser program. Update your database by opening it with a new CmUser program (version 6.10 or higher) if an error message notifies you that electronic signature will not be possible.

To sign a sequence proceed as follows:

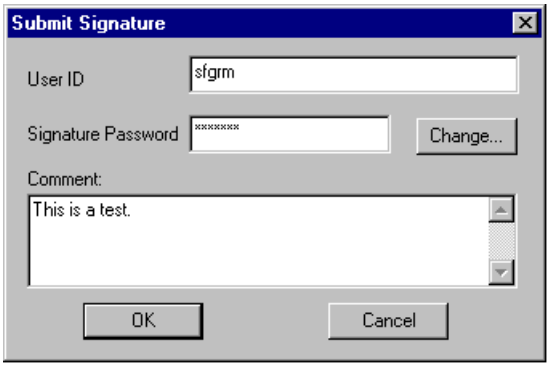
- Click the sequence and select the **Submit Results** command (first signature step) in the context menu.
- In the opening dialog, select the pages to be signed, the report definition file (RDF), and the channel:



- The **Check Signed Results** dialog box opens which allows you to check the reports to be signed. Use the arrow keys to toggle between the samples of the sequence. For each sample, the tabs for the selected report pages are displayed. Having terminated your checks, press **OK**:

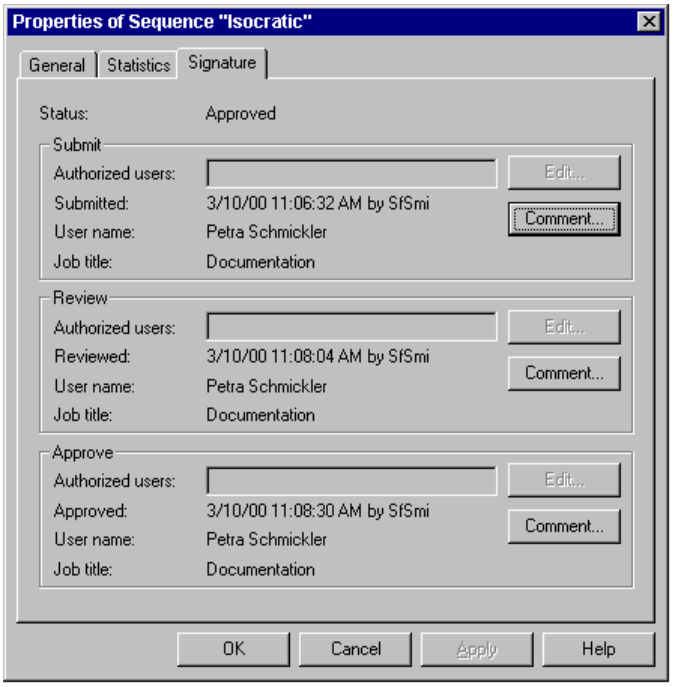


- Sign these pages by entering your User ID and your signature password in the opening dialog box.



- The extension of the newly created file is .SOR.
- Use the **Verify** command (see **File** menu: **Electronic Signature**) to let your chromatography management system check the signed report of the sequence once again, i.e. the sequence, the corresponding files (pgm, qnt, rdf, sor), and the individual samples.

The **Signature** tab in the sequence property dialog indicates the status of the current sequence:

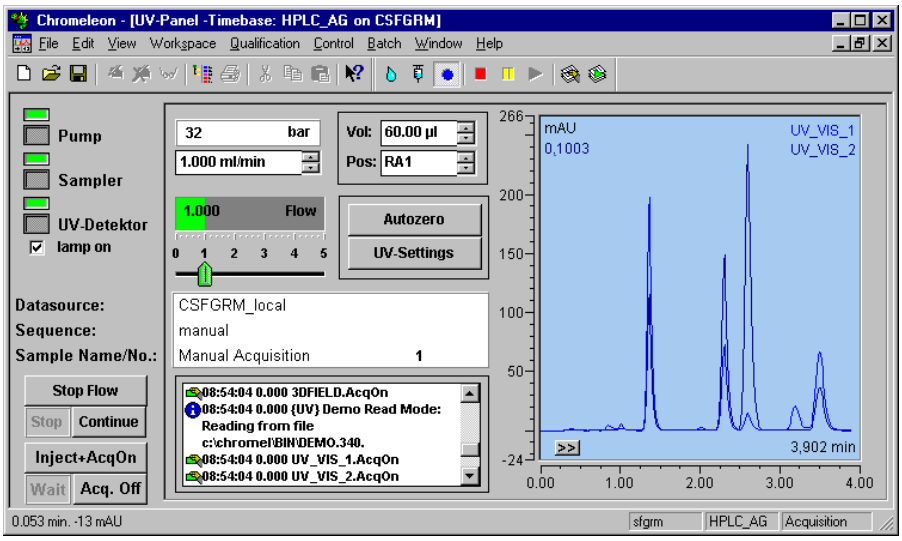


A signature can be removed only if the user has the corresponding privileges assigned. Removing the signature also deletes the corresponding SOR File.

III. Control

1a) The Control Panel

The Dionex Chromatography Management System allows controlling one or several analysis instruments via the **Control Panel**.



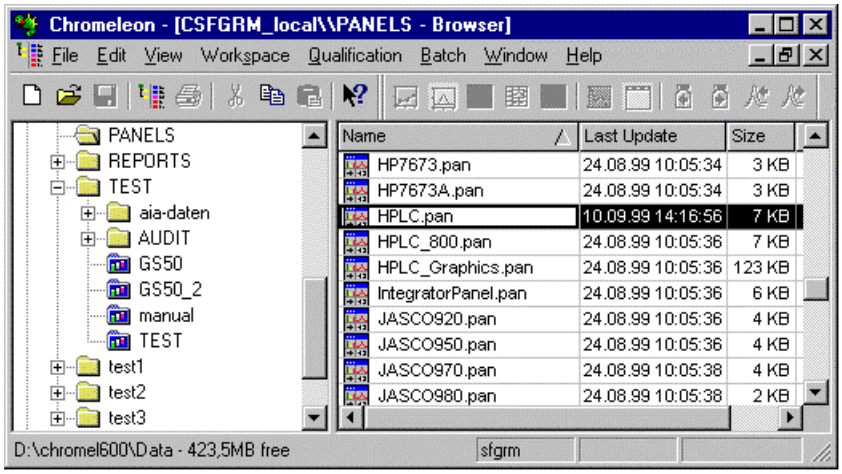
The above screen shows a control panel that allows controlling the basic functions of a pump, an autosampler, and a two-channel UV detector. On the right, you can see the detector signal.

The user can change the appearance and the functionality of a control panel. The Dionex Chromatography Management System includes numerous default control panels that cover most applications.

Opening a Default Control Panel

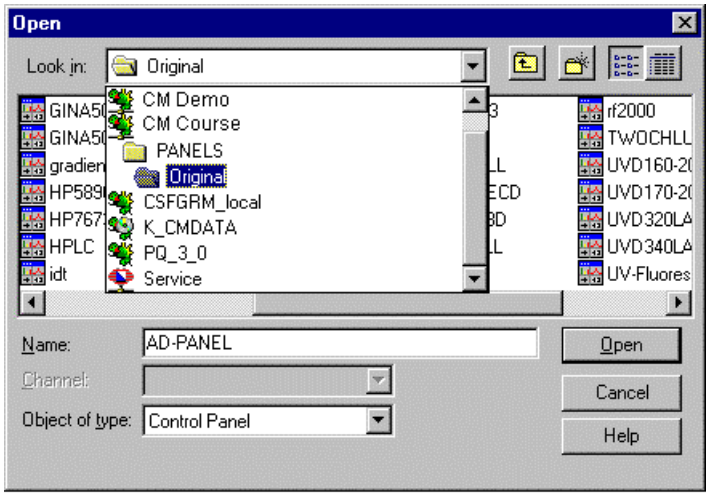
From the Browser

- Open the **Panels** directory and select the control panel corresponding to your system.
- Double-click the name of the window to open it.



From the File or context Menu

- Choose the **Open** command from the **File** menu.



- In the **Open** dialog box, select **Control Panel** under **Object of type**.
- Via the **Look in** field, choose the local ➔*Datasource* of the system. When installing the Dionex Chromatography Management System, this datasource is automatically saved on your computer.

The datasource has the name <NAME_LOCAL>, where <NAME> is replaced by the **Computer name** listed under **Network/Identification** in the Windows Control Panel. If the **Look In** field contains further datasources, you can also search here for an appropriate control panel.

- Open the **Panels** directory and choose one of the default control panels (*.**pan**).
- Double-click a name to open the window.

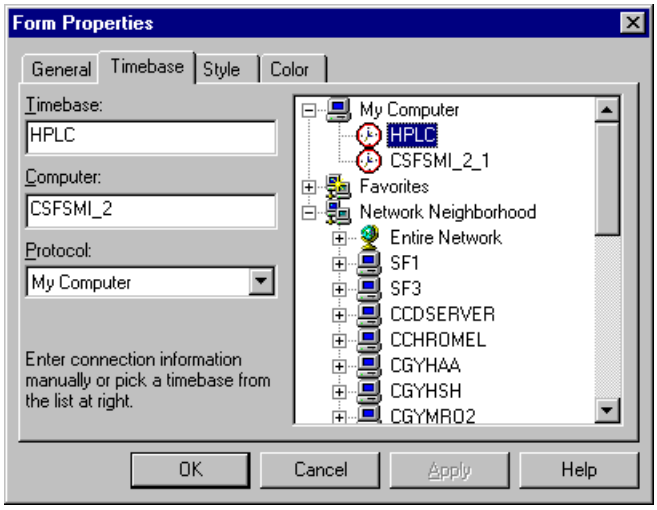
As soon as a control panel has been opened, the Dionex Chromatography Management System will attempt to establish a connection to a specific ➔*Timebase*. With the control panels that are included in the Dionex Chromatography Management System, a link to the **SYS1** timebase on the local server will be created.

If it is not possible to establish a connection, the control panel is grayed. The system shows an error message.

1b) Connecting a Control Panel with a Timebase

If a control panel is currently open, you can establish a connection to a timebase at any time. However, the server on which the timebase was installed needs to be started as described under ➔*Starting the Dionex Chromatography Management System*.

- Choose the **Connect to Timebase** command from the **Control** menu to create or change the timebase assignment (➔*Online Help*).
- Via the following dialog box, determine the ➔*Server* and the ➔*Timebase* to which you whish to connect the control panel.



- If the server is started locally on your computer, you can click the **+** character to open the **My Computer** submenu. If the server is running, the names of all timebases that are installed on the respective server will be displayed. If the server is not running, a corresponding message will be given. In this case, you need to start the server first before you can choose the desired timebase (e.g. SYS1). The **Computer** field will automatically show your PC, i.e. its name that was determined during the Windows installation. In the **Protocol** field, the entry **My Computer** will appear.
- If your PC is connected to other computers via a network or a modem, accessing a server that was not started on your local computer, but another PC is possible as well. In this case, open the **Network Neighborhood** submenu to browse for the required timebase. Under **Protocol**, the corresponding network protocol will be given.
- The Dionex Chromatography Management System remembers the servers that you have accessed on other computers. These servers can be selected under **Favorites**.

As soon as you complete the dialog, the Dionex Chromatography Management System will attempt to access the timebase you selected. If there is no communication, this may be due to several reasons.

Possible Problems when Connecting to a Timebase

Cannot connect to timebase ...

⇒ This error message indicates that the corresponding server is not running, that the selected timebase does not exist on this server, or that the wrong protocol was selected for the communication.

- Start the server as described under **Starting the Dionex Chromatography Management System** or select the required timebase or protocol.

☞ ***Tip*:** The Dionex Chromatography Management System can communicate via various network protocols such as IPX, TCP/IP, or NetBEUI. Communication between two stations is possible only if the same (!) network protocol is installed and selected. Generally, it is sufficient to install the corresponding Microsoft ("IPX/SPX-compatible protocol"; "NetBEUI"; "TCP/IP") or Novell ("Novell IPX ODI Protocol") network protocols via **Settings/Control Panel/Network/Configuration**. Which protocol is actually used depends on the current network installation. Please contact your network administrator. If a connection should be established to a Windows NT computer, this is frequently via the supplied **Named Pipes** protocol.

This timebase contains no object named...

⇒ The control panel attempts to access an instrument (or a function of this instrument) that is not part of the current installation environment. The control panel and installation environment do not correspond. Load an appropriate control panel or change the existing configuration of the timebase in the installation program (= Server Configuration). For details on how to change the server configuration, see **How to ...: Actions in the Server Configuration Program** in the User Manual and the Online Help.

Device is not remote.

⇒ The control panel attempts to access an instrument that is currently not ready to operate. Check whether all instruments listed in the configuration are actually connected to the server PC **and** that they are switched on. It may be necessary to restart the instrument to ensure the proper functionality.

The connection is established correctly (no error message), but the controls are grayed.

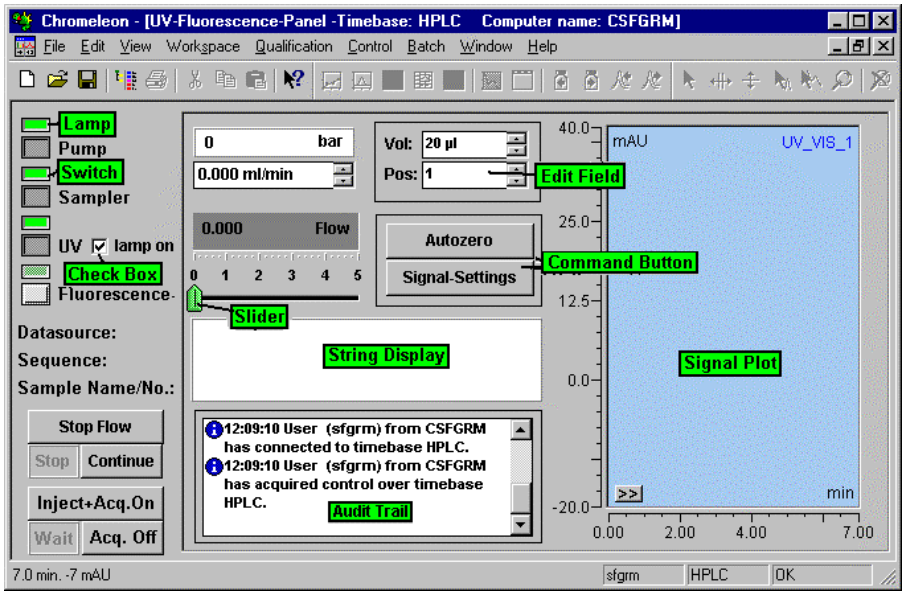
⇒ The **Monitor Only** mode is activated. The control panel cannot be actively operated. This is always the case when the selected timebase is already controlled by a different workstation. The **Monitor Only** mode can be deactivated via the **Control** menu. After that, actively controlling the timebase is possible (which indicated by the controls on the control panel). Simultaneously, the previously controlling workstation loses the control rights and is in the **Monitor Only** mode.

☞ ***Tip:*** Follow the **Audit Trail** entries. It is usually possible to draw conclusions about the error.

1c) Using the Control Panel

As soon as a control panel is correctly connected to a timebase, the individual instruments of this timebase can be operated via the controls shown in the window.

Depending on the currently used default control panel, various active and passive control and display elements (**Lamp**, ... **Signal Plot**) are available for controlling instruments and for displaying system functions. The appearance of the controls (size, shape, and color) can be altered.



The basic commands such as controlling the pump flow, the inject command, or starting the data acquisition are available via a separate toolbar. This toolbar is only active with an open control panel.

However, how will the system know that moving a slider should change the pump flow, and not the oven temperature? Very simple: It is not only possible to change the size, the color, and the shape of each control, but also its functionality. These assignments are preset for the controls of the default control panels. Of course, you can change them according to your requirements.

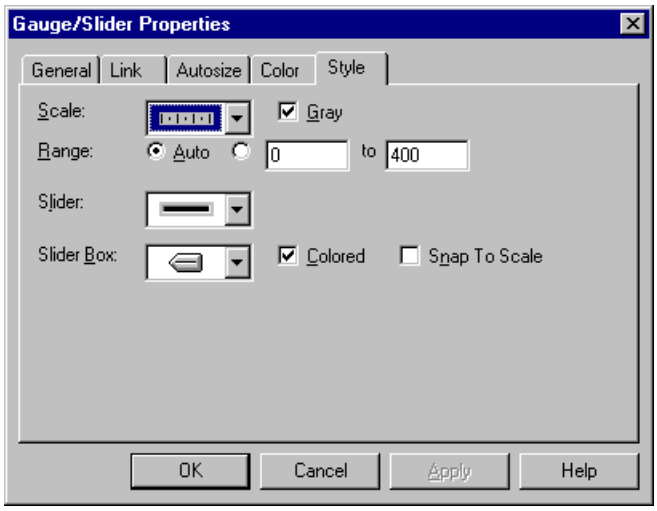
1d) Modifying the Control Panel

Changing the Functionality and the Shape of Controls

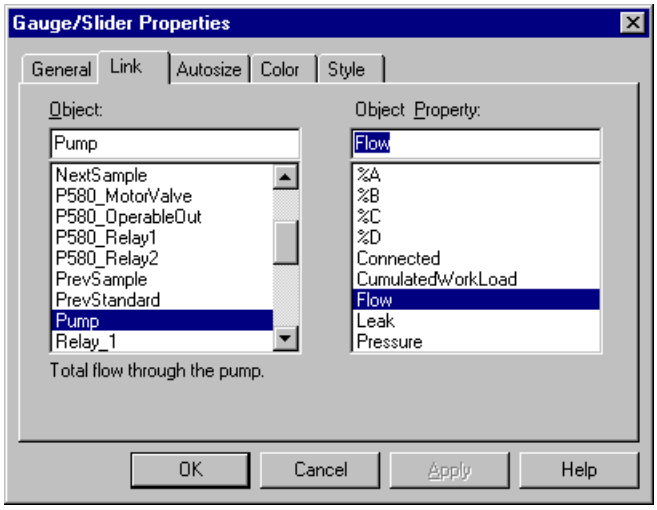
Note: If it is not possible to perform the following steps with your software version, you do not have the user privileges required for these actions. In this case, contact your system administrator.

- Move the mouse cursor on the corresponding control and open the context menu (right mouse button).
- Choose the **Properties** command to open the edit box.

Depending on the selected control, the **Properties** dialog box includes various tabs. For a slider, the **Style** tab will look as follows:



- Choose the **General**, **Color**, or **Style** tab to change the appearance such as the color, the shape, or the caption of the control.
- Choose the **Link** tab to determine the function and the instrument to be operated via the control.



- Under **Object**, choose the instrument itself and under **Object Property** choose the instrument's function. Instrument and function selection depend on the components installed with the timebase.

With the settings shown above, a slider can control the pump flow rate.

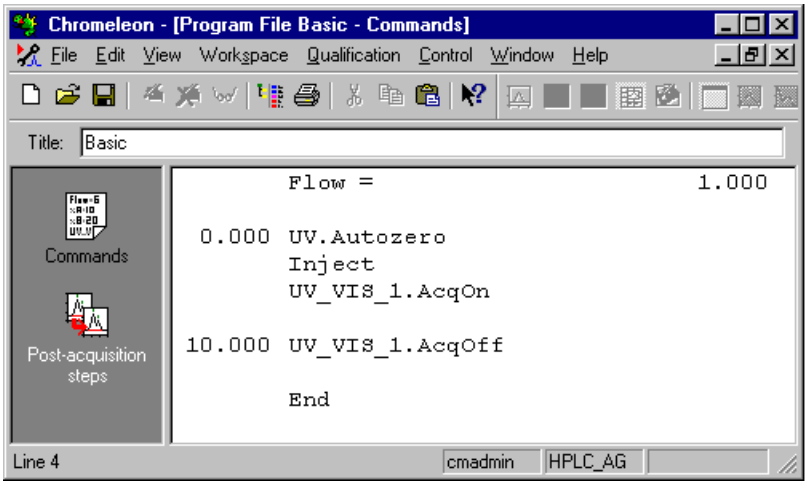
2. The Control File (PGM File)

By entering commands, the user can instruct individual instruments to perform specific tasks. Commands can be entered either via the controls on the control panel or by pressing the corresponding buttons.

As this can be time-consuming, it is also possible to list the series of required commands in a file. When starting the file, the listed commands are executed consecutively, observing the relative time differences. This file type is called control file or PGM file.

Control File Properties

The control file window will be similar to the following illustration:

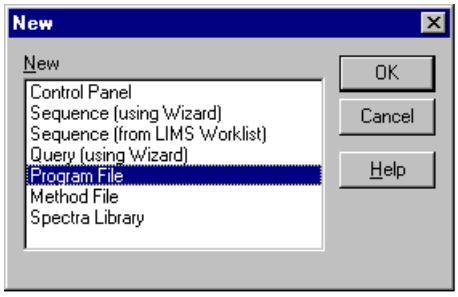


Below the **Title** line, there are various commands (starting with the time entry). For information on how to create a PGM file, see the following sections.

3. The Program Wizard

Using the Program Wizard is recommended for creating a basic program structure. This is especially true since a specific syntax must be observed for entering the commands.

- Check whether the server is running. If not, start the server as described under ➔*Starting the Dionex Chromatography Management System*.
- Choose the **New** command from the **File** menu.
- Choose **Program File** from the list and press **OK** to start the Program Wizard.

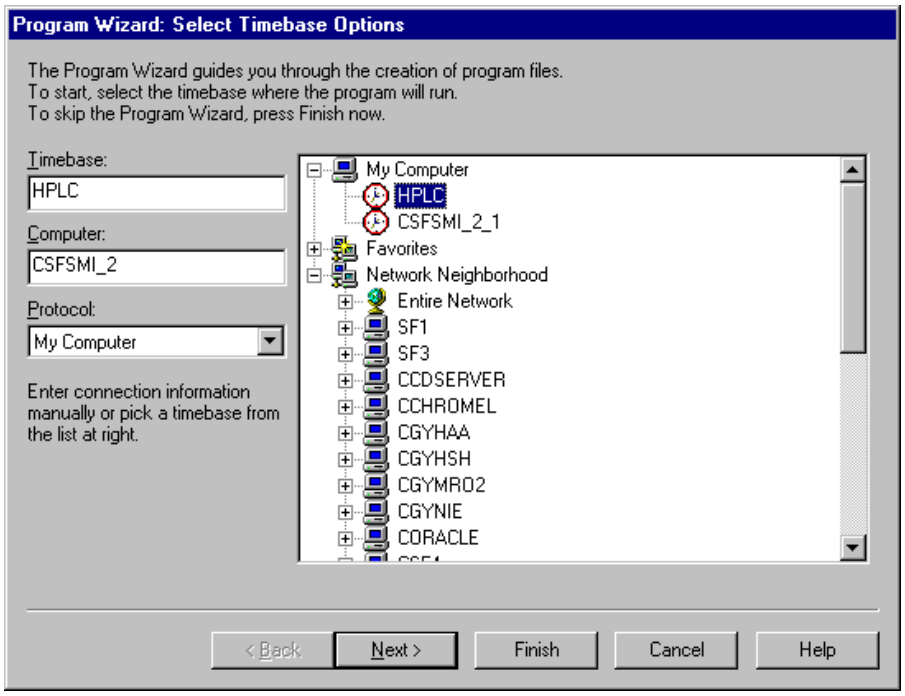


Depending on the installed instruments, various steps must be performed. For each screen, detailed information is available via the F1 key or the **Help** button. Pressing **Back** or **Next** allows you to toggle between the edit screens.

Step 1: Timebase and Server

Determine the server and the timebase to be used.

- If the server was started locally, click the **+** sign to open the **My Computer** submenu and select the desired timebase. Choose **My Computer** in the **Protocol** field. If you want to access a server that was not started on your computer but on a remote PC, open the **Network Neighborhood** submenu and click the appropriate timebase there. In this case, you have to select a network protocol under **Protocol**. For details, press the F1 key.

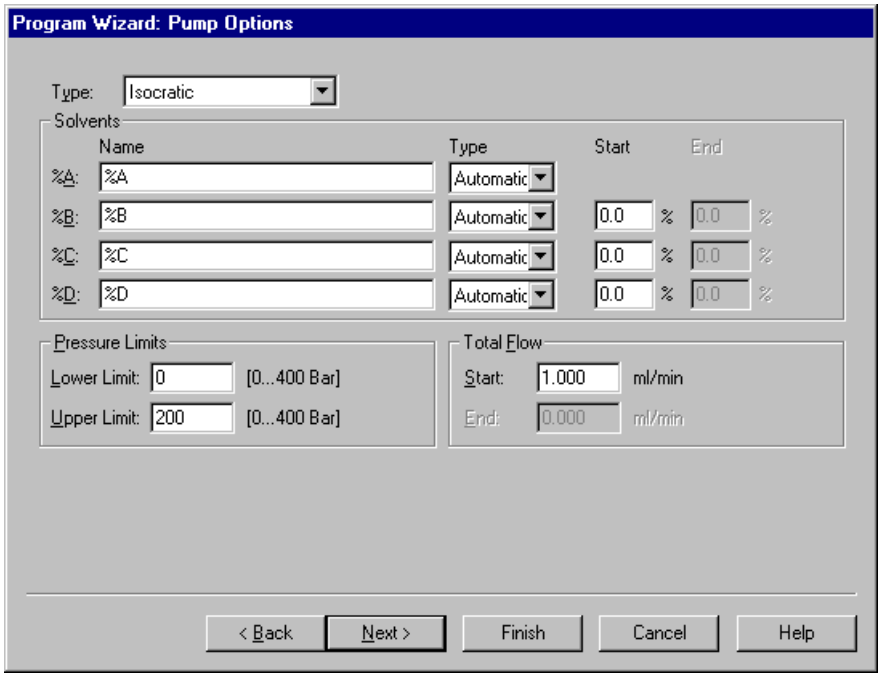


The **Next** button allows you to proceed to the next page of the **Program Wizard**. Press **Finish** to generate a program with the settings you made so far.

Step 2: Flow Conditions

If your chromatography system includes a controllable pump, define how to operate the pump.

- Choose **isocratic** to deliver a constant solvent composition. Under **%A**, **%B,** etc. you can enter the names of the currently used solvents. Instead of **%A**, **%B**, etc. the actual solvent name will be indicated in the control panel or in the report. If more than one solvent is used, the **Start** field determines the solvent composition in percent (e.g. B = 45%, C = 0%, D = 5%). %A is calculated by the system from the portions of B, C, and D. Enter the flow rate under **Total Flow**.



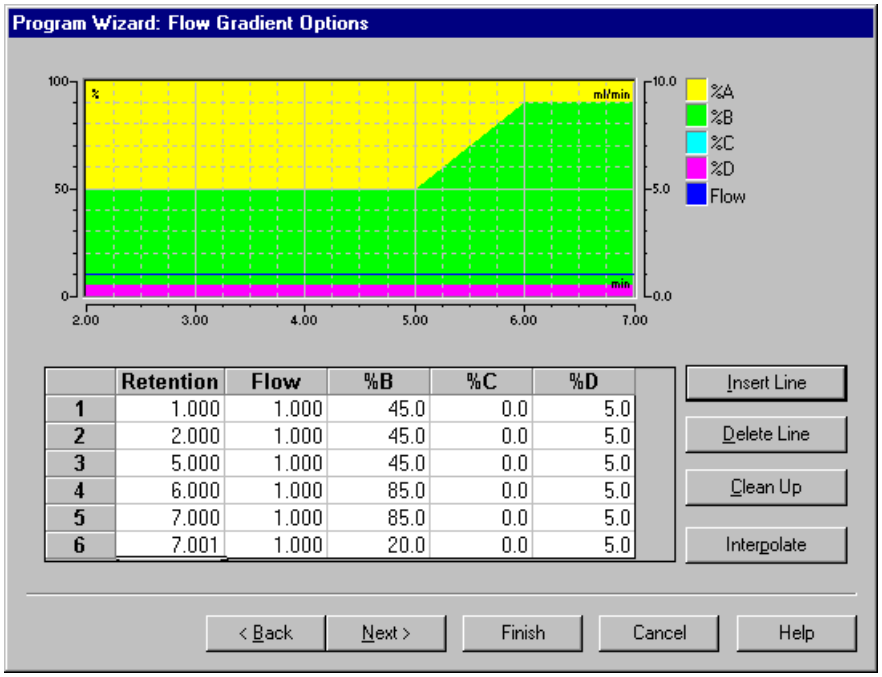
- If **Ramp** is selected as type instead of **Isocratic**, you can set the start and end time of the gradient ramp. You can also select a **multi-step gradient**. In this case, click **Next** to open another edit box.

Step 3: Gradient

The **Flow Gradient Options** window allows specifying a gradient. Enter the following data:

- Retention time
- Flow
- Solvent composition

To append lines to the table, press the down arrow key on your keyboard. The window will show a graphical representation of your gradient. A blue line indicates the flow, while the area represents the gradient composition. The following example shows a gradient at a flow rate of 1 ml/min, with a constant 5%D during the entire gradient.



Step 4: Data Acquisition

After that, determine the signals to be recorded during sample processing.

- Select the signals. Under **Acquisition Time**, enter how long an individual sample should be analyzed.

For a two-channel UV detector, e.g. the channels **UV_VIS_1** and **UV_VIS_2** are recorded for 30 minutes (**From 0.000 min to 30.00 min**). **0.000** means that data acquisition starts immediately after the injection (t = 0).

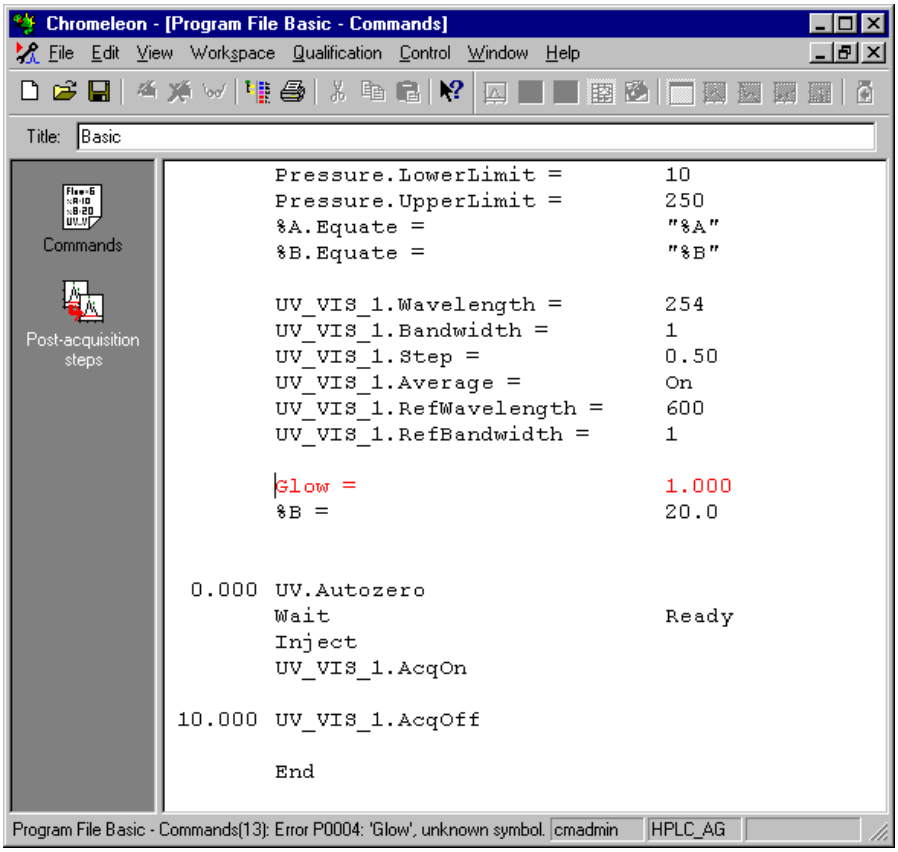
Step 5: Signal Parameters

Define the signal parameters for each signal that was selected under Step 4.

- Depending on the signal type, various parameters must be set (e.g. **Excitation Wavelength** for the fluorescence detector). In the case of a UV detector, the wavelength, the bandwidth, and the step used for recording (e.g. Wavelength = 225nm, Bandwidth = 1nm, Step = Auto, Average = On (selected) must be specified.

Step 6: Completing and Saving the Program

- Choose **Finish** to complete the Program Wizard. In addition to your input, the completed program that is displayed in the QNT editor also includes commands that are automatically added by the Dionex Chromatography Management System (e.g. **Inject** and **End** commands). These commands are required for executing the file. The completed program may have the following appearance:



- You can edit a completed program later, as necessary. If invalid commands are entered, the Dionex Chromatography Management System will recognize these and show the respective line in red (**Glow** instead of **Flow** in the above example).
- Save the PGM file under a descriptive name via the **Save as** command from the **File** menu.

4. Editing the Control File

Each line can be edited directly via the keyboard, provided the control file is connected with a timebase.

- Open the PGM file via the **Open** command from the **File** menu or double-click the corresponding file name directly in the Browser.
- Check whether your server is running. If not, start the server as described under ➔*Starting the Dionex Chromatography Management System*.
- Choose the **Connect to Timebase** command from the **Control** menu.

You can now edit the program. Instead of overwriting the command syntax directly in the PGM file, we recommend to proceed as follows:

- Move the mouse cursor in the line to be edited; press the F8 key. The Dionex Chromatography Management System opens the **Commands** dialog box for the currently selected command. You can now edit the input by selecting defined values, without having to worry about the correct syntax of each command.
- Save the edited PGM file (**Save as**).

Caution: If you have not specified a control file when creating a sequence (Step 4 of the Sequence Wizard), the fields of the **Program** column in the sample list will be empty! In this case, change to the Browser, select the sequence, and enter the name of the PGM file for each sample that is to be processed based on the created program. Copy each required PGM file to the sequence directory afterwards.

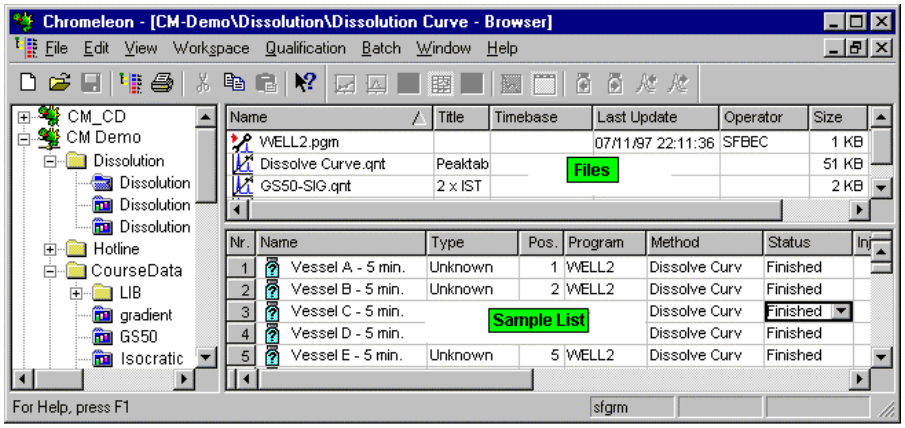
IV. The Analysis

1. The Sample List (Sequence)

Opening the Sample List (Sequence Table)

- Select a sequence (blue folder) in the left Browser section to view all samples and files contained in that sequence in the right Browser section.

The upper section is reserved for files that are (or were) required for processing a sample. The lower section lists all samples belonging to the selected sequence. This section is referred to as **Sample List**.



Sample List Contents

The sample list forms the basis for sample processing. It lists the samples intended for processing (one line corresponds to one sample) and how processing is or was performed (contents of individual columns).

For example, the table can contain the volume in µl (**Inj.Vol** column), the position (**Pos**), the program (**Program**) that is used for processing the sample, and the method (**Method**) used for evaluation purposes. The vial color in the **Name** column indicates whether the sample is an unknown sample (= **Unknown** (blue)) or a standard sample (= **Standard** (yellow)). The current sample status is indicated in the **Status** column. If the sample was already

processed, i.e. analyzed, it is labeled **finished**. Samples to be processed are labeled **single**. If the sample is currently processed, the entire line has a green background. The sample status is **running**. **Multiple** indicates that the sample can be processed several times, however, with the old run being overwritten each time.

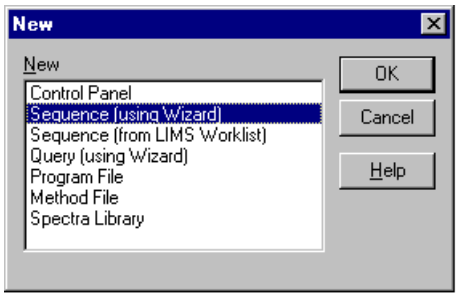
Samples are always processed in the order of their appearance in the sample list.

2. The Sequence Wizard

Start the Sequence Wizard to create the basic structure of a sample list.

Starting the Sequence Wizard

- Choose **New** from the **File** menu.
- From the list, choose **Sequence (using Wizard)**.
- Press **OK** to start the Sequence Wizard.



A sequence is created in **five steps**: Each step is performed on a separate page. For each page, detailed information is available via the F1 key or the **Help** button. Pressing **Back** or **Next** allows you to toggle between the pages.

Step 1

Specify the timebase on which the sequence to be created shall run. Select a timebase in the right window section. The corresponding entries for **Computer** and **Protocol** will be made automatically.

- Enter a name in the **Sequence Name** field, choose the local datasource <USERNAME_LOCAL> in the **Datasource** field, and generate a separate

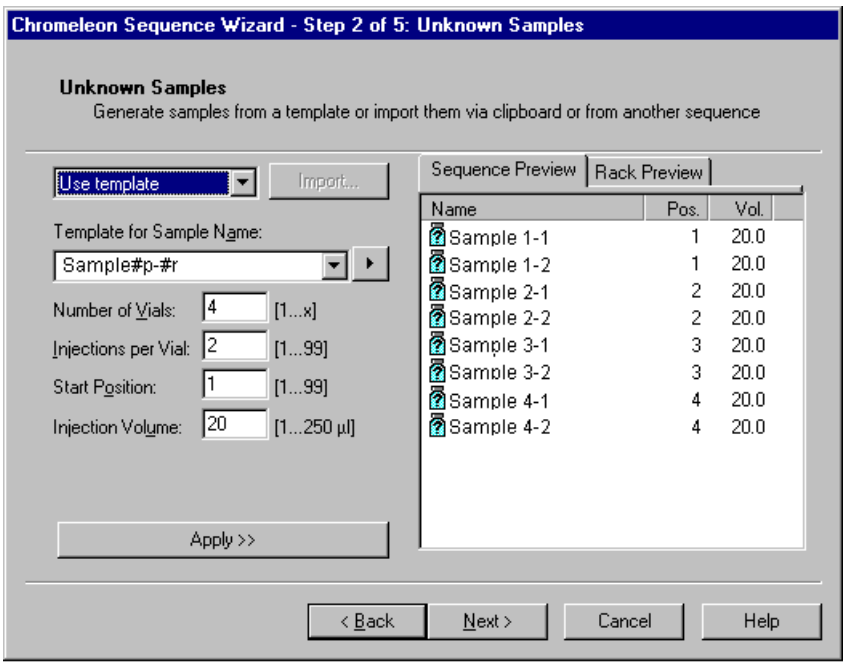
sequence directory in the **Directory** field (creating a new directory at this point is possible).

Caution: Do not use special characters (e.g. umlaut) for new directory names or sequences, as this may cause problems in Novell networks!

Step 2

Generate all unknown samples to be processed.

- Choose **Use Template**; enter the number of samples to be processed (**Number of Vials**), the sample volume to be injected (**Injection Volume**), the number of injections (**Injections per Vial**), and the position of the first sample (**Start position**). Then enter a sample name and use the arrow key to add e.g. "#n" to number the samples consecutively (e.g. "sample#n"). Press **Apply** to view the result of your input as sample list (**Sequence Preview**). If the result requires editing, e.g., because the injection volume should not always be the same or because the positions of the individual vials are not consecutive, you can change the information manually in the Browser after closing the Sequence Wizard. In the **Rack Preview**, you can also view the positions for the currently entered samples in the rack.



Step 3

Generate all standard samples to be processed.

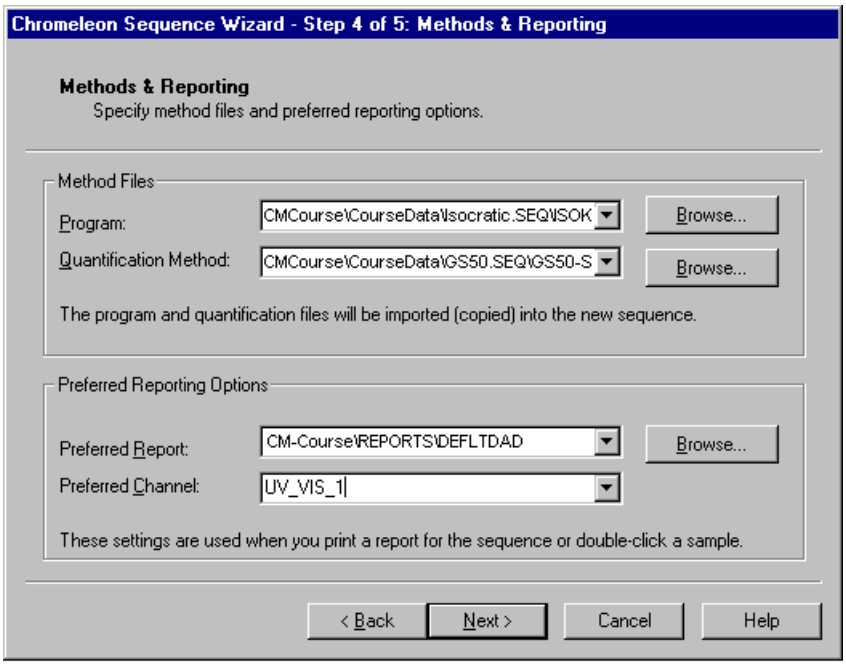
- Proceed as in step 2. In addition, you can specify any number of standards (**Variation**:) that shall be analyzed after a specified number of samples (**after each**).

Step 4

Determine how to process, evaluate, and print the sequence.

- Enter the name and the directory of the ➔*PGM file* and the ➔*QNT file* to be used (see the **Program** and **Quantification Method** fields) or choose a file via the **Browse...** button. If you have not generated a new PGM file or QNT file before, you can leave these fields empty for now.

- Under **Preferred Report**, choose the **DEFAULT.RDF** report template from the **REPORT** directory of the local database to open the default report. Choosing a **Preferred Channel** determines the channel whose the data are to be displayed.



Note: The **Quantification Method**, **Preferred Report**, and **Preferred Channel** fields are optional at this point.

Step 5

Specify the name for the sequence to be created and where to save it.

- Enter any name in the **Sequence Name** field and select the local data <BENUTZERNAME_LOCAL> in the **Datasource** field. Generate a separate sequence directory by specifying a directory name in the **Directory** field (a new directory can be created as well).

Caution: Do not use special characters (e.g. umlaut) in new sequences and directories names as this may cause problems in Novell networks!

- Press **Done** on the last page of the wizard to complete your input.

Editing the Sequence

Pressing **Finish** generates a sequence based on the entered information. The sequence is displayed in the Browser. As mentioned before, the sequence is a basic structure that needs to be adjusted to special requirements.

If, for example, you wish to inject different volumes, edit the sequence. Also, select a PGM and/or a QNT file if you have not specified these files in step 4 of the Sequence Wizard.

- Change to the Browser and select the name of the newly created sequence.
- In the sample list, change individual fields directly via the keyboard or open an edit box by pressing the F8 key.
- Adding samples is possible via **Append new line**.

3. Starting the Analysis

Analyzing one sample can be performed manually. For several samples, automatic sample processing is recommended.

***Tip*:** Creating the sample list, the control file, and the quantification method is only required for automatic sample processing!

Manual Sample Processing

The analysis is performed systematically by entering single commands.

- Open a control panel and connect to the desired timebase.
- Choose the **Flow ...** command from the **Control** menu (or use the corresponding button on the Online toolbar: ). Enter the flow rate and the solvent composition the pump should deliver.

- Choose the **Inject...** command from the **Control** menu (or use the corresponding button on the Online toolbar: ). Enter the injection volume in µl and the autosampler position.
- Choose the **Acquisition On** command from the **Control** menu (or use the corresponding button on the Online toolbar: ). Choose the signals to record and start data acquisition by pressing **OK**. The injected sample amount is transported over the column. The chromatography management system records the signals supplied by the detector.

These commands are also included in the **Online** toolbar. If your control panel supports this, you can execute these commands directly from the control panel.

- If you want to finish data acquisition and thus complete the analysis, choose the **Acquisition Off** command and stop the pump flow (**Stop Flow**).

If your control panel is connected to a timebase on the local server, the recorded data is saved to the **Manual** sequence in the <Timebase Name> directory of the local datasource.

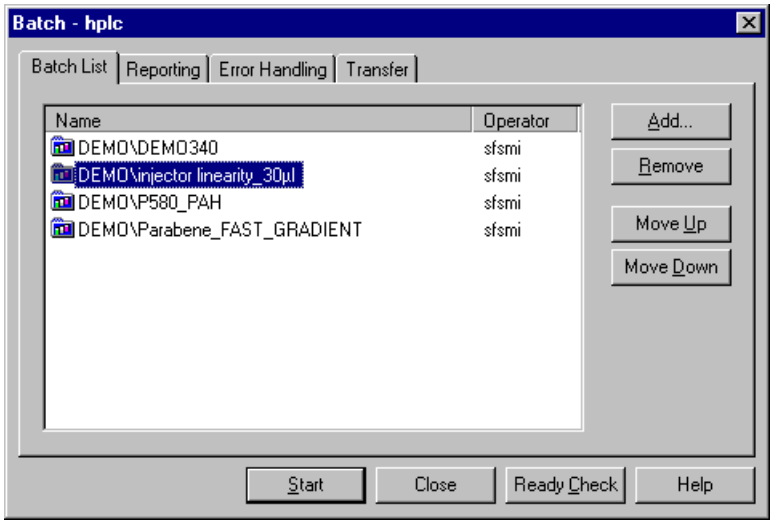
Creating this sequence is not required. The sequence is automatically generated during the installation; it contains one sample only. With each new manual sample processing, the data is overwritten by the newly analyzed sample. This type of sample processing should be used for test runs etc. only!

Automatic Sample Processing

Automatic sample processing can be started as soon as the chromatographic conditions, the samples to be processed, and their order have been defined during sequence creation.

Automatic sample processing is also called **Online Batch** or **Batch Processing**.

- Open a Control Panel and choose the **Edit** command from the **Batch** menu. Alternatively, press the  icon on the **Online** toolbar.



- Press the **Add** button on the **Batch List** tab and find the previously created sequence within your datasource via the **Open** dialog box.

The path and the name of the sequence are entered in the Batch dialog box. If a sequence contains a sufficient number of samples, sample processing is possible around the clock. Instead of listing all samples in one sequence, you can create several sequences. In this case, enter all required sequence names in the Batch List (max. 16).

- Add the sequences until all required sequences are displayed in the display field.

The order of the listed sequences determines the order of sample processing, i.e., when starting a batch, samples 1 to n of the first sequence are analyzed, followed by samples 1 to n of the second sequence, etc.

- Select a sequence and change the processing order via the **Move Up** and **Move Down** buttons.
- Press **Ready Check** to check whether automatic sample processing (batch) can be carried out, i.e., whether all devices to be used are ready for use (turned on, connected, lamp switched on, etc.) In addition, it is checked whether all data are available and whether the memory capacity is sufficient.
- Then start the analysis process by pressing **Start**.

As soon as the online batch is started, all samples of the sequence(s) that have the status **Single** or **Multiple** are analyzed in the listed order. During a running batch, the currently processed sequence is labeled with a green triangle in the batch list.

V. Data Reprocessing

Data reprocessing refers to the presentation of raw data under various aspects. This can include the display of an integrated chromatogram, manual chromatogram re-integration, and chromatogram comparison, checking peak purity, representing calibration curves, or searching individual spectra in a spectra library.

Each action is performed in a separate window. These windows are also called **partial methods**. Each partial method is intended for a specific task and has its own window arrangement and menu structure. Use the icons on the **Method** toolbar to quickly change from one view to another:

The following partial methods are available (order as on the toolbar):

- **Calibration**
- **Integration**
- **Peak Purity Analysis (PPA)**
  (opens a window for presenting data of a diode array detector)
- **Printer Layout**
- **Quantification Method (QNT Editor)**

The next tool allows you to view the signed results. Use the next icons to open another two window sections:

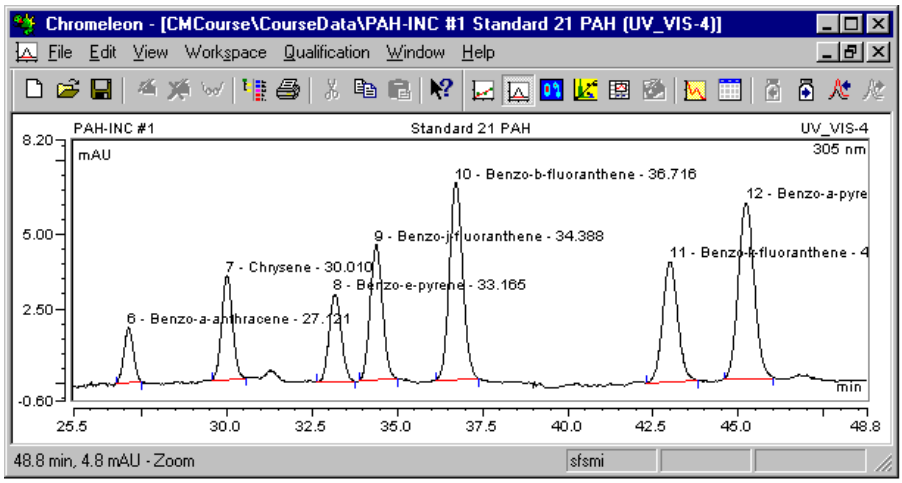
- **Spectra Plot** (opens a window for spectra representation)
- **Report** (opens a Report window)

Let us see the points that must be considered in the following example of the **Integration** partial method. Changing the other method windows is in the same way.

1. The Integration Window

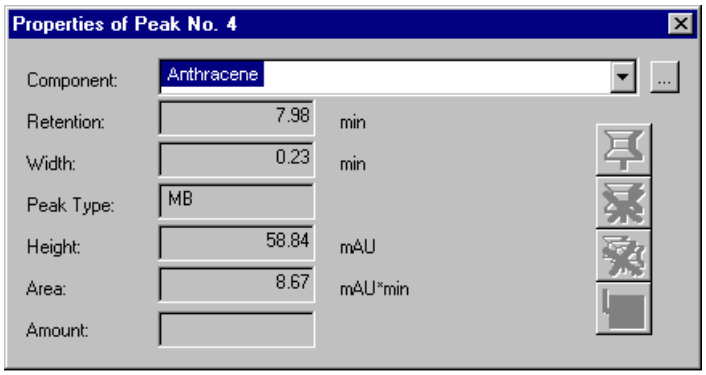
- Open a sample chromatogram by double-clicking the sample name in the Browser.

You will see the chromatogram of a sample, e.g.:

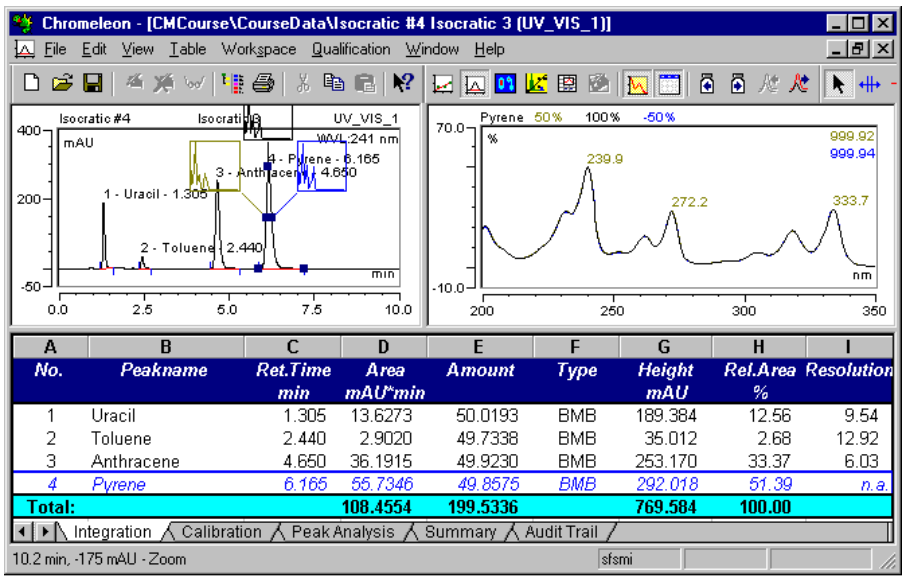


- Choose the **Decorations** command from the context menu to change the appearance of the chromatogram. The captions, axis ratios, and coloring can be changed as well as the actual chromatogram representation (display of peak heights, additional chromatograms or grid).

- Double-clicking an individual peak shows its properties:



- Select a peak and click the corresponding icons to view the **Spectra Plot** and the **Report**.



On the top right, the spectrum of the selected peak, e.g., anthracene (provided the analysis was performed with a diode array detector) is displayed; the lower section shows part of the integration report (three lines, the currently selected peak is highlighted by a different background color). As before, the Spectra Plot window can be changed via the **Decorations** command. Choose this

command to view the available options. This command also allows minimizing the spectrum in the chromatogram.

The displayed default report contains information on various parameters. Each worksheet has a number of default variables that are an integral part of a specific report type. For example, the integration report contains the columns **Ret.Time**, **Area** and **Amount**, the calibration report includes the columns **Offset (c0)**, **Slope (c1)**, and **Curve (c2)**, etc.

Double-clicking a peak name in a report window changes the selection of the current peak, i.e., instead of anthracene; pyrene is then highlighted by a different color. The spectra representation is also updated.

2. Modifying the Chromatogram

In individual cases, it may be useful to change the automatically performed integration of a sample, e.g., by moving peak delimiters. This is possible via the icons on the **Integration** toolbar:

The most important actions can be performed with the **Automatic Tool**. The shape of the mouse cursor indicates the performed action.

	Move left/right peak delimiter
	Change baseline point (left/right/center)
	Move baseline point (left/right/center)
	Move perpendicular line
	Move baseline segment
	Move detection parameter
	Insert peak
	Display spectra
	Zoom out an area
	Action not possible

The action that can be performed at the current position is indicated in the status bar:

Example:

Near the blue peak delimiters, the mouse cursor changes its shape. symbolizes the peak start, while marks the peak end.

- Press the left mouse button to change the integration limits of a peak by moving the peak delimiters.

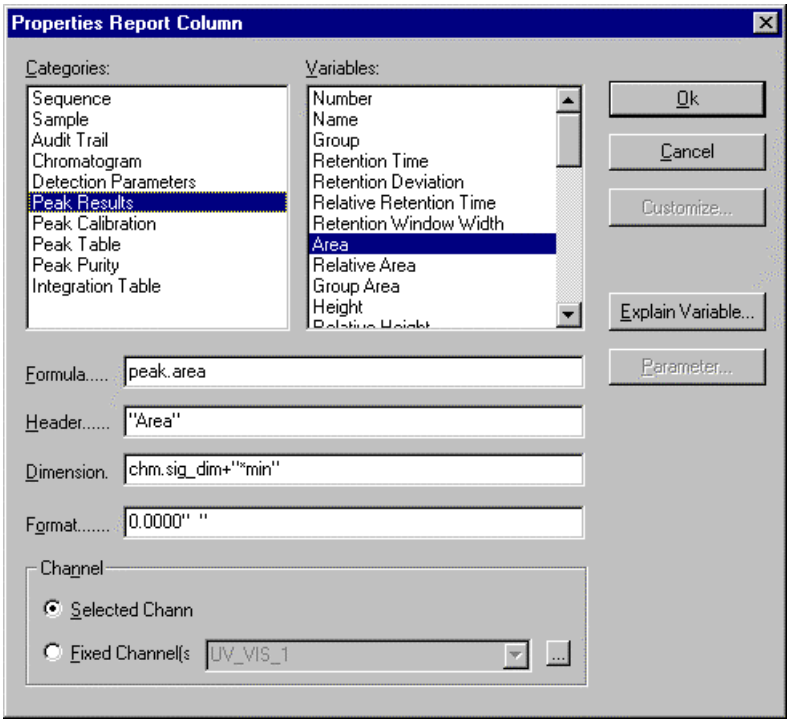
It is not possible to "run over" another peak delimiter. After moving a peak delimiter, the Dionex Chromatography Management System draws a new baseline between the peak start and the peak end. All peak properties such as area, width, substance amount etc. are recalculated. The integration report is immediately updated.

- Choose the **Save Manipulations** command (via the context or **Edit** menu) to save the reprocessing result.

Similar to moving peak delimiters, other actions can be performed, e.g., inserting or deleting peaks or changing the baseline.

3. Modifying the Report

In the report, choose the **Column Properties** command from the context menu to change the appearance of the current worksheet. You will see the following dialog box.



Divided in various categories, this dialog box offers all result variables that are calculated and evaluated by the Dionex Chromatography Management System. As soon as you have selected a variable, its properties (Formula..., Header..., Dimension..., Format...) are displayed.

Header.. shows the text of the column head, **Dimension..** shows the dimension name, and **Format..** defines the number of decimal places. Choose the **Selected Channel** option to display the values of the current channel, or choose **Fixed Channel** to output the data of a specific channel independently of the representation in the integration window.

- Press **OK** to extend the current report by an additional variable column.
- Select a column and choose **Delete Column(s)** to remove the column.

Caution: These report options influence the representation on the screen only. The appearance of the printed report is defined in the **Printer Layout**!

4. Saving Changes

The **Save Report Definition..** command allows saving all changes within a report under a separate name. The arrangement and the appearance of the individual report window sections are saved plus the variables to be displayed.

With each new start of the Dionex Chromatography Management System, the report is opened just as it was saved last. You can choose a different appearance via **Load Report Definition..** (provided that you have created your own Report Definition Files (RDF)).

Please note that each sequence is saved with a preferred profile. Then, upon opening a sample of the corresponding sequence, it is not the appearance of the window saved last that is used but the appearance of a specific report definition file (RDF). Proceed as follows to define a sequence for a preferred report:

- Select a sequence in the Browser and choose the **Properties** command via the context menu.
- Under **Preferred RDF File**, enter the name of the report definition to load.

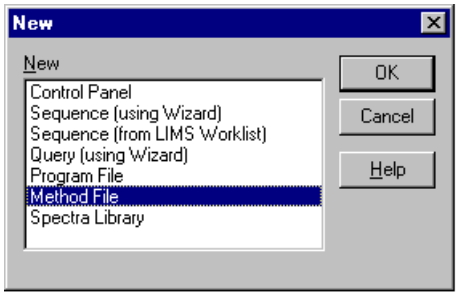
VI. Quantification Method (QNT File)

As soon as you want to present the results of sample processing, e.g. the chromatogram or a report, the Dionex Chromatography Management System searches the **Method** column of the sample list for the name of the quantification method. The settings made in this QNT file determine how substances are calibrated and how chromatogram peaks are integrated and identified.

Strictly speaking, the QNT file is required after the analysis only. However, it is recommended to create the file earlier. This allows you to follow and evaluate the course of the analysis.

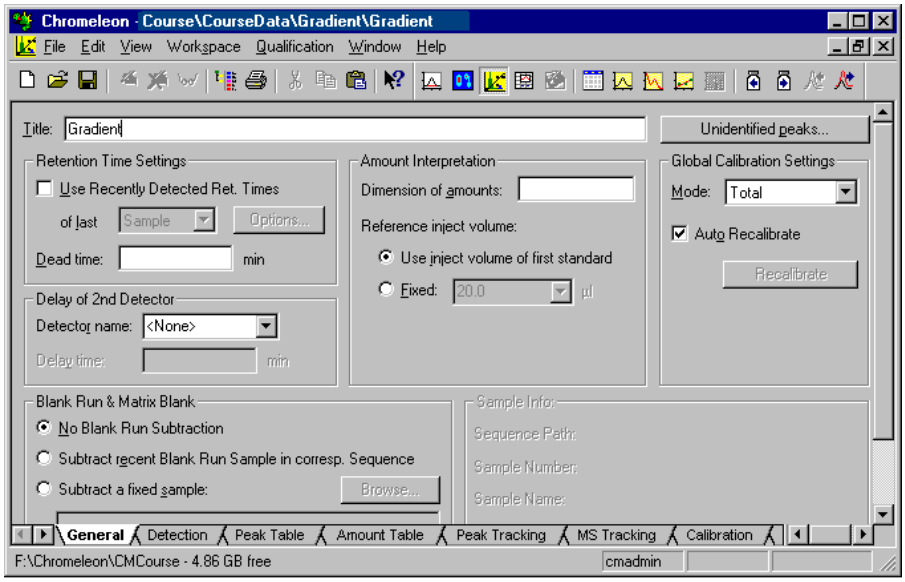
Creating a Quantification Method

- Choose the **New** command from the **File** menu.
- Choose **Method File** as file type and press **OK** to create a new method.



The QNT File Window

The QNT file window contains various worksheets **(General**, **Detection**, **Peak Table**, **Amount Table**, **Peak Tracking**, **MS Tracking, Calibration**, **Spectra Library Screening, SST, and MS**). Open the required worksheet by clicking the respective.



To create a simple evaluation method, it is sufficient to enter the **Peak Table** settings.

Creating a Peak Table

The peak table allows recognizing peaks (= ➔*Detect*), assigning names to the peaks in a chromatogram (= ➔*Identify*), and converting the determined peak areas into substance amounts (= ➔*Quantify*). The required information is usually entered before the analysis.

Saving the QNT File

Save the quantification method via **Save as** under a separate name.

Editing the QNT File

When the QNT file is edited, all changes will be implemented immediately in all involved components.

If you have opened a channel of a specific sample (see: ➔*Browser Appearance and Functions*) and you see the corresponding chromatogram, this representation is updated immediately after changing the QNT file. The same applies to the representation of numerical values as they appear in any report.

Caution: If you have not specified a quantification method when creating a sequence (Step 4 of the ➔*Sequence Wizard*), the fields of the **Method** column in the sample list will be empty! Enter the name of the desired QNT file for each of the samples. To evaluate all samples with the same QNT file, just select the QNT file for the first sample and copy the entry for all entries using F9.

1. Detecting Peaks

Before peaks can be identified and quantified, they have to be detected. Based on default values for the peak recognition algorithm the Dionex Chromatography Management System is able to detect even the smallest peaks. Normally, however, you will not be interested in these small peaks so that you may want to include certain filters to exclude them from being displayed. This and other detection tasks are defined on the **Detection** tab.

Usually, the **Minimum Area** filter will be sufficient. Normally, 1.000 mAU*min is an appropriate value for HPLC-UV. In addition, the detection parameters **Minimum Height**, **Minimum Width** as well as **Maximum Height** and **Maximum Width** can be used as filters.

Use the detection parameters **Rider Threshold** and **Maximum Rider Ratio** to define the peaks that shall be classified as riders. Use **Rider Skimming** to define how to divide a rider peak from the main peak.

Besides, you can use

Detect Negative Peaks to detect negative peaks,

Valley to Valley to enforce valley-to-valley integration,

Inhibit Integration to inhibit integration, and

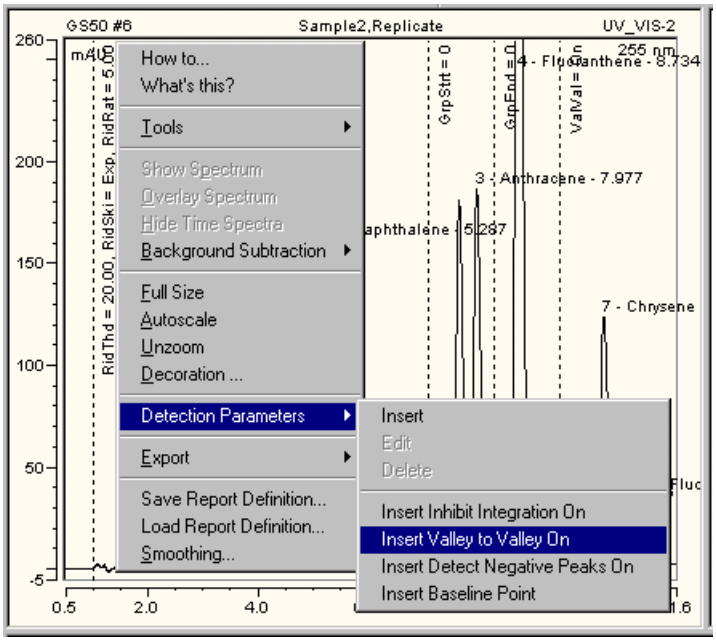
Fronting/Tailing Sensitivity Factor to influence the peak start and peak end determination.

Clicking the detection parameter tool allows viewing the position of the detection parameters in the chromatogram.

This is especially useful if you want to change the position of detection parameters or graphically insert additional parameters. Use the **Detection Parameter Tool** to change the position of detection parameters. Open the tool via the respective command of the context menu or via the {Tool_DetPar.bmp} icon. In the chromatogram, the parameters are marked by a dotted line at which the abbreviation for the parameter and the respective parameter value is indicated. The figure below, for example, shows the values for the Rider

Threshold (in short: RidThd), Rider Skimming (RidSki), and Maximum Rider Ratio (RidRat) at 1.000 min. Positioning the mouse on a detection parameter in the chromatogram activates the detection parameter tool so that you can move this parameter via the left mouse button.

Use the **Detection Parameters** command of the context menu to insert a detection parameter at the position of the mouse cursor:



This setting, for example enforces valley-to-valley integration as from the selected time.

Alternatively, you can enter detection parameters graphically by selecting a chromatogram area via the right mouse button. The opening context menu provides the following options:

- Set Averaged Baseline Start/End
- Set Minimum Area
- Set Minimum Height
- Set Minimum Width
- Set Peak Slice & Sensitivity
- Set Inhibit Integration Range

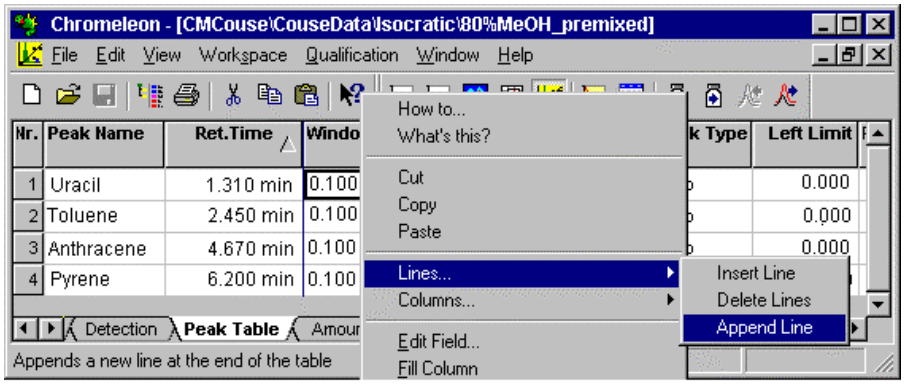
☞ ***Tip***: You can undo the graphical input of detection parameters. Click into one of the QNT editor tables and select the **Undo** command of the **Edit** menu. (In the chromatogram itself, you can undo changes only that were made in currently open chromatograms.)

2. Identifying Substances

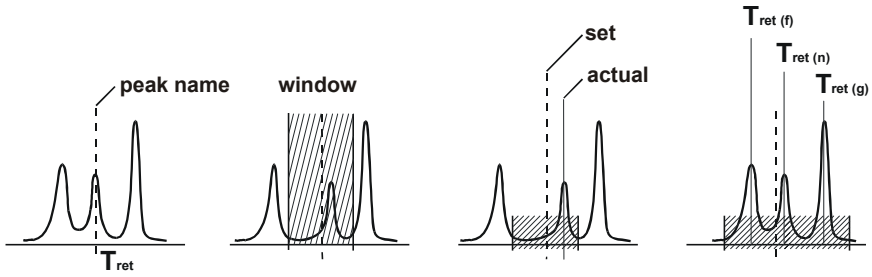
- Select the **Peak Table** tab to open the peak table.

Most frequently, peaks are identified via the retention time.

- Enter the names of **all** peaks to identify in the **Peak Name** column. Assign the expected retention time to each peak in the column **Ret.Time** (= nominal retention time (Tret)). *(**Tip:** additional lines can be added via the **Lines .../ Append Line** commands of the context menu)*.



If a peak is detected at the specified time, the name is assigned automatically (fig. a). An additional tolerance range is defined via the **Window** column (fig. b). The width corresponds to the double **Window** value. If a peak is detected in this range, it is identified even if the actual retention time does not correspond to the entered "set" (nominal) retention time (fig. c). If several peaks are detected within this range, the chromatography management system identifies the greatest, the first, or the nearest peak to the retention time (fig. D), depending on the extension of the **Window** parameter.



- In the **Window** column, enter e.g. **0.25 AG** for each peak to identify the largest peak within a 30-second window. Time input is in industry minutes, e.g. the value 1.00 corresponds to 60 s. The value 0.25 thus corresponds to 15 s, which means a window range of 30 s. The setting **0.25AF** identifies the first peak; the setting **0.25AN** identifies the nearest peak to the set retention time.

Note: To create the peak table automatically, use the **Autogenerate Peak Table** command of the context menu. You can also have the peaks numbered consecutively or use the results of the ➔*Spectra Library Screening*.

3. Quantifying Substances

Each substance that should not only be identified but also quantified requires a standard substance. The known substance amount of this sample needs to be entered in the peak table together with the standard method. Enter this information in the **Amount** and **Standard** columns.

"Amount" Column

- Search the peak table for the substance name of the standard substance(s). If the required names are not listed, enter the names and the retention times as described under **Identifying Substances**.
- Move along the line until you reach the **Amount** column.
- Enter the amount values of the substances (Substance A, Substance B, etc.).

No.	Peak Name	Ret.Time	Standard	Int.Type	Cal.Type	Amount
1	Substance A	1.500 min	External	Area	Lin	12.00000
2	Substance B	2.600 min	External	Area	Lin	17.00000

Either a concentration value (e.g. µg/µl) or an absolute value (e.g. µg) can be entered. If standards are available in various concentrations, i.e. in several vials, the concentration of each vial from which to inject "must" be entered in a separate **Amount** column.

- Choose the **Columns.../ New Amount Column...** commands of the context menu to add additional **Amount** columns.
- Enter the concentration value of the second vial in the new **Amount** column.

No.	Peak Name	Ret.Time	Window	Standard	Int.Type	Cal.Type	Amount Standard 1	Amount Standard 2
1	Substance A	1.500 min	0.400 AG	External	Area	Lin	12.00000	48.00000
2	Substance B	2.600 min	0.400 AG	External	Area	Lin	17.00000	56.00000

However, if injection is several times from the same sample vial (multiple injection), one amount value is sufficient, as the concentration is constant. This is also true if a different volume and thus different substance amounts are

injected, as the chromatography management system considers this automatically!

"Standard" Column

The standard method determines how a calibration is performed. A general distinction is made between calibrations based on an *external* or *internal* standard.

External standard means that the calibration is performed based on one or several standard samples (= normal case). *Internal* standard means adding a known amount of standard to the unknown sample (= special case that is not described in this Tutorial!).

- Ensure that the correct standard method for each peak to calibrate is entered in the **Standard** column (= **external** = default value).

For information on further calibration options (internal or internal/external), see the Online Help or the User Manual (in the **Calibration** section).

Further Columns

All other peak table columns determine how the determined area values are converted into the resulting substance amount values. Generally, the standard settings can be used, i.e. *no changes* are required.

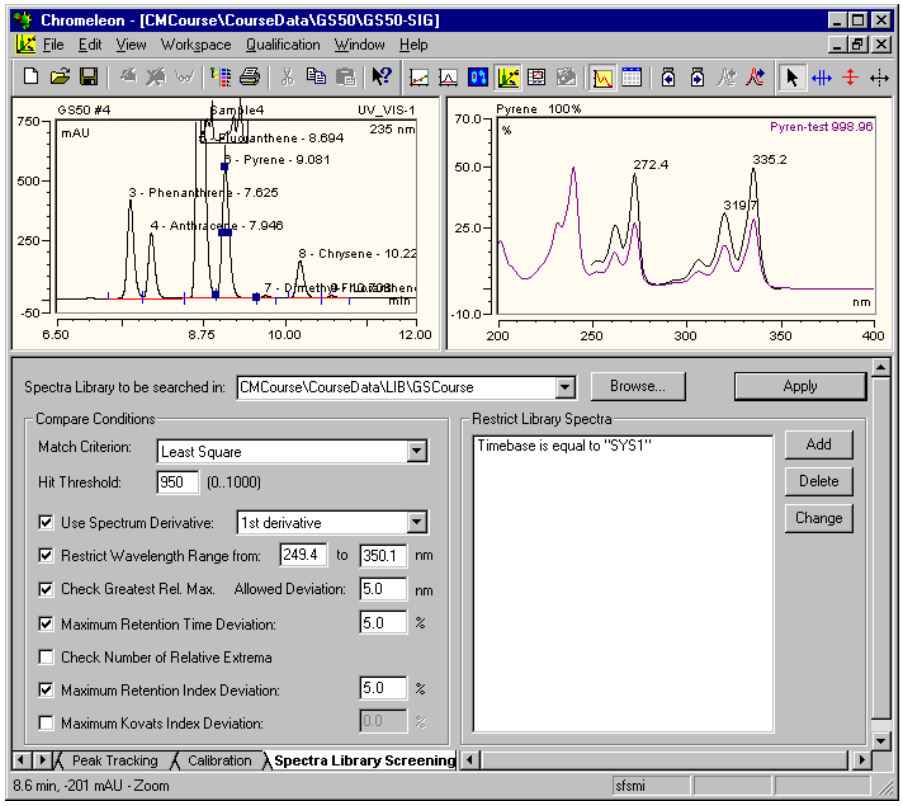
Ensure the following settings:

- **Calibration Type = Lin**
- **Integr. Type = Area**
- **Right/Left Limit = 0,000**
- **Group = --**
- **Response Factor = 1,000**

4. Spectra Library Screening

The **Spectra Library Screening** tab of the QNT editor allows searching spectra libraries for reference spectra for the different peaks of the current chromatogram. As the chromatographic conditions, considerably influence the spectra, we recommend filling your library with spectra from chromatograms that were recorded under the same conditions as the current chromatogram.

On the **Spectra Library Screening** tab, select the spectra library in which to search for the reference spectra. In addition, enter the comparison criteria for the spectra search. Normally, the default values of the **Match Criterion** (Least Squares) and **Hit Threshold** (950) will be sufficient. However, you can also specify many additional search criteria.



Start the spectra search by pressing **Apply**. The retention spectrum of the actual peaks is compared to the reference spectrum that was found. To the top

right of the spectra plot, the corresponding match factor is displayed. The match factor indicates the correspondence of the two spectra. A value of 1000 indicates that the spectra are identical while they would be completely different with a match factor of 0. If no corresponding spectrum is found based on the selected criteria, the **No spectra library hits found!** message will be given.

 ***Note:*** You can use the spectra library screening results for automatic peak table creation (see ➔*Identifying Substances*).

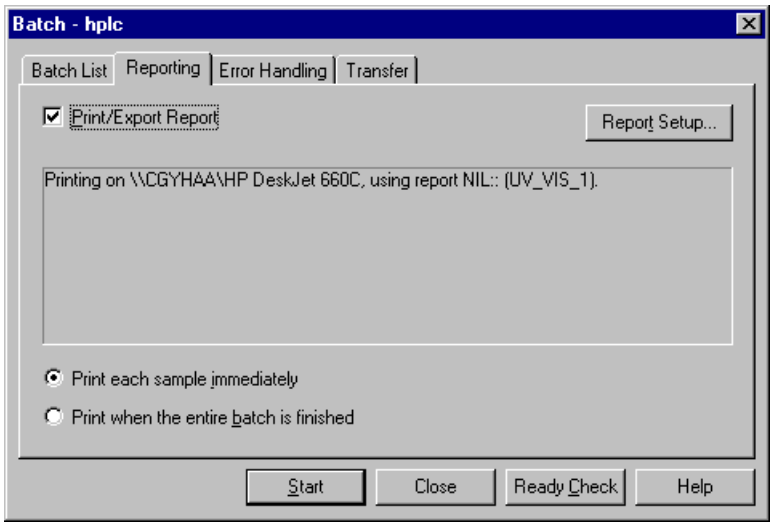
VII. Printing Results

1. General

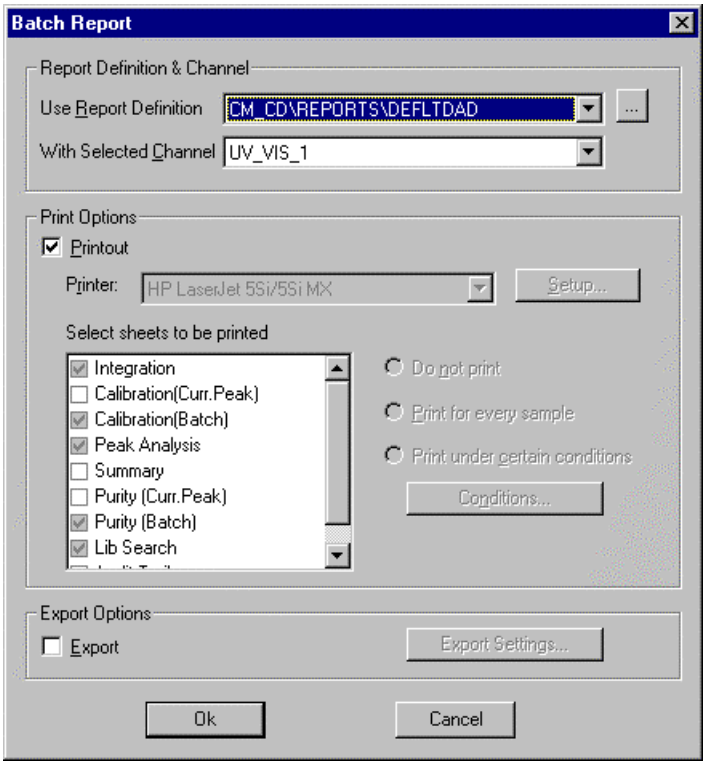
Printing in Automatic Batch Operation

As mentioned in the previous chapter, printing results can be started together with automatic sample processing (**Online Batch**). Let us have another look at the **Batch** dialog box.

- Change to the **Reporting** tab.
- Activate the **Print/Export Report** check box to print the sample processing results.
- Choose **Print each sample immediately** to start printing after each sample. Choose **Print when the entire batch has finished** to print all sample results after the entire sequence is completed.



- The report type and the extent of the printed output are determined via the **Report Setup** button and the following dialog box.



Choose a report template in the **Use Report Definition** field. The default report template DEFAULT.RDF of the Dionex Chromatography Management System is stored in the **REPORT** directory.

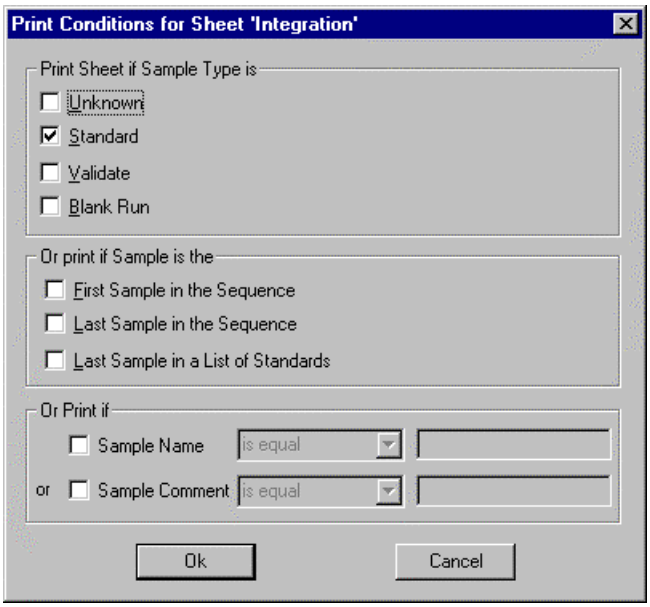
- From the **With Selected Channel** field, choose the channel to print (e.g. UV_VIS_1). If the field remains empty, the preferred channel (see ➔*The Browser: Appearance and Function*) will be printed.
- Select the **Printout** option to print the sheets.
- The **Printer** field shows the name of the previously selected default printer. Choose **Setup** to select another printer.

So far, you have specified the channel, the printer, and the report definition for the printed output. However, what is included in the selected template? Is it possible to change the appearance of the printed results? Yes, it is!

As described in detail in ➔*The Printer Layout* section, a report template contains several special sheets for different print data. The sheets included in the selected report template can be viewed in the **Selected sheets to be printed** field. The **Integration**, **Calibration (Curr.Peak), Calibration (Batch)**, **Peak Analysis**, **Summary**, and **Audit Trail** sheets are included in the default report template.

- Under **Selected sheets to be printed**, choose the worksheets of the report template you wish to print.
- For each selected worksheet, it is necessary to determine whether all samples or only samples of a specific type should be printed.
- Choose **Print for every sample** to print results for each sample type.
- Choose **Print under certain conditions** to print results for a specific sample type only.

If you want to print, for example, the **Calibration** worksheet for standard samples only, choose the **Print under certain conditions** option and press the **Conditions** button. In the following dialog box, activate the **Standard** check box.



The other options of these two dialog boxes are for later use.

- Press **OK** to return to the **Batch Report** dialog box and define the other worksheets.
- Then start sample processing by pressing **Start**, as described under ➔*Starting the Analysis*.

Printing Samples

Of course, sample-processing results can be printed independently of the online batch. This applies to all samples for which raw data are available. The Dionex Chromatography Management System assigns **Finished** as sample status in the sample list. Proceed as follows to print the results of any samples.

- Open the **Browser** and choose the **Print Setup** command to select a printer for printing the results.
- Open the sequence directory and select the name of a sequence to print the results of all included samples.
- If you want to print specific samples of a sequence only, select them one by one with the mouse. Use the CTRL key to select several samples.
- Choose the **Batch Report...** command from the **File** or context menu and determine how to print the report (see **Printing in Automatic Batch Operation** above).

Printing with your own Report Templates

The Dionex Chromatography Management System allows each user to change the default report that was created with the DEFAULT.RDF report template according to individual requirements. This requires creating a new report template in the **Printer Layout** window. The new template is saved under a new name and is now available as a separate template. The new report template can be selected in the **Using Report Definition** field instead of the file DEFAULT.RDF.

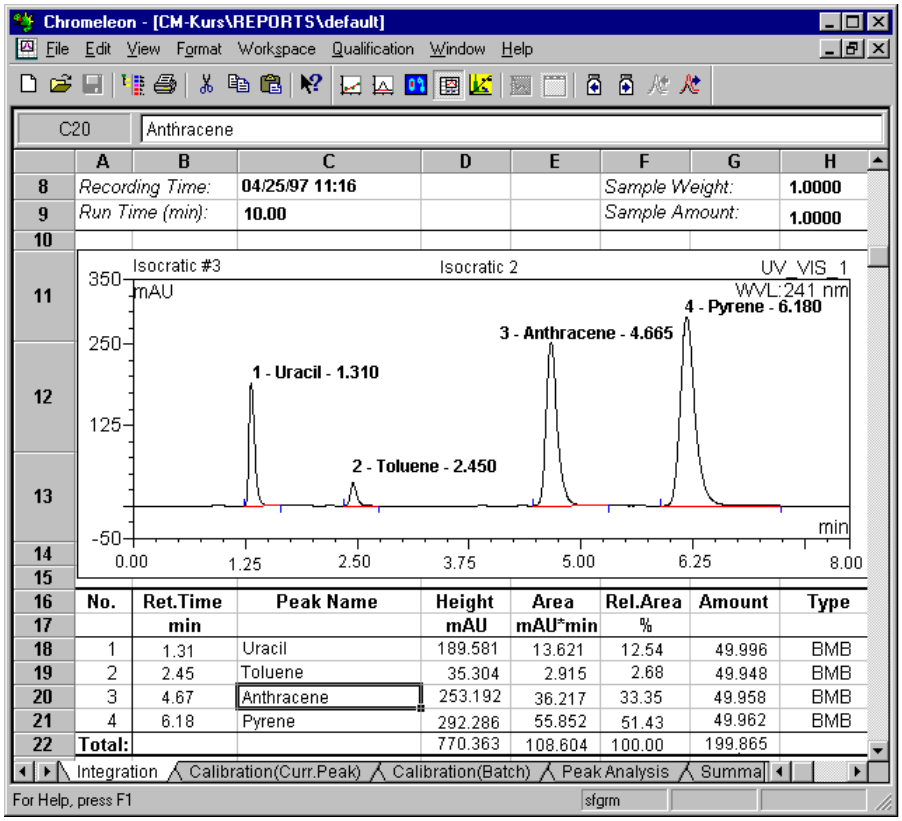
2. Printer Layout

The **Printer Layout** window serves to create custom print templates. Proceed as follows:

- Double-click a sample name in the **Browser** to open the sample chromatogram. For representing the chromatogram, the Dionex Chromatography Management System opens the **Integration** window.
- Use the **Printer Layout** command (**View** menu) to change from the **Integration** view to the **Printer Layout** view.

☞ ***Tip:*** To quickly change from one view to another, the Dionex Chromatography Management System offers a Method toolbar (described under ➔*Data Reprocessing*) Place the mouse cursor over an icon to read its label in the quick info.

The following view shows a section of a report based on the default report template DEFAULT.RDF:



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	1.31	Uracil	189.581	13.621	12.54	49.996	BMB
2	2.45	Toluene	35.304	2.915	2.68	49.948	BMB
3	4.67	Anthracene	253.192	36.217	33.35	49.958	BMB
4	6.18	Pyrene	292.286	55.852	51.43	49.962	BMB
Total:			770.363	108.604	100.00	199.865	

The **Integration**, **Calibration (Curr. Peak)**, **Calibration (Batch)**, **Peak Analysis**, **Summary**, and **Audit Trail** worksheets are part of the DEFAULT.RDF report template.

- Choose one of the tabs on the window bottom to change between the individual sheets of a report template and to view the different worksheets.

The appearance and the structure of an individual worksheet are very similar to **Microsoft Excel** spreadsheets. Each sheet consists of a large number of columns (256) and lines (16000) and thus is much larger than a single printed page. A worksheet can consist of many horizontally or vertically arranged printed pages.

Chromatograms or tables that exceed one printed page are automatically printed on two or more pages. The order in which the pages are printed is defined in the **Page Setup** (**File** menu).

Editing an Existing DEFAULT.RDF Template

It is much easier to change an existing report template rather than to create a completely new one. As only the DEFAULT.RDF template (and the DEFLTDAD.RDF template) is available at first, copy this template, and then modify it.

- Choose the **Save Report Definition** command from the context or **Workspace** menu and save the template under a new name.

You can now perform changes without overwriting the default report template. For an overview on how to proceed and on the available options, see below. For a detailed description on the individual steps, see the **How to ...: Actions in the Window Printer Layout** section in the User Manual or the Online Help system.

- Choose the **Layout Mode** command from the **Edit** menu.

This command serves as write protection for the report templates. Only after having activated the **Layout Mode**, you can change report templates or individual worksheets.

- Choose the worksheet you wish to edit or add an additional (empty) worksheet via the **Insert Sheet** command (**Edit** menu).
- Choose the **Delete Sheet** command (**Edit** menu) to delete an unnecessary worksheet.
- Double-click a tab to assign it a different name (e.g. **Integration Special**).

- Choose the **Insert Row(s)/Column(s)** or **Delete Row(s)/Column(s)** commands to add or remove single rows or columns on the worksheet (not of an included table).
- Select a field, a column or an area and choose the **Clear ...** command from the context menu to clear unnecessary information from the worksheet.

Having removed all unnecessary parts, you can now fill cells, columns, or areas of the worksheet with new contents. You can either use the Windows clipboard (**copy** / **paste**) or the **Insert ...** command of the context menu.

- **Insert ... Chromatogram** reserves an area for a chromatogram.
- **Insert ... CHROMELEON Report Table** reserves an area for a complete report table.
- **Insert ... CHROMELEON Report Column** inserts a column for a new report variable in an existing table.
- **Insert ... Spectra Plot** reserves an area for a spectrum.
- **Insert ... Chart** reserves an area for a chart, etc.

"Reserved area" means that a section is reserved for inserting a specific chromatogram, spectrum, etc. instead of actually inserting it. For tables, the number and the contents of all columns are defined. When printing a sample, the reserved area is filled with the actual chromatogram, the spectrum, or the table values.

- Choose the **Save Report Definition** command from the context menu or the **Workspace** menu and save the result of your changes.

VIII. Online Help

When working with the Dionex Chromatography Management System, there may be issues and questions that are not discussed in this Tutorial. In this case, refer to the User Manual and to the Online Help for more detailed information. You can access the Online Help system anywhere in the program. Choose one of the following ways to view help information.

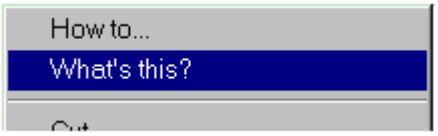
- ➔*Context-sensitive Help* answers your questions regarding any topics of your current position.
- ➔*Systematic Help* allows
    - selecting an interesting topic from the contents tab or
    - searching the index for any required information.

1. Viewing Context-sensitive Online Help

Depending on your current cursor position, you can view different online help windows. If a help window is opened, you can access systematic help. In other cases, a popup window opens providing a short context-sensitive description. Usually, you can jump to related topics.

Help via the Context Menu

The right mouse button allows you to view help on the topic that is currently selected:



Select **How to ...** to view detailed information on actions that are possible at the current position. Click **What's this?** for a description of the selected item, command, etc. In some cases, **What's this?** topics offer information that is more general. Normally, various links are available for specific information.

Help via the Help Button and Icon

After clicking the  icon on the toolbar, a question mark is appended to the cursor. With this special cursor, you can now click any item on the screen to view specific information on the selected topic.

Several screens offer a **Help** button instead of the context menu or the question mark. This button allows you to view information on the current screen. In the QNT editor, where you can enter parameters and variables, the **Explain Param.** and **Explain Variable** buttons provide explanations on the selected parameter or variable.

Help via the F1 Key

Finally, you always have the possibility to view help information via the **F1 key**. This help information corresponds to the context-sensitive help available via the question mark cursor or the **Help** button.

2. Viewing Systematic Online Help

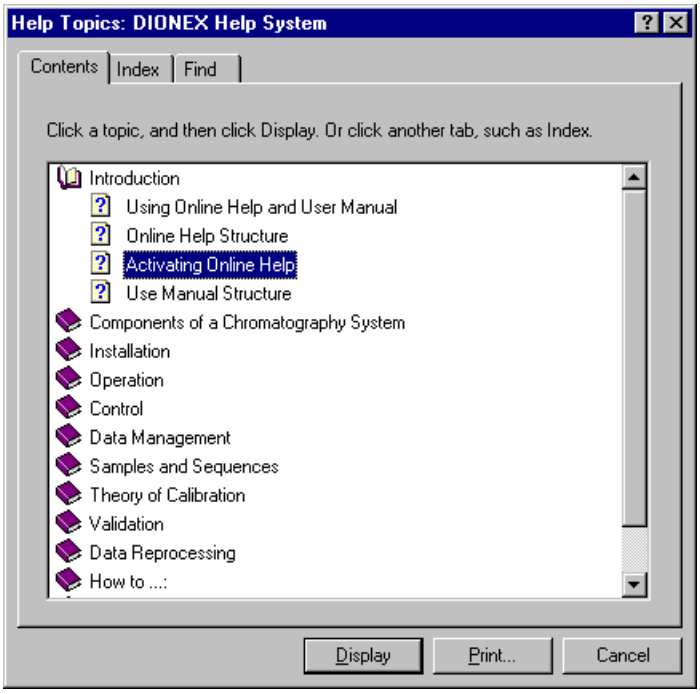
Open the **Help** menu and click **Index** for a topic overview in the Help system. The help window offers the following tabs:

- **Contents**
- **Index**
- **Find**

Contents Tab

This tab shows the Help system's table of contents. Double-click the book symbol to view the topic titles contained in the chapter. Double-click the opened book symbol to close the book (chapter) again.

Topic titles are indicated by a page symbol with a blue question mark. Double-clicking a topic title allows viewing the topic.



Index Tab

This tab assists you in finding a specific term via index entries in the entire Help. Enter the first few letters in the first field until the required term appears in the second field. To view the topic, press **View** as soon as you have selected the topic. If several topics are found, you can open one of them in the **Topics Found** window.

Find Tab

This tab assists you in finding a specific key word in the entire help system. First, the Dionex Chromatography Management System generates a list containing all words in the entire Online Help. Similar to the index, you can search the resulting list for a specific term.

Addendum: Short Glossary

Datasource and Database

The term datasource is used for a database that is registered on a server. Setting up (registering) a datasource is performed in the Browser. The user specifies the format and the location of the database.

During the initial installation, a local default datasource is created on each client PC. In network operation, the datasource name is composed of the computer name and the extension **LOCAL** (<PC-NAME_LOCAL>). On a local station that is not included in a network, the name that is stated in the operating system below **Control Panel / Network / Identification** is used. If no identification is entered, the datasource is named DEFAULT_LOCAL.

Normally, Dionex Chromatography Management System data is stored in an Access database, i.e. in a MDB (**Microsoft Data Base**) container. The default datasource is based on an Access database, too. The ODBC capability of the chromatography management system allows using various other formats (dBASE, SQL, Oracle, etc.) as well. Independently of the chosen format, data of single samples (**Sample data**) is saved in a datasource as well as data of sequences (**Sequence data**). Databases can be saved on a local hard disk or any other mass storage device.

In the Dionex Chromatography Management System, the **Directory** command allows creating individual subdirectories below a datasource. The directories are used for saving ➔*Sequences* and the corresponding data and programs.

If the datasource is located on a centralized network PC, the database is accessible by all clients that have the appropriate access rights assigned by the system administrator. If the datasource is stored on a local hard disk, it is up to the corresponding client to decide whether the database can be accessed via the **File Sharing** option. The Dionex Chromatography Management System also offers the possibility to lock datasources, directories, or sequences.

Note: "Old" GynkoSoft data has the required database structure. The Dionex Chromatography Management System is therefore capable of handling this data as "real" data of the Dionex Chromatography Management System. The user simply establishes a connection (**Connect**) to the data stored under **Drive....** (see: ➔*Installing Datasources*). For details on creating a datasource, see the Online Help and the User Manual.

Raw Data

Raw data refers to all analog and digital data points that are digitally stored on a PC. Raw data therefore exists for signals or channels only that were selected by the user before data acquisition.

The scope and accuracy of the stored raw data depends on the selected **Sampling Rate** and **Step**.

Sequence

A sequence combines samples that belong together due to their origin or processing. The names of all samples belonging to one sequence are entered in the sample list (also called sequence table). A sequence is thus a container for various samples.

Theoretically, the number of samples is not limited, but 100 sample entries should be exceeded only in exceptions. Creating more sequences reduces the number of samples included in one sequence, thus accelerating access to the individual samples. In addition, it is easier for the user to keep track of the processed samples.

The sequence table also defines how to process a sample. This includes information on the sample itself (injection volume, position, amount, dilution factor, etc.) as well as references to chromatographic methods that specify the program (PGM file) to be performed for the analysis and the evaluation parameters to be used (QNT method).

The entire data collected in connection with creating and processing a sequence, including raw data and protocol data recorded during the analysis, is saved in the sequence directory of a datasource or in the underlying database. Of course, this includes the raw data and the protocol data that were recorded during the analysis.

Similar to ➔*Datasources*, sequences can be "locked." In this status, data and results are read-only; they cannot be modified or extended.

(Chromatography) Server

PCs connected to the components of a system via a serial interface can be used as chromatography servers.

A chromatography server is automatically installed on the PC during the installation. The chromatography server controls the data exchange between the system and the PC. Upon starting, each server is capable of serving up to six controlled or 16 non-controlled systems (➔*Timebases*). The server receives the commands entered by a client PC in a control panel and executes them at the specified time (e.g., by transmitting them to the corresponding device driver of the HPC system). In the opposite direction, the server also assumes this buffer function. Thus, the raw data of each system is stored at the location specified by the client and the entire system-relevant data is forwarded to the client.

Configuring a server and installing a timebase is performed via the Server Configuration program. If the server and the client software of the chromatography management system are located on the same PC, this is called a local installation; if they are not, it is a network installation.

☞ ***Tip:*** In case of manual data acquisition, the ➔*Raw Data* from the system is always stored in the server directory PCNAME_LOCAL. In the case of a batch, the user can choose where to store the data. To minimize the risk of losing data, raw data should always be stored temporarily on the server. In the course of archiving, it can be transferred to a different computer.

Timebase

All components combined in a chromatography system to enable the chromatographic separation and related in a time context with each other, are assigned to the same timebase.

A timebase can be a very complex system (that includes e.g. two pumps, one autosampler, one column oven, and two detectors switched in series). However, an isolated integrator or a gas chromatograph can represent a timebase as well.

Another system that is completely independent from the first one represents a new timebase. Administration of different timebases is on one or several ➔*Chromatography Servers*. The name for a timebase is assigned in the Server Configuration program.

PeakNet 6 Tutorial Index

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PeakNet 6 User's Guide

Contents

Introduction

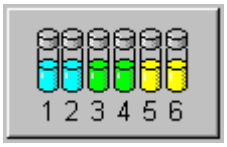
Tutorial

To become familiar with the Dionex Chromatography Management System we recommend you to work through the **Tutorial**. From there, proceed to the desired topics via **Contents Overview**. Besides, you can also open the Tutorial directly via Start>Programs>CHROMELEON>Tutorials.

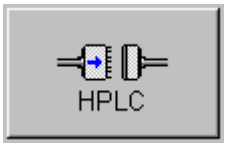
The Tutorial has the following sections:

I. 

Starting the Program: As soon as your computer and one of the operating systems Windows 98 or Windows NT/2000 are running, the Dionex Chromatography Management System can be started via the Windows Start button on the task bar.

II. 

Managing Data: The Dionex Chromatography Management System allows you to manage data in folders and directories similar to Microsoft Windows. The tool that helps you to handle your chromatography data is the **Browser**.

III. 

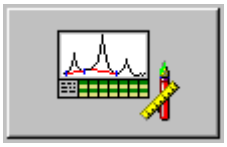
Controlling your HPLC system: Ensure that your chromatography, HPLC, GC, or CE instruments are correctly connected to the PC via a serial port. Using the ➢*Control Panel* allows you to operate the pump, ➢*Autosampler*, detector, etc. from your PC. In addition, you can create a ➢*PGM File* to control your system automatically.

IV. 

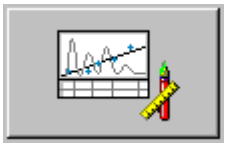
Analyzing Samples: Are your instruments controllable via the PC? Then, you can start your first analysis. Create a **Sample List** (= ➢*Sequence*) to use all capabilities the Dionex Data System offers.

First, use the **Sequence Wizard** to include the samples to process in the sample list. The Wizard allows you to define the order of sample processing, the injection volumes, the sample type (analysis or standard), and where the Dionex Chromatography Management System finds information on how to perform the analysis. The latter is by entering a program and a method name, and by creating the corresponding files (PGM File, QNT File, see below).

As soon as you have created the sample list, the program file, and the quantification method, you can start the **Analysis**. The resulting data is automatically saved.

V. 

Reprocessing Data: The analysis result can be viewed and edited on the screen. **Data Reprocessing** allows you to manually change integration limits directly in the chromatogram or to evaluate samples again ("offline") based on new parameters.

VI. 

Quantifying: Using a ➢*Quantification Method* (QNT file**)** allows you to minimize the reprocessing effort for individual chromatograms. The QNT method defines the detection parameters, the peak identification, and the calibration of the substances in the sequence.

VII. 

Printing Results: Analysis data can be printed at any time. For perfect adjustment to your personal requirements, you can create your own report templates in the **Printer Layout**, define your own result variables, or embed your company logo.

VIII. 

Online Help: This Tutorial can deal with selected aspects of the Dionex Chromatography Management System, only. For further information, see the detailed description in the **Online Help** or the User Manual.

Using the Online Help System and the Manual

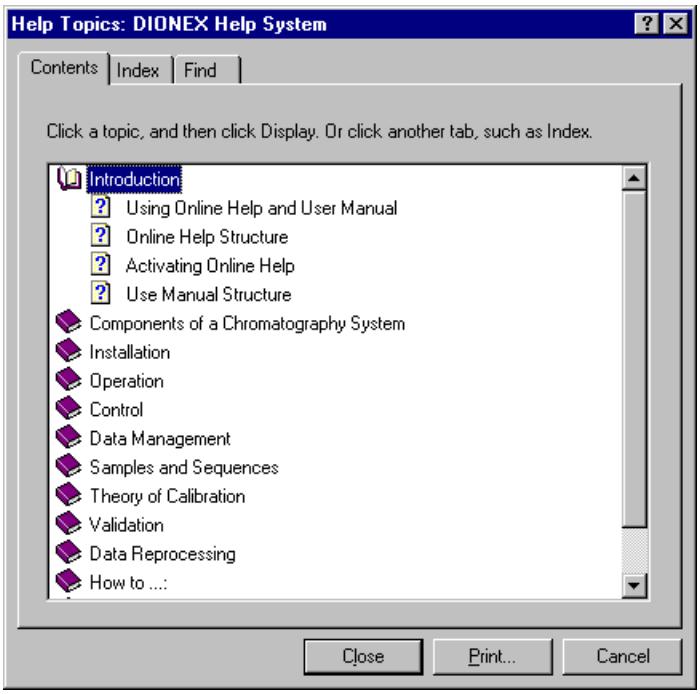
The Online Help system and this user manual differ only slightly in their respective contents, but they are intended for different situations.

- Refer to the Online Help system to look up terms or find information on how to use the application in a specific situation on the ***current screen***. The easiest and quickest way to receive help is by pressing the ➢*F1 Key*. For further information, see **Activating Online Help.**
- Look up information in the user manual to become familiar with the ***fundamental features*** and operation of the data system. We recommend that you read the topics of the first two sections and look up unfamiliar terms in the glossary.

Overview: Online Help

As with most Windows programs, the Online Help features various windows and levels. These largely correspond to the various parts of the user manual, such as table of contents, main section, appendix, and index. In addition to the manual, the Online Help provides many context-sensitive tips that open only from the respective program window.

The overview displayed via the **Contents** button corresponds to the table of contents in the user manual:



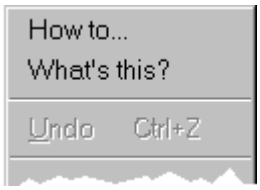
- Double-click a **book symbol** to view further levels ("branches").
- Double-click a **question mark symbol** to open the corresponding topic.
- Click the **Index** tab to search Online Help for an index term.
- Select the **Find** tab to search Online Help for any non-indexed string.

The selected topic appears in a separate Help window. This window will have a white background if the topic deals with questions regarding theory, installation, and operation. The background color will be yellow if tips that are more practical are opened (**How to ...:**). Both windows can be displayed simultaneously.

☞ ***Tip***: Online Help is automatically displayed in the language (German or English) of the current language setting (see Windows Control Panel/International Settings). As default, the system loads the English version.

Activating Online Help

There are several ways to access Online Help.

➢***F1-Key***	Pressing the F1 key opens a Help topic containing context-sensitive Help information.
	Choose **How to ...** from the context menu to view information on the currently possible operations (practical tips). Choose **What's this**? to view a description of the corresponding control or the currently displayed window (theory).
Help menu	The ➢*Index* option in the Help menu opens the contents overview of Online Help. The **Using Help** option shows how to use Online Help.
	After clicking this button, the mouse cursor changes to a question mark. Click any screen element to display the corresponding description.
	The **Help** button in dialog boxes opens the corresponding explanations for this dialog box.

When viewing a Help topic in the Online Help, you can ➢*jump to another Help topic* by clicking the hyperlink term underlined with a single line or by clicking a shortcut symbol.

Topics underlined with a dotted line can be viewed simultaneously with the current window.

Overview: User Manual

The user manual contains the sections **Theory, Installation, Operation**, **How to ...:** and the **Glossary**. Use **Contents** and **Index** to search for specific terms and to get an overview over the various topics described in the manual.

1. Section: Theory, Installation, and Operation

This section describes the structure and the functions of the Dionex Chromatography Management System as well as basic chromatographic facts and methods. Where appropriate, the user is referred to related topics.

These references are indicated as follows:

	***Jump term***	Refers to technical terms in the glossary section.
⇒	***Jump term***	Refers to topics in the reference manual.
	**Shortcut symbol**	Refers to topics in the **Theory, Installation, Operation** or **How to ....** sections.
	**"Installation" link**	Refers to topics in the **Installation Instructions for Different Devices** section.

2. Section: How to ...:

In this section, you will find helpful answers to frequently asked questions, for example:

"How do I perform external calibrations?"

"How do I generate program files?" or

"How do I re-integrate chromatograms manually?"

3. Section: Installations Instructions

The installation section provides detailed information on how to install:

- All third-party devices that can be controlled.
- All Dionex PC plug-in boards and interfaces.
- An appendix on cables and pin assignments.

4. Section: Reference Manual

The reference manual includes tabular descriptions on Commands, Parameters, Variables, and Report Categories.

Appendix: Glossary

The glossary section contains an alphabetically sorted list of chromatographic and program-related terms.

Refer to the glossary to view exact definitions of technical terms (e.g., Blank Run Subtraction), a command (e.g., **Draw**), or a parameter (e.g., **Skewness**).

Index

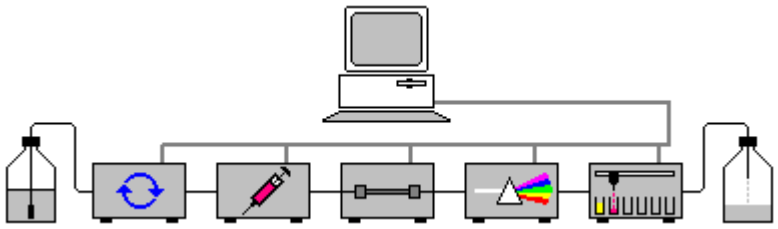
Refer to the index to locate information on a specific term. In addition to the page numbers that refer to the first two sections, page numbers preceded by the letter **A** refer to the glossary section, e.g.:

Theory, Installation, Operation

Hardware and Software Chromatography Components

Overview: Components of a Chromatography System

A modern HPLC (High Pressure/Performance Liquid Chromatography) system or IC (Ion Chromatography) system consists of the following components:



From one or several reservoirs (**a**), up to four solvents are drawn via the pump (**b**), mixed to supply a defined solvent mixture and are then directed to the system with a different flow rate. In this liquid flow, the solution to be analyzed is injected via the injection unit (**c**). On the column (**d**), the contained substances are separated into individual fractions or components. Using a thermostat-controlled oven can optimize the separation process. When a substance reaches the detector flow cell (**e**), a signal is produced that is proportional to the measured concentration. Additionally, a ➢*Suppressor* is added before the detector in suppressed conductivity mode IC. The signal whose profile corresponds to a Gaussian distribution is called a peak. By determining the peak area and by means of a previously acquired calibration curve, the exact quantity of each individual substance can be calculated (quantitative analysis). Optionally, a fraction collector (**f**) can then distribute individual substances or fractions to different containers (**g**).

Determination of the peak area is performed by the chromatography data system installed on a PC (**h**). In addition, the data system

- controls and monitors all connected chromatography instruments, collects data and status messages, and
- enables quantitative and qualitative evaluation of the data when used together with photodiode array detectors.

Communication between chromatography instruments on the one hand and computer and data system on the other hand is via serial interfaces or via additional boards such as A/D converter and the pump control board.

If several PCs are connected via a network, systems can be controlled from remote locations in the network. Data can be managed centrally and can be retrieved from any workstation.

For detailed information on the components of a chromatography system, see the topics below:

Chromatography Instruments

Device Communication

PC and Operating System

Network

Data System

Chromatography Instruments

The Dionex Chromatography Management System is especially designed to control and monitor the following Dionex instruments. Appropriate instrument control options may need to be purchased and installed in order to control the particular instrument.

HPLC pumps:	M480, P580
IC pumps:	GP40, GP50, GS50, IP20, IP25, IS25
Autosamplers:	GINA 50, GINA 50T, GINA 160, AS50, AS3500, ASI-100
UV/VIS detectors:	
Single wavelength	AD20, AD25
Multiple wavelength	UVD 160S, UVD 170S
Full-spectrum (PDA)	UVD 320S, UVD 340S, PDA-100

Electrochemical detectors:	CD20, CD25, CD25A, ED40, ED50, ED50A
Instrument/PC interface:	UI20 Universal Interface, UCI-100 Universal Chromatography Interface
Eluent generator:	EG40 Eluent Generator (installed via the IC pumps)
Temperature control modules:	LC25, LC30, AS50 Thermal Compartment
System modules:	DX-120, IC20, IC25, IC25A

In addition, the following instruments, which are available from Dionex, are supported.

Fluorescence detectors:	RF1002, RF2000
Refractive index detector:	RI-71 (data acquisition only)
Column oven:	STH-585

Third-party analytical instruments are also supported. See the following examples. Appropriate instrument control options may need to be purchased and installed in order to control these instruments.

Gas chromatographs:	e.g. Agilent (formerly HP) HP5890; HP6890
Radioactivity detectors:	e.g. Berthold LB507A
Electrochem. detectors:	ANTEC DECADE, ANTEC INTRO
HPLC systems	Agilent (formerly HP) HP1100

Should you have any questions regarding product support, please contact your Dionex sales representative.

Device Communication

To control a chromatography system and to record chromatograms and spectra, the Dionex Chromatography Management System constantly communicates with peripherals such as ➢*Autosamplers*, pumps, and ➢*Photodiode Array Detectors*.

On the one hand, the data system sends control commands to the instruments; on the other hand, the detector transmits large quantities of data (3D-fields, chromatograms, and spectra) to the data system. Depending on the type of the exchanged data, various transmission methods are used.

Also, see the topics below:

A/D Converter

Pump Control Board (Frequency/Pulse Width Modulation)

Serial Interface (Digital)

Dionex Universal Chromatography Interface (UCI-100)

DX LAN

A/D Converter

Chromatographic detectors convert ➢*Signals*, e.g., absorption or conductivity, into electric voltage. As a PC can only process digital information, the electric voltage must be converted into digital data by an additional interface board. If the detector is not capable of this conversion, an analog/digital converter (the A/D converter) performs the conversion.

The ➢*A/D Converter* has 16 analog inputs and several (digital) ➢*Remote Inputs*. Analog signals of the detector are recorded via the analog inputs, and external events (for example, injection of a sample) are communicated via the remote inputs.

Modern photodiode array detectors such as the Dionex **UVD 320S** and **340S** detectors are capable of generating digital data. Detectors of this type do not require an additional A/D interface board. Transmission of the data to the data system is digitally via a **Serial (RS232) Interface** or a separate PC board.

For installation information, see **Installing the A/D Converter**.

Caution: Wrong polarity (remote inputs) and input voltages outside the valid range will destroy the board!

Pump Control Board

Pumps without a built-in serial RS232 or DX-LAN interface receive their flow commands via special control lines (9-pin SUB-D-connector). The signals transmitted on these lines, such as the required frequencies for operating a frequency-controlled pump, are generated in the PC by the pump control board. The Dionex Chromatography Management System is thus capable of controlling the flow of up to three pumps simultaneously. Furthermore, the pump control board is fitted with four relay outputs that are available for transmitting events to other instruments.

You need the board to run flow or percent gradients with the Gynkotek pump M300. You can also use the pump control board to control the flow of the Dionex pumps M480 and P580. However, the flow of these two Dionex pumps can be controlled without the pump control board as well. For further details, see **Installing the Pump Control Board**.

Serial Interface

The operating systems Windows 98 and Windows NT/2000 allow direct data exchange via serial interfaces. Without any problems, several serial interfaces and thus a large number of chromatography instruments can be controlled from the PC. If more ports are required, additional interface boards can be installed (for further details, see **Installing a Serial Interface Board**.)

Drawbacks of this type of data transmission are the relatively short range (< 10m) and limited speed. When transmitting large quantities of data, as does the Dionex photodiode array detector UVD340S, special interface boards must be used.

Dionex Universal Chromatography Interface (UCI-100)

In chromatographic systems, different interfaces are required for data acquisition and device control. The Universal Chromatography Interface (➢*UCI-100*) provides these different interface types and makes them available to the chromatography server. For communication with the chromatographic data system of the server, either a USB or an Ethernet connection can be used.

This chromatography interface, which is designed to meet the requirements of modern chromatographic systems controlled by the Dionex Chromatography Management System, is equipped with 8 analog inputs, 8 (digital) ➢*Remote Inputs*, 8 digital outputs (relay outputs), as well as BCD inputs for the sample position. In addition, 4 RS232 ports are available.

Tip: Use the RS232 interfaces (COM ports) via USB only (**no** TCP/IP)! NT4 computers do not support USB. Thus, if LAN connections are required, additional Equinox boards must be used for instrument control via RS232. We recommend using a peer-to-peer connection for analog data acquisition via LAN (= installation of a second network interface card (= NIC; in the operating system = adapter) in the server PC - see **Connecting the UCI-100 via a Peer-to-Peer Connection**

under NT4).

For installation information, see **Installing the Dionex Universal Chromatography Interface (UCI-100)**.

DX-LAN

Many Dionex instruments can communicate with the Dionex Chromatography Management System through a Dionex local area network (DX-LAN). The DX-LAN network consists of a PC equipped with a DX-LAN interface card and at least one additional device, for example, a GP50 pump, AS50 autosampler, or ED40 detector. The additional device must also be equipped with a DX-LAN interface card.

For installation information, see **Installing the DX-LAN Card**.

Timebase

If you intend to operate a single chromatographic system with the Dionex Chromatography Management System, you will work with a single **timebase**. All instruments (sampler, pumps, detector etc.) are time-dependent on each other and are synchronized during operation, i.e., they have a common clock. If you control several systems, the individual systems work independently (asynchronously) from each other: the Dionex Chromatography Management System must manage a separate timebase for each system, i.e., the systems behave as if they were controlled by separate PCs.

PC

To work with the Dionex Chromatography Management System, a Windows PC with a Pentium processor (minimum 100 MHz) with a 32-bit **Operating System** Windows 98, Windows NT or Windows 2000) is required. To work efficiently, we recommend at least 32MByte RAM for Windows 98 and 64 Mbytes for Windows NT/Windows 2000. For graphical representation, you need a graphic board with a resolution of minimum 800 x 600 pixels. However, for a clear and ergonomically representation a 17" monitor with a resolution of 1024 x 768 pixels is recommended. An industry-standard mouse and sufficient hard disc capacity (at least 200 Mbytes free capacity should be available) are necessary for comfortably working with the data system.

These requirements apply to systems with one or two timebases without the diode array option. If you use several timebases or diode array detectors, higher requirements must be met. In this case, we recommend a Pentium II PC (266 MHz or higher) with 64 Mbytes RAM and a free disc capacity of at least 1 Gbyte.

PC requirements for acquiring mass spectra

The complete XC system (REV 1.2) must be installed on every computer (also pure Remote Clients of the Dionex Chromatography Management System) that should be able to access MS data. That is why the minimum system requirements for an LC/MS System are as follows:

- 400 MHz PII CPU
- 128 MB RAM
- 10 GB hard disc
- 1024 x 768 x 16 screen resolution

Operating System

The Dionex Chromatography Management System supports the following operating systems:

- Windows 98
- Windows NT 4.0/Windows 2000.

In contrast to the earlier operating systems Windows 3.0 and 3.1, these are 32-bit ➢*Multi-Tasking* operating systems, i.e., several programs can be executed simultaneously. This is especially important for instrument control, data acquisition, and comfortable printer support.

Caution: Note the differences between the operation of the Dionex Chromatography Management System under Windows 98 and Windows NT/Windows 2000. See **The Dionex Chromatography Management System under Windows 98 and Windows NT/2000** in the **Installation** section.

Network

The network capability of the Dionex Chromatography Management System allows operation of the data system within local and global networks, also referred to as LAN ("local area network") or WAN ("wide area network").

The Dionex Chromatography Management System cannot only be operated locally in a single-user installation, but also within a network. This includes data transfer and remote operation via ISDN. The stations of the Dionex Chromatography Management System can be linked around the world (Wide Area Network).

To use all advantages and possibilities offered by network operation, such as centralized data storage, backup and administration, shared access to methods and worldwide availability, safe and fast data exchange is essential.

Sometimes even state-of-the-art networks have difficulty coping with the enormous amount of data. That is why client/server systems offer decisive advantages by specifically selecting transferred data.

Client/Server System

From a decentralized PC (client), sub-programs are started on a central computer (➢*Server* or Chromatography Server) via ➢*RPC* commands (Remote Procedure Calls). The server executes the actual "work," e.g., searching for data in a database or running an application. The client merely receives the search result or the status of the application. This means that the client provides the user interface, and the actual operation is performed on the server via "remote control." The Dionex Chromatography Management System also uses this "division of labor."

The user starts the Dionex Chromatography Management System on a local PC, the ➢*Client*. Now the user can perform all server-independent tasks. This includes re-processing of raw data, creating sequences, or searching individual spectra in a library.

If a Chromatography ➢*Server* has been activated via the ➢*Server Monitor Program*, controlling and monitoring the chromatography instruments connected to the server is possible. Theoretically, each client that is connected with a running server via a ➢*Control Panel* can perform this control. In practice, the first client using this possibility also has control rights. From this point, all other users of the Dionex Chromatography Management System can only monitor the system status.

Via device drivers, the server converts the control commands entered on the first client PC for the analytical instruments. Inversely, the server receives information from the system and forwards it to the appropriate locations. Thus, status information, such as the current flow rate, appears on all client PCs connected with this chromatography system. Raw data is automatically stored in the directory of a ➢*Datasource* and the underlying database.

Depending on whether the client and the server are located on the same PC or on different PCs in a network, a distinction is made between the following installation types: local client/server installation and network installation. For further details, see the topics below:

Local Client/Server Installation

Network Installation

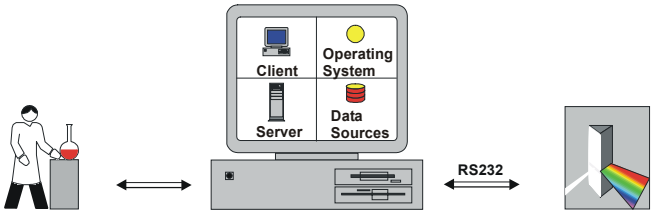
Local Client/Server Installation

The ➢*Client* and the (Chromatography) ➢*Server* are located on the same PC. They must be started separately.

The controlled instruments in the chromatography system are connected to the PC via RS232 ports or a ➢*DX-LAN*. Additional interface boards can supply a sufficient number of ports. Each chromatography server can operate a maximum of 6 controlled or 16 non-controlled ➢*Timebases* (chromatography systems).

Saving data is on the local PC. During the initial installation of the Dionex Chromatography Management System, a local datasource is installed on each local computer.

If the PC is part of a local network (LAN = **L**ocal **A**rea **N**etwork or WAN = **W**ide **A**rea **N**etwork), data can also be saved externally. In the same way, external data can be used for data editing.



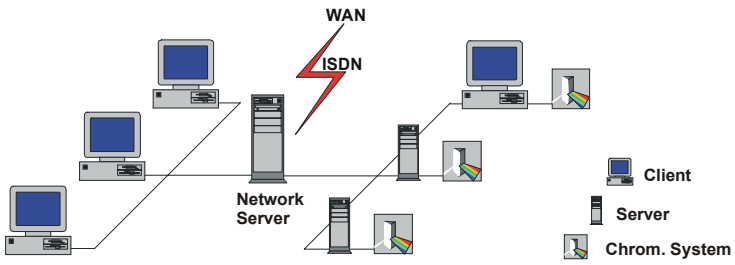
If the local PC is connected to a network, all options of a network installation are available.

Network Installation

The ➢*Client*, the Chromatography ➢*Server,* and the ➢*Datasource* can be installed on different computers. They are connected via the network and the corresponding network server (generally a Windows NT/2000 server). Each

chromatography server can operate up to 6 controlled or 16 non-controlled chromatography systems (➢*Timebases*).

Client, Server and Datasource are independent units within the network.



On each PC, a server, a client, and a local datasource are set up during the installation of the Dionex Chromatography Management System. Independently of this, each PC can act as "server only" or "client only." Theoretically, each client can access each datasource and each server. In practice, this may not be desirable for safety reasons. Therefore, various options are available to restrict user access.

- The ➢*Server Configuration* program allows defining the extent of network operation for each ➢*Server* and for each timebase. A server can be made available for the entire network or ➢*Access Groups*, only, or the server can be locked partly or completely. If the server is partly locked, e.g., monitoring the server is possible, but controlling the connected instruments is disabled. In this case, control is reserved for the local client. This distinction also applies to the timebases. If three timebases (TIME1/2/3) are installed on a server, TIME1 could be completely shared, TIME2 could be excluded from the network operation, and TIME3 could be shared for monitoring only.

- Datasources and/or their subdirectories can also be protected from undesired access. Depending on the location of the corresponding database (on the local hard disk or a network PC), the respective user or the network administrator decides (by "sharing" a directory) who which data can be accessed and by whom. In addition, datasources shared in Windows can be locked in the Dionex Chromatography Management System.

- Another type of access restriction is possible via the ➢*User Mode* or User Management of the Dionex Chromatography Management System. If

access control is activated (the CmSecure program is available for administrators), the user must be identified via password input. From this point, the user can only perform specific operations assigned by the network administrator via the CmUser program. Thus, it is possible to deny controlling rights or prohibit "locking" of datasources.

Important data are often stored on central data server PCs. If, during data acquisition, the network connection is interrupted or the data server PC crashes, data acquisition should be continued, nevertheless. All data that are relevant for the server of the Dionex Chromatography Management System are locally stored on the server's hard disc thus ensuring that the data acquisition will not be interrupted in case of a network failure. The ➢*Network Failure Protection* is available **for Windows NT and Windows 2000, only**.

In addition to allowing data exchange within a local area on a Windows, Novell, DEC, or UNIX network (LAN), data transfer across huge distances (WAN) via ISDN is of course also possible. The basic requirement for any type of network operation is the availability of the corresponding network drivers for Windows 98 or Windows NT/2000.

Caution: Note the differences between the operation of the Dionex Chromatography Management System under Windows 98 and Windows NT/2000. Also, see **Dionex Chromatography Management System under Windows 98 and Windows NT/2000** in the **Installation** section.

Overview: Chromatography Data System

The data system is the control center of a modern chromatography system.

Tasks of a Data System

- It converts user input into time-precise control commands.
- It monitors the state of the connected chromatography instruments.
- It logs all user entries and modifications to the system.
- It saves and archives all data.
- It graphically represents data and allows the user to check the system status and system results.
- It allows the user to thoroughly check and evaluate data.

Components

- The basis for precise control is a real-time capable **Operating System**.
- Installation and configuration is the task of the **Server Configuration**.
- Communication with the different instruments and device types is enabled by the **Chromatography BIOS** and various **Device Drivers** as well as **Virtual Channel Drivers**.
- Each operation, for example, execution of a command or display of an error message, is included in the **Audit Trail**.
- Depending on the required scope of performance, the Dionex Chromatography Management System offers various **Options**.

User Interface of the Dionex Chromatography Management System

- Regarding the menu structure, screen elements and operation, the Dionex Chromatography Management System offers all typical Windows properties. A homogeneous, situation-related menu structure is as evident as the Windows technology, toolbars, and context-sensitive use of the right mouse button (see **The Client User Interface**).
- Each user can save and activate a "personal" screen (**User Profile/Workspace**).
- The user can modify the graphical representation of the online control windows (see **Control Panel**).

Operation

- Before the **Program Start**, the correct hardware configuration, connections between the PC and the system and between the PC and a datasource must be ensured.
- In **Network Operation**, the client PC can control systems and datasources that are not directly connected with the PC.
- Operating the data system is facilitated by various assistants, the ➢*Wizards*.

New Features Compared to GynkoSoft

The Dionex Chromatography Management System for Windows 95/98 and Windows NT/Windows 2000 offers a variety of new features and enhancements in comparison with the previous product (GynkoSoft), including the following:

- Modern control technology via Client/Server Architecture and Windows RPC technology (see **Network**)
- Complete **Network Installation**
- Individual subprogram for user management: *CmUser* (The Online Help provides further assistance if this program is installed on your PC).
- Query-based data access via an integrated ➢*Database*
- Connection to standard ➢*ODBC* / SQL databases

- Tele-service (Remote maintenance)
- Freely definable workspace in the **Control Panel**
- ➢*Mass Spectrometer* control and MS data evaluation
- ➢*Sample-Oriented Operation*
- ➢*Electronic Signature* of sequences
- GLP compliant: automated ➢*Instrument Qualification (IQ)* and ➢*Operational Qualification (OQ)* as well as Instrument OQ and ➢*Performance Qualification (PQ)* of the Dionex Chromatography Management System
- ➢*Year 2000 Conformity* (either 2- or 4-digit year formats are supported, e.g., 1-1-00 or 1-1-2000)

User interface and operation correspond to the standard Windows requirements:

- Comprehensive ➢*Online Help*
- Easy operation due to ➢*Toolbars*, Windows Technology (see **Basic Operation Working with Several Windows**) and ➢*Wizards*
- Comprehensive context menus via the ➢*Right Mouse Button*
- ➢*Drag & Drop* functionality
- Real ➢*Multi-Tasking* and ➢*Multi-Threading*

In addition, the new chromatographic interface now features special novelties and enhancements:

- Optical representation of the gradient profile
- Online zooming beyond the current time
- Grid in online window
- Additional peak variables
- Determination of reference wavelength for individual channels
- Wavelength compensation via holmium oxide filter
- Enhanced data compression and restoration of old data

- Baseline subtraction, now called blank run
- Base area correction/base area recognition
- Comprehensive Online Help for any situation

For detailed information on any differences that might occur when creating programs, also see **How to ...: Actions in the PGM Editor Differences Compared to GynkoSoft**

Options of the Dionex Chromatography Management System

The Dionex Chromatography Management System's scope of performance can be adjusted to the requirements of a specific application. In addition to the basic software package, various options can be purchased.

The purchased scope of performance is coded in a copy protection chip or from the ➢*License Server* (see **Software Protection**). The Dionex Chromatography Management System can only be started with the full range of features if a protection device was detected, i.e., a ➢*Dongle* on the parallel PC interface or a ➢*PAL* on the A/D converter, or if a license was detected, which was provided by the license server.

The following options are available for the Dionex Chromatography Management System:

Basic:

The basic license (without additional features) includes:

Signal acquisition with one timebase from any number of synchronous channels; Multi-Tasking; Reports from the following partial methods: single and multiple point calibration with various fit models, integration, ratio test, user programs, etc.

The following drivers are available if only the basic license is available:

1. Sharable Devices

   "Dionex 16 Chl. A/D Converter" (**A/D Converter** for ports only):

   "Dionex 16 Relays ISA Board (ME63)"

   "Dionex 16 Relays PCI Board (ME630)"

   "Dionex Digital I/O ISA Board (ME14)"

   "Dionex Digital I/O PCI Board (ME1400)"

   "Dionex PDA DA Converter (16 Bit)"

   "Dionex Pump Control Board" (**Pump Control Board** for relays and inputs only; pump control is not supported)

Basic (c'ntd)

2. ➢*UV* and Photodiode Array Detectors (properties cannot be changed in the PGM or commands cannot be changed during the data

acquisition):

"Dionex UVD340S"

"Dionex UVD170S"

"Dionex UVD320S"

"Dionex UVD160S"

3. In addition, the following general ➢*Device Drivers* are available:

   Integrator Driver (provides A/D channels for the timebase)

   Remote Inject (input required)

   ➢*Shared Relays and Inputs*

   ➢*Virtual Channel Driver*

Therefore, the basic license does not provide most of the device drivers that are available with a **Control** or **Extended Device Control** license. This also means that the corresponding commands are not available, e.g., ⇒*Wait* or ⇒*Delay*. In addition, you cannot ⇒*trigger* commands.

Control: Control allows controlling chromatography systems. The software module must be purchased once to control any number of timebases.

Extended Device Control The Extended Device Control option allows controlling additional chromatography instruments not supported by Control (Control licenses included)

RPC: With the RPC extension, the Dionex Chromatography Management System can be controlled network-wide. For each installed Chromatography ➢*Server* one option is required.

Timebase: Additional license for extending the Dionex Chromatography Management System by one timebase. Per PC, a maximum of 6 timebases can be installed.

Client: Additional single-user license for data reprocessing on a network PC including control of any number of systems in the network.

Data: Additional single-user license for data reprocessing on a network PC *without* control.

PDA: Additional single-user license for photodiode array detectors: digital data acquisition of a three-dimensional data field which is required for the representation as 3D-plot as well as for peak purity control

Library: Additional single-user license for the access to special spectra libraries.

IC Control: Module for controlling ion chromatography timebases (IC Control SE license included).

IC Control SE: Special control module for stand-alone ion chromatography systems, such as DX-120 Ion Chromatography System.

Chromatography BIOS

BIOS is the abbreviation for **B**asic **I**nput/**O**utput **S**ystem. As a (software) component of each MS-DOS PC, it serves for a uniform control of all PC peripherals, i.e. the screen, disks, keyboard etc. BIOS allows the operating system MS-DOS to communicate with disk drives or keyboards from different manufacturers. From the viewpoint of a PC user, a keyboard delivers command strings to a PC; a disk provides a certain amount of storage capacity. The technical realization of these components is irrelevant.

The Dionex Chromatography Management System implements this reliable and well-proven concept in its unique chromatography BIOS:

From the viewpoint of the user, the fluidic system of an HPLC pump consists of a flow total and several partial flows that are usually referred to as %A, %B, and %C. The sampler injects varying volume quantities from different positions and performs additional derivation steps, as necessary. Analysis by a conventional UV detector offers the following functions: The user specifies one (or several) wavelength(s), varies the full scale, and executes Autozero etc. How the individual functions are realized technically, is of no interest for the operation. The user assumes that the commands are executed, regardless whether they were entered manually via the user interface or via a control program (**Control Program**).

The Dionex Chromatography Management System control therefore only knows "virtual" commands, e.g., ⇒*Flow (Flow Rate)* or ⇒*Partial Flows*. The chromatography BIOS converts these commands into control commands readable by the instruments. To the user, it is thus irrelevant whether a command (for example, **%B**) is directed to a low-pressure gradient pump or a high-pressure gradient system.

This is possible by conversion programs that are available for each instrument and device type, the **Device Drivers**.

Device Drivers

The Dionex Chromatography Management System is capable of operating a number of different analytical instruments via a uniform, device-independent control language. The Dionex Chromatography Management System uses the driver concept, which means that the appropriate ➢*Device Driver* must be loaded for each controlled device. This is done automatically when the data system is started.

The device driver determines the instrument's scope of functions. The driver is responsible for all device-specific tasks such as sending commands in the

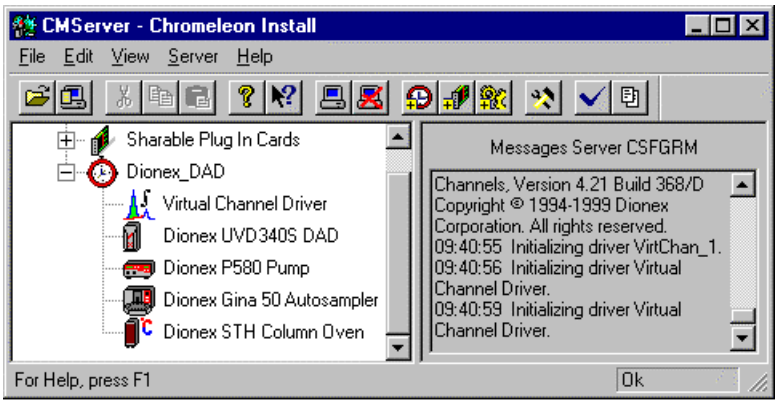
command language of the device or deciphering the data sent by the device. Thus, the control ➢*Program* of the data system does not have to deal with specifics but prompts the driver to execute certain instrument functions (for example, inject 9 ml from vial 17).

All drivers are stored in the BIN directory. They have a version number assigned that can be viewed in the Explorer via the **Properties** context menu.

Third-party instruments can be controlled if the corresponding driver support is available. Please contact Dionex Service for information on supported instruments.

Virtual Channel Drivers

In addition to the ➢*Device Drivers*, the Dionex Chromatography Management System offers the possibility to install a driver for virtual channels (➢*Virtual Channel Driver*). Similar to device drivers, this driver is installed in the **Server Configuration**. Also, see **Virtual Channel Driver: Installation**.



By default, the Dionex Chromatography Management System generates 16 virtual channels. All individual channels have the same sampling step. If you require different sampling steps, install another instance of the virtual channel driver.

Following the installation, delete any channels you do not need. Open the context menu (right mouse button), click **Properties**, and then choose the **Signals** tab. To change the default channel name, click the **Change** button.

As ➢*Virtual Signals* cannot be generated manually, the corresponding ➢*Program* must be started. For information on how to enter commands, see **How to ...: Device Control Virtual Channel Commands**.

Audit Trail

The Dionex Chromatography Management System device drivers do not only send the parameters specified in the control file to the corresponding devices, but also constantly monitor the device parameters and compare the nominal values with the actual values. Deviations from the nominal values are either corrected or indicated by an error message.

Each command, each correction, and each error message is both, recorded and stored by the Dionex Chromatography Management System with split-second accuracy and displayed in the Audit Trail window of the **Control Panel**.

Caution: Complete documentation of all performed commands and status messages is only possible with Dionex instruments. Not all third party instruments are capable of communicating current device parameters regularly or upon request.

For further information on storing protocol data, see **Protocol Data (Audit Trail)** in the **Data** chapter.

Installation: Software

Tips for Software Installation

In general, the Dionex Service or an Authorized Dionex Distributor installs the Dionex Chromatography Management System.

If this is not the case, proceed as described in the **Initial Installation and Update** section. After the installation, see **Program Start**.

Initial Installation and Update

Note: Please note that the PC Power Management features must be switched off in the BIOS! Otherwise, problems may occur when controlling instruments.

Note: Please note the information on using **Dionex Chromatography Management System under Windows 98 and Windows NT/Windows 2000** The installation under Windows NT/Windows 2000 is only possible if the user performing the setup has administrator rights!

Setup of the Dionex Chromatography Management System

Opening the Dionex Chromatography Management System Setup program SETUP.EXE starts initial installation of the Dionex Chromatography Management System. If CD Autostart is active on your PC, the installation is started automatically upon insertion of the CD into the respective drive.

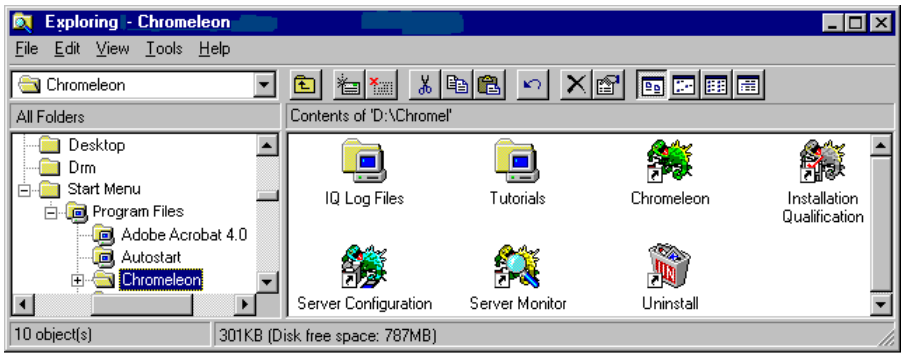
Caution: Neither the ➢*Server*, nor the ➢*Client*, nor the server monitor must be active during the Setup procedure. Ensure that there are no minimized program buttons on the Windows task bar and that there is no server monitor icon!

Caution: Controlling an aQa ➢*Mass Spectrometer* requires installing the ➢*Xcalibur* software before you install the software of the Dionex Chromatography Management System. For information on how to proceed, see **How to..: Actions Related to the aQa-MS Installing MS Components**.

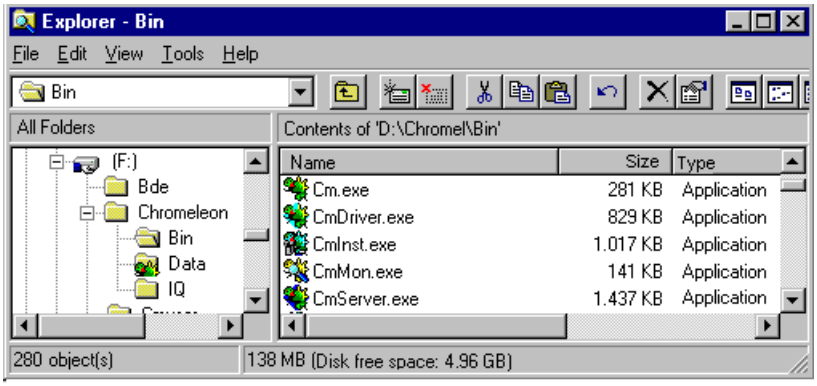
Follow the installation steps to correctly install the Dionex Chromatography Management System. Please note:

- Answer **Yes** to the question **Enable mass spectrometry support in the server** if Xcalibur is already installed.
- Take a note of the directory name in which the Dionex Chromatography Management System is installed.
- When prompted whether to create a link to the **Server Monitor** program in the **Autostart** group, choose **Yes**.

At the end of the installation process, a program group <NAME of DIRECTORY> is generated in which you find five links to start the different program parts and to uninstall the Dionex Chromatography Management System.

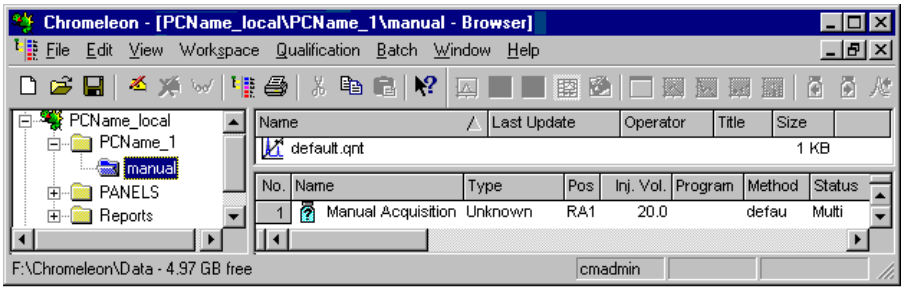


The programs on which the links are based are located in the BIN directory in the directory structure created by the Dionex Chromatography Management System:



The DATA directory contains various subdirectories (PANELS, REPORTS, PROGRAMS, PCNAME_1) that serve to save default templates. A default ➢*Datasource* is also created. The underlying database is located directly in the DATA directory under the name CM_LOCAL.mdb.

Datasources are only visible in the Browser of the Dionex Chromatography Management System (see **Data** **Browser**). The environment created by the Setup program has the following structure:



The local datasource has the name <PCNAME_local>. It contains the subdirectory **PCNAME_1** in which the ➢*Sequence* "**manual**" is located. The sequence consists of a single default sample and enables the manual data acquisition. To access default templates directly in the Dionex Chromatography Management System, subdirectories of the DATA directory are mapped (PANELS, REPORT...).

Modifications to the described directory structure are realized by creating new:

- Datasources and sequences (in the Browser)
- Timebases (in the **Server Configuration**).

Caution: If the Dionex Chromatography Management System is not started correctly, there may be a version conflict between the system files in the Windows system directory. In this case, install MDAC_TYP.EXE once again. The **Installation Qualification Manager** (described in the **Validation** section) provides an overview on the version numbers used

Updating the Dionex Chromatography Management System

Updating the Dionex Chromatography Management System is started by file SETUP.EXE.

Tip: When updating the Dionex Chromatography Management System, uninstalling a previous Dionex Chromatography Management System version is not required and not recommended, as this would delete all entries in the Registry of the Dionex Chromatography Management System (e.g., key code, PAL location, and datasources). Before updating the version, close the server, the client, the Server Monitor Program, and all other applications!

If the Setup program detects "old" PAN files (control panel) or RDFs (report definition files) in the directories PANELS and REPORT, the user is prompted whether to overwrite existing destination files. Therefore, it is highly recommended to save personal PAN files, RDFs, and, if necessary, GEN files to prevent inadvertent overwriting.

Tip: Before performing an update, copy all PAN files, RDFs, and GEN files you created to a separate directory to prevent inadvertently overwriting the files.

The Dionex Chromatography Management System under Windows 98 and Windows NT/Windows 2000

The Dionex Chromatography Management System supports the operating systems Windows 98 or Windows NT/Windows 2000. Although Windows NT/Windows 2000 and Windows 98 have similar user interfaces, their cores differ considerably. Windows NT resembles more the "large" operating systems such as UNIX or VMS, while traces of DOS can still be found in Windows 98. The focus of Windows NT/Windows 2000 has been stability, safety, and security. These properties are responsible for the higher storage capacity demands of Windows NT and Windows 2000.

When operating the Dionex Chromatography Management System under Windows NT or Windows 2000, note the following aspects:

Setup

For performing the Setup of the Dionex Chromatography Management System, PC administrator privileges are required on the Windows NT computer.

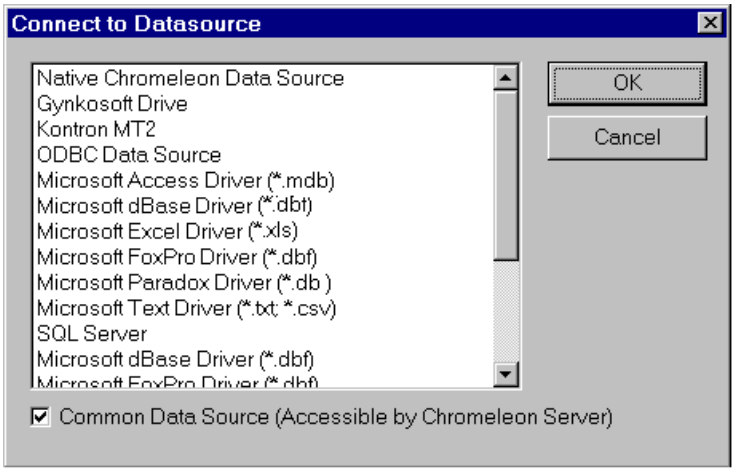
Otherwise, it is not possible to create ➢*Datasources* or install various system programs. The Dionex Chromatography Management System cannot operate correctly without these settings.

Under Windows NT/Windows 2000, SETUP creates the user group **Chromeleon Operators**. The user currently logged onto the system is immediately included in this group. All users wishing to work with the Dionex Chromatography Management System must also be members of this group. Under Windows NT, adding new users and assigning them to various groups is via the **User Manager**. Access the **User Manager** by pressing **Start menu → Programs → Administrative Tools**. The registered users can be added to a group.

Datasources

When generating a new datasource or when connecting to an existing datasource, activate the check box **Common Datasource** for system-wide access sharing. Instead of being assigned to a specific user, the datasource is recognized in the entire system as a system datasource. Creating system datasources also requires administrator rights on the local PC.

All datasources that are accessed by the server of the Dionex Chromatography Management System to process sequences must be system datasources.



Server Access to the Network

Users logging onto a PC have a personal Windows NT user account defining the currently granted rights. Under Windows 98, this user account is not required.

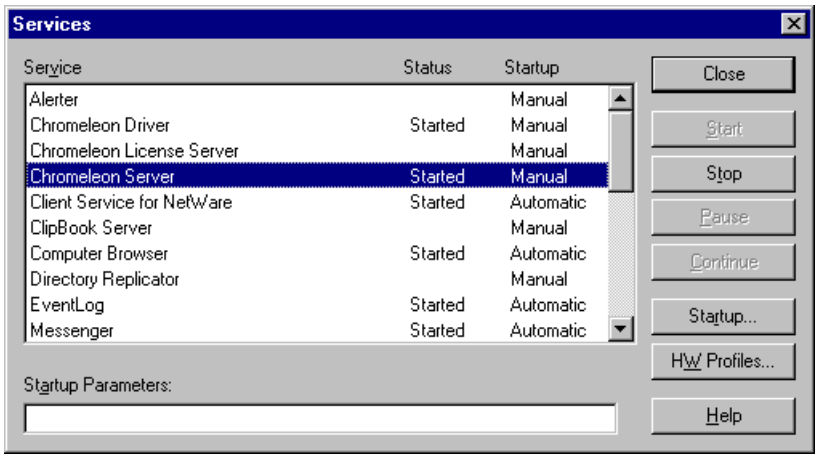
If a server is installed simultaneously on the PC, it will automatically have the same rights under Windows 98 as the current user. As soon as the user logs off, the server looses the network access.

Under Windows NT, this is not the case. Here, the server is installed as a system-inherent service. As long as the server only works on the local datasource, this will have no negative effects. In contrast, the server will continue operation even if a user logs off the system.

Problems occur when the server is to perform operations via the network. If the server should process sequences located on a network datasource, a special procedure may be necessary under Windows NT. The server must be assigned a user account for its network accesses. This is only possible if the user has administrator rights.

Proceed as follows:

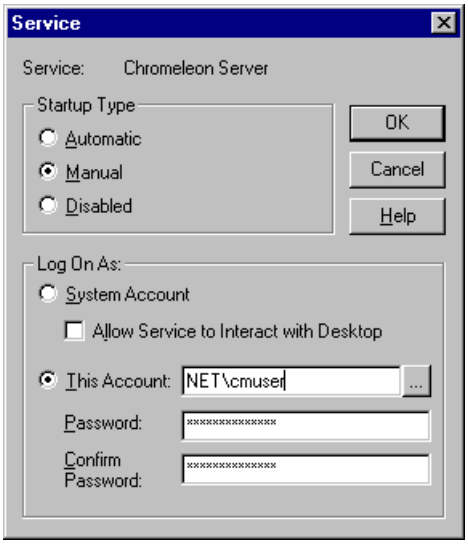
- Click the **Services** icon in the control panel.
- Choose the **Chromeleon Server** item from the list and press the "**Start**..." button.
- Caution: do not modify the **Chromeleon Driver** entry!



- In the **Services** dialog box, activate **This Account**. Enter a user name and password with access to the corresponding network directory. With the button on the right of the edit field, you can choose a user name from the list.

☞ ***Tip:*** The selected user must be a member of the **CHROMELEON Operators** group.

If users have to change their passwords at regular intervals, establishing a separate account for the server is recommended as this saves the effort to change the passwords for the server service of the Dionex Chromatography Management System at regular intervals as well.



After completion and restarting the system, the server of the Dionex Chromatography Management System is automatically logged on under the new user account.

Network Failure Protection

A ➢*Network Failure Protection* is available for Windows NT and Windows 2000. It is disabled on Windows 98 because these systems are unstable under network failure conditions.

The network failure protection ensures uninterrupted data acquisition on an external server PC in case of a network failure. For this purpose, the server of the Dionex Chromatography Management System stores all relevant data on its local hard disc. The ➢*Server* of the Dionex Chromatography System continues processing these sequences even in case of a network failure. In addition, the failure of the network connection is logged in the Audit Trail (**Protocol Data**).

Software Protection

Each station of the Dionex Chromatography Management System, regardless of whether it is a server and/or a client, is protected by a copy protection chip (➢*Dongle*) or a hard-protect plug-in board (➢*PAL*). PALs and dongles store the licensed serial number for *one* Dionex Chromatography Management System station.

For large installations, a ➢*License Server* has been developed for the Dionex Chromatography Management System to manage the availability of licenses.

Each user of a dongle or PAL-protected station must enter a 12-digit or a 24-digit ➢*Key Code* during the installation of the Dionex Chromatography Management System. The key code includes all functions and  **Options of the Dionex Chromatography Management System** made available to a specific user. A key code matches exactly one serial number.

 ***Caution***: It is not possible to operate several stations of the Dionex Chromatography Management System with the same key code or to expand the scope of functions on a different station. Only if the entered key code matches the dongle or the PAL plug-in board, operation of the Dionex Chromatography Management System is possible beyond the one-hour demo mode.

If the functions of the Dionex Chromatography Management System are upgraded by acquiring the corresponding license, the user receives a new key code. The extended scope of functions is made available upon entering the new code.

Also, see **How to ...: Actions in the Server Configuration**  **Selecting the Copy Protection Location and Entering the Key Code**.

Access Control

The network capabilities of the Dionex Chromatography Management System allow the user to perform any operation from any workstation (Client). As the network itself, the Dionex Chromatography Management System has a comprehensive system of user management. The ➢*CmUser and CmSecure* programs enable the system administrator to control access to data, systems, and stations.

This is to guarantee that only authorized users can access specific ➢*Timebases*, data, ➢*Datasources*, directories, ➢*Sequences*, templates, etc.

Access-protected operations include:

- Creating, modifying, and deleting ➢*Clients*, datasources, directories, sequences, samples, work lists, workspaces, ➢*Queries*, server configurations, timebases, spectra libraries, ➢*Control Panel*, report definitions, and quantification methods (QNT files)
- Starting data acquisition and batch processing, exporting and printing batch data
- ➢*Electronic Signature* of sequences
- Saving and deleting peak manipulations
- ➢*Backup* and restoring datasources, directories and sequences (see: ➢*Restore*)
- Importing and exporting data
- Access to ➢*Servers* and timebases

Granting Privileges

The administrator performs granting privileges. When access control is activated, the administrator thus defines the scope of functions available to each user and assigns passwords.

When the user logs onto a station subject to access control with his/her ➢*Password*, the "personal" privileges are available. It is irrelevant on which station the user logs onto the system.

Caution: Client stations that are not subject to access control have free network access to any unprotected objects of other clients' stations. In the case of a datasource, this means that access is possible as soon as the datasource directory is shared in the Windows Explorer. Access is restricted as soon as an ➢*Access Group* is assigned in the Browser of the Dionex Chromatography Management System. This is possible after selecting the datasource and choosing the **Properties** command (context menu or Edit menu).

In the ➢*Server Configuration* program, the **Properties** dialog allows limiting the operations that can be performed from another PC. For example, to allow monitoring but not controlling a timebase, deactivate the **Control** checkbox under **Allow Remote** (see example below).

Executing Privileges

In general, personal access options and ➢*Privileges* are already defined when the user of the Dionex Chromatography Management System logs onto the system. This means that the user can perform all tasks available on the screen or accessible via mouse click. The user has no influence on the status of the entire system.

This can be different for users who are granted extensive privileges. These users are able to change access to datasources, directories, sequences, servers, and timebases in the Dionex Chromatography Management System or in the **Server Configuration**. The corresponding object is selected in the Browser or the Server Configuration and can then be supplied with a new access group assignment via the **Properties** (context menu). In addition, datasources, directories, and sequences can be locked. A red lock () on an icon indicates that the respective item is locked.

CmUser.EXE and CmSecure.EXE

Two separate programs are available to the Administrator, the CmUser program (CmUser.EXE), and a program for enabling the ➢*User Mode* (CmSecure.EXE). Both programs are included in the CmUser directory of the Setup, but are **not** automatically copied to the program directory.

The CmUser program is password-protected as well and can be opened only by the Administrator or persons with similar functions.

☞ ***Tip***: Authorized persons should copy the CmUser directory to a floppy disk to enable on-site changes to the user management. This directory also contains an Online Help file describing all steps and options of the user management.

The main task of the CmUser program is administration of *User*, *Privileges,* and *AccessGroups*. The following operations are possible:

- Creating and editing ➢*Access Groups* (A-group)
- Creating and editing ➢*Privileges* (privilege group or P-Group)
- Creating and editing new users in the Dionex Chromatography Management System. The user's name and title, the logon and signature ➢*Password*, and the reaction on a failed ➢*Logon* can be defined.

The CmSecure program allows enabling and disabling the User Mode on the clients of the Dionex Chromatography Management System. In addition, a

CmUser database containing the status of each user and his/her rights is selected in the CmSecure program. Starting the Dionex Chromatography Management System requires a password when the User Mode is enabled. Signing sequences electronically is possible with enabled User Mode only (see ➢*Electronic Signature*).

The CmSecure program serves to create a CmUser database that contains the status of each user and the rights granted to him/her. In addition, user control is enabled and disabled on regular stations of the Dionex Chromatography Management System. With enabled CmUser mode, a password is required to start the Dionex Chromatography Management System.

Users can work with an object if they are members of an A-group granting access to this object. The actions they are allowed to perform are determined by the assigned privileges (to members of a P-group).

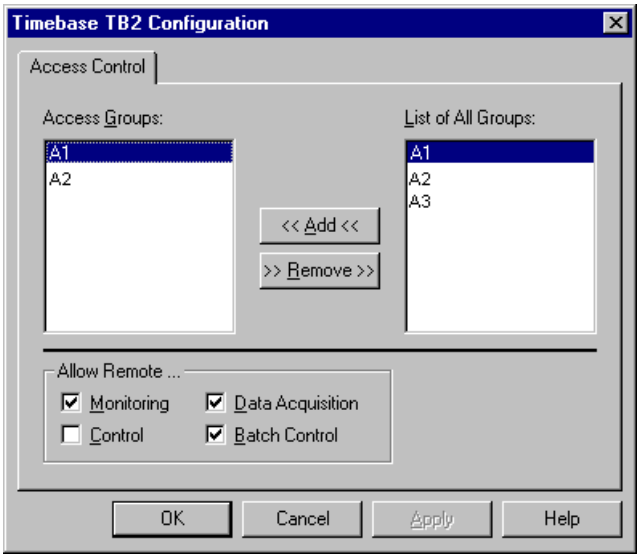
Example

A Dionex Chromatography Management System with the two timebases TB1 and TB2 is to be operated by five users, U1, U21, U22, U31, and U32. U1 is the system administrator with unlimited access to all objects of the Dionex Chromatography Management System. U21 and U22 are authorized to record data with both timebases; U31 and U32 can only use TB1 for analyses. The administrator sets up the following users, A-groups and P-groups in the **CmUser** program:

- Users: U1, U21, U22, U31, and U32,
- A-groups: A1 (contains only U1), A2 (members: U1, U21, and U22) and A3 (U1, U31, and U32),
- P-groups: P1 (U1), P2 (U1, U21, and U22) and P3 (U1, U31, and U32).

After that, the administrator assigns the access privileges for the timebases TB1 and TB2 in the ➢*Server Configuration* program. To perform this task, click the corresponding timebase and select the **Properties** in the context menu or from the **Edit** menu.

In the example, the properties of TB2 are as follows:



Only the members of the A1 and A2 groups can access the timebase TB2. From other network computers, it is possible to view the results, start data acquisition and control batches. However, controlling the timebase from other computers is not possible.

The Server Configuration

Function

The ➢*Server Configuration* program serves to install ➢*Timebases* on a ➢*Server*. It is only required by users who use the Dionex Chromatography Management System to control a chromatography system and who wish to change the current instrument configuration.

For users who exclusively perform data evaluation it is not necessary to be familiar with this program part.

Starting the Server Configuration

- To start the Server Configuration and perform changes to the server configuration, select Server Configuration from the Start/Programs menu on the task bar. For example, for CHROMELEON, choose Start > Programs > Chromeleon > Server Configuration.

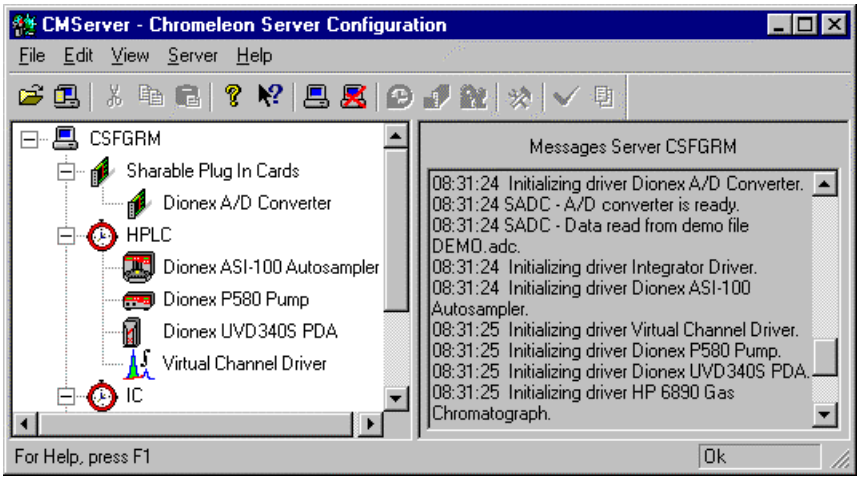
Caution: Modifications of the installation are possible only if the server to

be configured is started (see Program Start in the Installation section) and if no sequences or samples are currently processed on this server.

When opening the Server Configuration for the first time or when changing an existing server configuration, there are also changes in the directory structure.

Description

The user interface of the Server Configuration has two partial windows (see figure below). The left window section lists the names of all currently active (started) chromatography servers. The right-hand section of the Server Configuration logs the configuration process (Audit Trail).



A running server is shown in the shape of a PC icon; an inactive server is crossed out red. A red prohibitive sign (red circle with white line) indicates that a server is active (for example, processing samples).

Click the "+" character next to any server name to see its timebases and hardware components (**Timebase**, **Hardware**). In the same way, the chromatography instruments assigned to a timebase (**Devices**) are made visible. Information on the type and number of all installed components is, together with their configuration, stored in the file CMSERVER.CFG.

Installation/Configuration Procedure

Access to a server (and thus changing its configuration) is only possible after it is started. In addition, sequence or sample processing is not possible at the same time!

If this is ensured, the Server Configuration allows adding and removing timebases, hardware and instrument components. The configuration of each component can be changed here. The changes are saved in the ➢*Server Configuration*.

- Select **Connect Remote Computer** in the **Server** menu to establish a connection to a specific server. Enter the computer name of the server and the protocol to use. As soon as there is a connection to the server, its name and symbol appear in the left window section of the **Server Configuration**.
- Select **Add Timebase / Add Device / Add Sharable Device** in the **Edit** menu to add new components to the system.
- Select a component in the file structure and double-click to change its configuration. Alternatively, you can choose the **Properties** option in the context menu. In both cases, a dialog box is opened with several tab dialog boxes; these contain all configuration options.

When opening the **Server Configuration** for the first time or changing an existing server configuration, the directory structure also changes.

- The Dionex Chromatography Management System creates a local datasource under <PCNAME_local>.
- For each timebase on the current server, the datasource receives a separate subdirectory for storing the corresponding raw data.
- Below each timebase, a sequence directory with a corresponding sequence is created. The sequence contains a sample for manual data acquisition.

For detailed information on the server configuration, see **How to ... Actions in the Server Configuration**  **Changing the Server Configuration**

Installing Dionex Instruments

The following instruments are installed via the ➢*Server Configuration*:

Pumps and connected components

Instruments	Driver Names	Remarks
M480, P580	Dionex M480/P580 Pump	HPLC gradient pumps
GP40, GP50, GS50	Dionex GP40/GP50/GS50 Pump	IC gradient pumps
IP20, IP25, IS20, IS25	Dionex IP20/IP25/IS20/IS25 Pump	IC isocratic pumps
EG40	Dionex GP40/GP50/GS50 IP20/IP25/IS20/IS25 Pump	Eluent generator (installed via the IC pump drivers)
LC25, LC30	Dionex GP40/GP50/GS50/ IP20/IP25/IS20/IS25 Pump	Temperature control modules (installed via the IC pump drivers)

For information on the respective control commands, see **Dionex Pumps**

Autosamplers

Instruments	Driver Names	Remarks
GINA 50	Dionex GINA50 Autosampler	Autosampler (50 positions; cooling option: GINA50T)
GINA 160	Dionex GINA160 Autosampler	Autosampler (160 positions)
ASI-100 / ASI-100T	Dionex ASI-100 Autosampler	Autosampler (100 positions) / ASI-100 = with temperature control
AS50	Dionex AS50 Autosampler	Autosampler (50 positions, optionally available with temperature control)
AS 3500	Dionex AS 3500 Autosampler	Autosampler (160 positions)

For information on the respective control commands, see

Dionex Autosamplers GINA 50 and GINA 160

Dionex Autosamplers ASI-100 / ASI-100T

Dionex Autosamplers AS50

Detectors

Instrument	Driver Names	Remarks
AD20, AD25	Dionex AD20/AD25 Detector	UV detectors (single wavelength)
UVD 160S, UVD 170S	Dionex 160S /170S Detector	UV detectors (several wavelengths - can be upgraded to PDA functions)
UVD 320S, UVD 340S,	Dionex 320S/340S PDA	PDA detectors (200-595 nm)
PDA-100	Dionex PDA-100 Detector	PDA detectors (190-800 nm)
CD20/CD25/ CD25A	Dionex CD20/CD25/CD25A Detector	Electrochemical detectors (conductivity)
ED40/ED50/ ED50A	Dionex ED40/ED50/ED50A Conductivity Detector Dionex ED40/ED50/ED50A DC Amperometry Detector Dionex ED40/ED50/ED50A Integrated Amperometry Detector	Electrochemical detectors in the respective versions
RF1002, RF2000	Dionex RF1002/2000 Fluorescence Detector	Fluorescence detectors (available via Dionex)

In addition, the Finnigan aQa ➢*Mass Spectrometer* is available from Dionex as well. For installation information, see **FINNIGAN** in the **Installation** section.

For information on the control commands for Dionex detectors, see

Dionex Absorbance Detectors AD20/AD25

Dionex UV/PDA Detectors UVD 160S/320S and UVD 170S/340S

Dionex Photodiode Array Detector PDA-100

Dionex Electrochemical Detectors CD20/CD25/CD25A, ED40/ED50/ED50A, and IC20/IC25/IC25A

Dionex Fluorescence Detectors RF1002/RF2000

IC systems and other components

Instruments	Driver Names	Remarks
DX-120	Dionex DX-120 System	Integrated IC system module with injector, pump, and detector
IC20/IC25/ IC25A	Dionex IC20/IC25/IC25A System	Integrated IC system modules with pump and detector
UI20	Dionex UI20 Universal Interface	Instrument/PC interface
UCI-100	Dionex UCI-100 Universal Chromatography Interface	Instrument/PC interface
STH-585	Dionex STH Column Oven	Column oven

For information on the respective control commands for the DX-120, see

Dionex DX-120 Ion Chromatograph

For information on the respective control commands for the IC20 and IC25, see

Dionex Electrochemical Detectors

Dionex Pumps

In order to control the instruments, the respective control options must be available.

Should you have any questions, please contact your Dionex sales representative.

Basic Operation

Operation via the Keyboard

All menu items can be reached via the keyboard. Open the desired pull-down menu by simultaneously pressing the **Alt** key and the underlined letter (= hotkey). Enter another hotkey to select a menu item. You can also move to the desired menu item via the arrow keys. Then, confirm your choice by pressing the **Enter** key.

Example: To execute the **Align Left** function in the **Edit** menu, subsequently press the keys **E**, **A**, and **L** while you press and hold the **Alt** key. Alternatively, you can enter **Alt+E** and select a menu item via the ↓ and → arrow keys.

In addition, important commands have "shortcuts." Shortcuts are displayed on the right-hand side of menu items and functions. Entering the key combination directly executes the corresponding function.

Example: Press the keys **Control** and **C** (Ctrl+C) to copy a selected item.

For a list of available shortcuts, see

How to ...: Device Control  **Using Keyboard Shortcuts**.

Operation via the Mouse

The Dionex Chromatography Management System features all windows-typical properties and capabilities of a two-button mouse.

The **left mouse button** serves to point and select menus, menu items and icon buttons, for the operation of display and control elements as well as to modify windows (increase / reduce the size of window, zoom, modify display and control elements etc.). Double-click the left-hand mouse button to execute the selected function.

Press the **left mouse button and the SHIFT key** to simultaneously select several cells in a table. Select the first cell with the left mouse button, then press the SHIFT-key, and select a new cell. All cells between the two will be selected.

Use the **left mouse button and the CTRL key** to select cells in a table that are not adjacent. Select the first cell with the left mouse button, then press the CTRL key, and select a new cell. Keep the CTRL key depressed and repeat until all required cells are selected.

Click an object with the left mouse button and drag it to the desired position (**Drag and Drop**). Thus, you can move selected text items or entire samples. Perform this operation while pressing the CTRL key to copy the corresponding object.

The **right mouse button** is reserved for opening context-sensitive menus. These menus contain functions that are required or allowed in the current situation. After a very short time, even users not accustomed to Windows will appreciate this new and comfortable way to access menus.

For further information, refer to your Windows manual.

Undo / Redo Commands

The Dionex Chromatography Management System "remembers" the user's last modification. The operation can be undone via the **Undo** command in the **Edit** menu. Select **Redo** to repeat the last operation.

Program Start

The Dionex Chromatography Management System is operated exclusively via a PC equipped with Windows 98 or Windows NT/Windows 2000. As of Windows NT 4.0, both operating systems feature the same (Windows 98) user interface. A correctly installed Dionex Chromatography Management System is started as follows:

Start

- Click the Start button to open the Start menu. Move the mouse cursor to the **Programs** option and wait until the submenus display.
- Move the mouse cursor to **CHROMELEON** or **PeakNet**. A submenu displays with several choices.

Client (CHROMELEON or PeakNet)

- Choose **CHROMELEON** or **PeakNet** to start the data system and the data evaluation.
- If the Dionex Chromatography Management System was installed with integrated access control, users must be identified via user name and password input. If you have any questions regarding system access, please contact your system administrator.

☞ ***Tip***: If you wish to control your chromatography system via the Dionex Chromatography Management System you must start the server of the Dionex Chromatography Management System.

Server (Server Monitor)

- Choose **Server Monitor** to start the ➢*Sever Monitor Program*. On the Windows task bar, the Dionex Chromatography Management System icon will appear next to the Windows system clock.

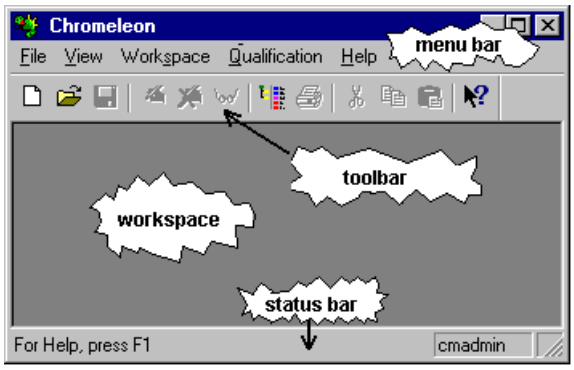
☞ ***Tip***: Normally, the Dionex Chromatography Management System will have created a link in the Autostart group during installation. The program is thus started as soon as the computer is started. You will see the corresponding icon.

- Move the mouse cursor over the icon. You will see a quick info message: **Chromeleon (or PeakNet) Server is not running**.
- Choose the **Start Server** command in the context menu (or double-click the icon and then press **Start**). The icon will show various color steps according to its status. The gray coloring indicates that the server is running (and the message is displayed: **Chromeleon (or PeakNet) Server is running idle**). From this point, you will have direct access (via control panels) to the devices installed below a timebase. Provided the instruments are correctly installed, they can be operated online.

☞ ***Tip***: Any problems occurring when controlling single instruments may be caused by an incorrect server configuration. Start the  **Server Configuration** to check the configuration.

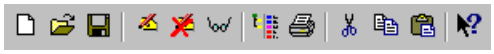
The Client User Interface

The user interface of the Dionex Chromatography Management System features all known Windows elements such as menu bar, ➢*Toolbar*, and ➢*Status Bar*.



Via the **View** menu, display of the individual bars listed below can be enabled or disabled.

Standard Toolbar for various standard functions



Online Tools for using the control panel

Layout Tools for designing the control panel

Method Tools for selecting a method window

Integration Tools for the most important operations in the **Chromatogram**

Move the mouse cursor over one of the buttons to view their description.

The space between the task and the status bar represents the workspace. It serves to display various windows. Five different **Window Types** are available in the Dionex Chromatography Management System.

Window Types

In the Dionex Chromatography Management System, there are five different window types with different appearances and functions. For descriptions, see the topics below:

Control Panel
Browser
Method Window
Table Editor
PGM Editor

Control Panel

A ➢*Control Panel* (in short: panel, also referred to as online plot or online window) controls and monitors the chromatography instruments of a ➢*Timebase*. With regard to appearance and function, it is a special type of window. In accordance to the Dionex Chromatography Management System philosophy, you are free to design its appearance in any way to meet the user requirements. For details, see

Appearance
Function
Audit Trail

Appearance

➢*Control Panels* do not have a uniform user interface. The appearance is determined by a combination of various default controls.

These controls can include:

- A slider to change the pump flow or another variable parameter.
- A separate field to display status information such as the running retention time.
- A screen LED to indicate the active detector lamp.
- A command buttons to execute the inject command.
- A signal plot to monitor the detector signal.
- The current ➢*3D Field* and the current ➢*Mass Spectrum*.
- The Audit Trail to follow the execution of an operation.

The user can determine the number of available controls and their functionality, depending on individual requirements. Each user thus "designs" a personal interface. The available functions depend on the functionality of the analytical instruments that are combined in a timebase. If a user integrated a controllable column oven into the system, the temperature of the oven can be controlled.

The system administrator determines via user-specific ➢*Privileges* in the ➢*CmUser* program whether a user is authorized to create his "personal" user interface. The organization of the panel allows locking certain functions on the user interface or disabling the display of irrelevant information.

A new user interface can be saved as a separate file (*.pan). Each user who has access to the directory containing the file can select and use the file via **File/Open**.

If this type of screen arrangement seems confusing at first, the system offers several default control panels that cannot be modified. These do not only cover all standard control functions but they can also be used easily and intuitively.

For details on creating control panels, see **How to ...: Actions in the Control Panel**.

Function

➢*Control Panels* serve to control and monitor individual ➢*Timebases*. The timebase to be controlled is specified when creating the control panel. As soon as the control panel is opened, establishing a connection with the specified timebase is automatically attempted. If this is not possible, e.g., because the corresponding timebase was renamed or because the corresponding Chromatography ➢*Server* is not in operation, the user is informed by a message. In this case, assignment must be changed manually. Proceed as follows:

- Open the desired control panel via **File/Open**.
- Choose **Connect to Timebase** from the **Control** menu and specify the name of the timebase to be connected with the control panel or select the name from the available list.

The new assignment is valid until the window is closed. Store the window to have the current assignment available next time you open the window.

The currently selected timebase is displayed in the status bar.

Tip: You can also view the report for the running sample from within the panel via the **Integrate** command of the **View** menu.

Signal Plot

The signal plot is an essential part of the **Control Panel**. The ➢*Signals* of the channels, which have been selected by the user, are displayed online, i.e., during data acquisition.

Different commands are available via the context menu (right mouse button) allowing you to define how the signals shall be displayed:

Autoscale Each time when performed, the ➢Autoscale command adjusts the scaling of the signal axis exactly to the current chromatogram or a section thereof.

Double-clicking the signal axis also executes the Autoscale command.

Auto Autoscale The ➢*Auto Autoscale* option automatically adjusts the scaling of the signal axis exactly to the current chromatogram or a section thereof whenever the signal leaves the signal plot

Auto Plot Speed Select the **Auto Plot Speed** option to prolong the time axis automatically by the period defined on the **Axis/Decoration** tab as soon as the end of the signal plot is reached.

Replot from Beginning Performing the ➢Replot from Beginning command has the following effect:

When the signal leaves the right border of the signal plot, the window is enlarged by the period defined on the **Axis/Decoration** tab so that always the complete recorded chromatogram will be displayed.

Audit Trail

The **Audit Trail** in a ➢*Control Panel* logs all commands performed during sample processing and saves information regarding the entire system. This includes graphical and text information. The Dionex Chromatography Management System classifies ⇒*Control Commands*, status information, and error messages as indicated below:

- System Message
- Warning
- Error
- Abort Error
- Next command

  (Symbol appears only during the batch and only if there is a connection to a datasource containing the ⇒*Sequence* to process!)
- Executed instruction. The color indicates the filter level. The message is displayed from this level on:

  Green: Normal

  Yellow: Advanced

  Red: Expert

  This color code is not yet valid for manual and triggered commands.
- Protocol; comments program steps or describes chromatographic conditions
- ⇒*Message* on the screen that must be confirmed by the user
- Fulfilled ⇒*Trigger* condition
- Triggered command
- Manually executed command
- ⇒*Log* (performed manually / by the device driver)

After starting data acquisition, the Audit Trail window shows the start time and any subsequently performed commands (⇒*AcqOn/Off*, ⇒*Inject*, etc.).

Even commands and status messages that are not automatically recorded (e.g., the current system pressure) can be periodically retrieved and displayed using the Log command.

Of course, each event included in the Audit Trail window is stored. Storage is very precise and comprehensive. This allows determining later how a sample was processed and which events occurred during sample processing. For further information, see **Protocol Data (Audit Trail)** in the **Data** chapter.

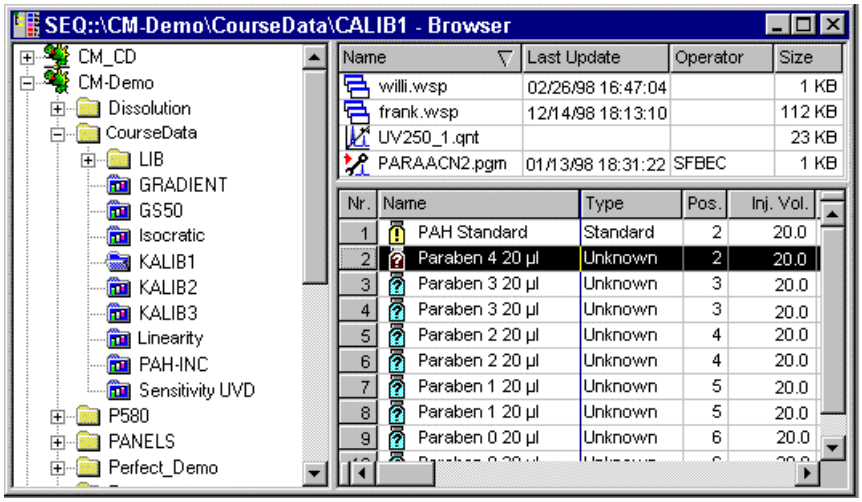
For documentation purposes, single events can be included in a report. For details see **How to ...: Actions in the Report Audit Trail**.

Browser

The ➢*Browser* of the Dionex Chromatography Management System is the tool for data management. It displays the directories in which chromatographic data is located and that can be accessed.

The browser allows opening, moving, and deleting chromatographic data as well as searching for specific data in various databases. When a file is selected, it can be opened and its contents can be viewed in a separate window.

Caution: Functions and structure are similar to the Windows Explorer. However, do not confuse the Browser window with the Windows Explorer! Do not use the Windows Explorer for operations within ➢*Datasources* of the Dionex Chromatography Management System!



For further details, see the topics below:

Common Features with the Windows Explorer

Differences from the Windows Explorer

Function

Common Features with the Windows Explorer

The window has two separate sections. As in the Explorer, the directory structure of all selectable directories is displayed on the left. Detailed information on files and ➢*Sequences* is shown on the right. Operation is also identical to the Explorer:

- Click the + and - symbols next to each directory name to expand or collapse the subdirectory structure.
- Select a directory to view its contents in the right-hand window section. Files and single samples are displayed.
- Double-click a file or sample in the right-hand window section to open the appropriate editor for a file or the corresponding chromatogram for a sample.

For convenient identification, each file type (sequence, ➢*PGM File*, ➢*Quantification Method,* ...) has a type-specific icon. The Dionex Chromatography Management System automatically recognizes the ⇒*Type* (Sample Type) (standard sample, unknown sample, Program File (PGM file) or the stored data format (3D-field etc.) and displays the data appropriately, i.e. in the respective chromatographic environment.

- Select a subdirectory, a sequence, or a file to drag it with the mouse to a different directory.

Caution: For safety reasons, the corresponding data is always copied. To move files, copy them and then delete the original files. Directly moving files is currently not supported.

Differences from the Windows Explorer

Structure

Only the chromatographic data that is part of a ➢*Datasource* is presented (for details see **Data** chapter) in the Browser.

A datasource always represents the top level of the Browser hierarchy. The datasource can be created exclusively with the Browser and cannot be compared to the "normal" subdirectory in the Windows Explorer. A small icon indicates the type of data on which it is based (CHROMELEON, GynkoSoft data, etc.). Users can only see those datasources for which they have the appropriate access rights.

Below the datasource level, there is the familiar Explorer directory structure (yellow file folder). The directory structure serves to manage different ➢*Sequences* in a datasource. A blue file folder represents a sequence. It is not possible to create a subdirectory below the sequence level.

Operation

- Select a datasource, any subdirectory, or sequence to view its contents in the right pane of the browser.

In the case of the datasource or subdirectory, you see the usual list of all directories and files. If you select a sequence, the right-hand window half is divided in two horizontal sections. These include the header with general properties of the selected sequence and a list of all analysis and standard samples and their sample data (**Sequence Editor**).

Caution: The sample data can be edited directly here! GynkoSoft users recognize the **Sample (SMP) File**. Additional samples can be included in the sequence, existing sample data can be modified, or old samples can be removed. For a detailed description of the sequence editor, refer to the **Sequences** section.

- Choose the **Query** command in the context menu to search for specific sequences, data or samples (also simultaneously in several datasources). This is a true ➢*Query* that can also search for specific properties, e.g., "all samples starting with PAK."

Moving, deleting, or copying directories, data, and files largely corresponds to the Microsoft Explorer (see **Browser** **Common Features with the Windows Explorer**). Note the following warning:

Caution: Moving, deleting, or opening chromatographic files must be performed ***exclusively*** in the Browser, as processes below the surface are performed apart from the visible result!

Function

- Use the Browser to set up ➢*Datasources* and create subdirectories, to move files via **Drag & Drop** or to delete files.
- Select a ➢*Sequence* in the left window (blue folder) to view a list of its contents on the right.
- Double-click a sample name to view the corresponding chromatogram.
- Double-click a ➢*PGM File* name to open the PGM editor.
- Select a file and press the right mouse button for further functions.
- Select several files (as in the Windows Explorer) and press the right mouse button to perform a function for several files simultaneously.
- Select a file, press the right mouse button, and start a ➢*Query* for several sequences and/or datasources. The result of the query, i.e. different files or samples with at least one common feature, is displayed in the right pane of the Browser.

Method Window

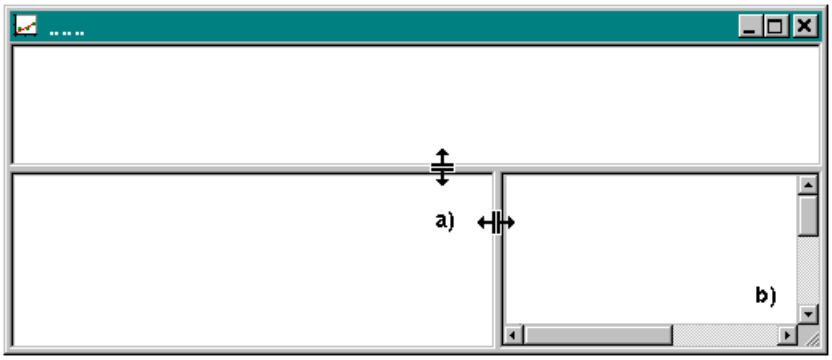
Offline windows serve to represent chromatographic results. They show chromatograms, 3D-fields, spectra, calibration data and result lists.

General

Method windows are opened via:

- The **View** menu,
- The respective toolbar icons or
- A double-click on a file

The appearance of different method windows can vary considerably. A window can have various window sections of which the borders can be moved (a). If the size of the window section is not large enough to show the entire information, the hidden area can be viewed via the scroll arrows or bars (b).



The contents of the window section depends on the type of the represented data. Table or text editors can also be integrated as a window section in a method window. Window sections with a graphical representation show the coordinates of the mouse cursor in the status bar.

Types

There are currently five different method windows:

- ⇒*Quantification Method* (QNT editor)
- Control window (see **PGM Editor** below)
- Integration
- Peak Purity Analysis (PPA)
- Printer Layout
- Spectra Library

Each window can be opened any number of times and shows the current data from various viewpoints.

It certainly makes sense not to limit the display of chromatograms to the method window Integration, but to enable it in the Calibration Curve or PPA methods. The same applies to the output of numerical data in the form of a report that can be displayed in any window.

Table Editor

The table editor is used for representation and entry of various parameters and variables. This includes creating sequences in the sequence table, determination of integration, calibration and peak table parameters as well as representation of all result and report variables.

- Appearance and use of all tables correspond to the Windows standard. Editing is by cell, column, or line.
- Selected columns can be moved, hidden, or made visible at the current cursor position. The width of a column is adjusted by moving the left or right delimiter or by applying the **Optimum column width** function.
- Adding or removing selected lines is possible anywhere in the table.
- The described functions can be accessed conveniently in the context menu.
- The font size can be changed. Choose a smaller font to display more information on the screen.
- Press the F1 key to view Online Help information on a specific column.

- Press the F8 key to open an Edit dialog box for a specific field. This prevents the input of incorrect or invalid values and names.
- Press the F9 key to fill an entire column with the value of the current field. Logical rows of numbers can also be extended with this method. If the input is 2, 4, and 6 in the first three fields, the row is continued with 8, 10, 12, etc.

PGM Editor

The PGM editor is used for editing a PGM file. It includes three views that can be accessed via the corresponding icons in the left pane (the so-called shortcut bar):

- **Commands**
- **Finnigan AQA**
- **Post-acquisition steps**

Commands

The **Commands** view is the actual program editor, a normal text editor, similar to the Windows **Wordpad** text editor. It serves to create a ⇒*Program*. Apart from comment lines, this file contains all commands that are executed exactly at the time indicated in automatic routine operation.

- As in most word processors, input is line by line.
- The **Cut & Paste** function is available for comfortable editing.
- The Dionex Chromatography Management System interprets pure ASCII text only. Formatted texts cannot be generated with this editor, nor can formatting be integrated with imported texts.

Different colors are used to facilitate orientation in the program. Distinctions are made between control commands **(black text)**, comment lines **(green text)**, ⇒*Trigger* commands **(blue text)**, and incorrect instructions **(red text)**.

A program can be modified directly or via the edit box. Open the edit box by pressing the **F8** key.

☞ ***Tip***: Editing the file is only possible after connecting the PGM file with a timebase while the server is active (see: **Connect to Timebase** command in the Control menu). If there is no connection to a ➢*Timebase*, all program lines are displayed in **gray print**.

For detailed information on creating and editing PGM files, see the chapter **Control** under:

Control Program

Program Syntax

Program Wizard

For a description of the different ⇒*Control Commands*, see **How to ...:**

Actions in the PGM Editor **Creating a Program**

Device Control **Extending a Program**

Finnigan AQA

This view of the PGM editor is part of ➢*Xcalibur* and serves to specify the method that is used by the aQa mass spectrometer.

On the **Ionization Mode** tab, specify the mode of ionization (Electrospray / APCI). On the **Analysis** tab, specify the sensitivity and fine-tune the mass spectrometer.

⚠ ***Caution:*** When using the Xcalibur method editor, the **Other detectors** section is irrelevant. Do not use this section for data acquisition with other detectors (e.g. UV detector)! In this case, perform data acquisition as usual.

The **Acquisition** tab allows setting the aQa-specific signal parameters for ➢*Mass Spectra* acquisition.

☞ ***Tip***: This view of the PGM editor is part of Xcalibur. Thus, you can open the Xcalibur help via either the **Help** menu or the **Help** button. The Xcalibur help provides detailed information on mass spectra acquisition.

Post-acquisition steps

Post-acquisition steps are extraction and smoothing steps that are performed by the PGM file after data acquisition. These steps can be performed online after data acquisition of offline outside of the chromatogram, UV spectrum, and mass spectrum.

Working with Several Windows

The Dionex Chromatography Management System not only supports working efficiently with several open windows as is typical in Windows programs, but also introduces what has become possible with object-oriented programming of applications and was not common before:

The display of data is always updated in all windows!

Below please find two examples of samples with chromatograms; Specific detection parameters were used for integration and analysis.

Example 1: If the ⇒*Minimum Area* detection parameter is corrected in the QNT method window by entering a smaller value, the corresponding chromatogram is immediately adjusted, i.e. peaks with an area smaller than the minimum are not considered.

Example 2: Similarly, the result of a manually modified baseline can be seen immediately in the window of the integration report.

User Profiles (Workspaces)

The Dionex Chromatography Management System offers the possibility to save the window arrangement of any work situation, i.e. the combination of different windows, in a workspace.

This facilitates opening single files or windows and allows the user to work with his/her own work environment on the screen.

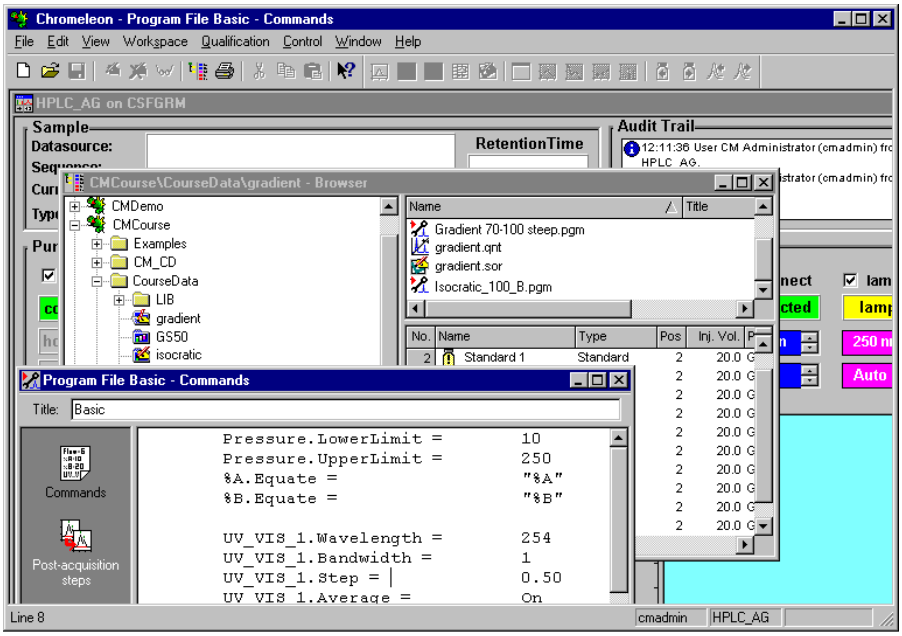
The information, which windows should be used, is stored in a WSP file. Users who want to start working with a specific workspace, open the corresponding WSP file or generate it by storing the screen contents.

- Choose the **Open Workspace** command from the Workspace menu to open an existing workspace.

- Choose the **Save Workspace** command to save the current workspace.
- Select the **Save Workspace as** command to save the current workspace with a new name.
- Select the **Autosave Workspace** command to always save the most recent workspace as the default workspace.

The number of **Windows** saved with each workspace is not restricted.

A possible and useful workspace arrangement combines, for example, the PGM editor, a control panel, and the Browser (see illustration).



The appearance of each individual window is stored in the **Report Definition**.

☞ ***Tip***: When the Dionex Chromatography Management System is started, the most recently used workspace is loaded.

Increasing the number of displayed windows and data in a workspace also increases the loading time!

Report Definition

The ➢*Report Definition File* (**RDF**) comprises the current settings such as the names and scaling of axes, the representation of chromatograms and spectra, display of additional information or auxiliary lines, setting various font types and sizes as well as arranging columns in a table. The report definition also determines how the current screen contents (Hardcopy) or online batch results are printed (see **Printing**).

In contrast to the workspace, a report definition can be used for individual windows. The report definition is required whenever a window is not opened via the workspace. The most recent report definition will be opened. If a user has not saved a RDF, the default report definition supplied with the Dionex Chromatography Management System (DEFAULT.RDF) is used. It is located in the REPORT directory.

- Choose **Save Report Definition** from the context or **View** menu to save the current settings.
- Choose **Load Report Definition** from the context or **View** menu to open a previously saved report definition.

Create/Open Files, Windows, and Templates

There are several ways to open or create files, windows, and templates. Frequently, other information is required for this.

For example, when being opened, each control panel searches "its" timebase, i.e. the correct link between the client PC and a certain chromatography system (➢*Timebase*) and each method window searches data from a specific ➢*Datasource*.

☞ ***Tip***: If problems arise in this context, they may be caused by the fact that the user later renames timebases or datasources that are correctly installed by the Dionex Service.

Similar problems may occur if databases are located on a network PC to which no link can be currently established or for which the user has no share authorization.

In this case, see **How to ...: Actions in the Browser**  **Connecting a Database**.

Automatically Loading the Most Recent User Profile

The Dionex Chromatography Management System automatically loads the most recently used workspace. If this is not possible, the Browser is started.

Opening Existing File Types and Windows

Choose the **Open** command of the **File** menu; select the datasource and the directory containing the file to open and the file type to represent. Refer to Online Help for further help on the opened dialog box.

Alternatively, a file can be opened by selecting it in the ➢*Browser* (File menu) and double-clicking it.

Open Most Recent Files and Templates

The lower section of the File and Workspace menu lists the most recently used templates and files. Click a template or file to open it. This is the most simple and quickest way to continue an interrupted task.

New

Select the **New** command of the **File** menu to receive a list of all possible file types and chromatographic operations.

- Select **Control Panel** to open a window for the control of chromatography devices of a specific timebase.
- Select **Sequence File (using Wizard)** to start the  **Sequence Wizard** for creating a ➢*Sequence*. The samples to be analyzed are entered in the sequence.
- Select **Sequence (from LIMS Worklist)** to include data and a ➢*Sequence* of a ➢*LIMS* in the ➢*Worklist* format.

- A ➢*PGM File* includes all ⇒*Control Commands* that must be transferred to the different chromatography devices to process a sample or a series of samples. Select **Program File** to start the **Program Wizard** for creating a **Control Program**.
- Select **Method File** to create a new quantification method.
- Select **Spectra Library** to create a new spectra library.

Printing

The ➢*Printer Layout* of the Dionex Chromatography Management System offers numerous options for presenting results. Similar to a word processor, the user can choose between printing screen contents and printing based on defined templates.

Printing the Screen Contents

The contents of the currently active window can be printed via the respective **Print ...** command. Via **Print Sequence,** you can print in the Browser the current sample list either with the corresponding PGM or QNT files. If a ➢*PGM File* is open, you can print the required views via **Print...** In the same way, you can print the selected pages of a ➢*Quantification Method (QNT Method)* via **Print QNT Method** in the QNT editor.

Printing Based on Report Templates

If one or several samples or sequences are selected in the Browser, **Batch Report** starts the printed output. The user specifies the report template (➢*Report Definition File (RDF)*) to be used and which pages of the printer layout shall be printed for which sample type and for which channel from the selected report template. Creating a report template is performed with the **Printer Layout** method.

Note: Use the Setup button in the Printer Layout to define the page format (see **How to ...: Actions in the Printer Layout Changing the Page Format**)

Printing in an Online Batch

If several samples are processed in an automatic sample batch (➢*Batch Processing*) it is possible to define whether and, if yes, for which channel and how to output results after completing the process.

Printing can be started either after processing a single sample or after processing a complete sequence.

Note: The report template used for printing is stored with other settings (e.g., screen settings) in the Report Definition File (RDF). Future versions of the Dionex Chromatography Management System versions will save the screen and the print settings separately.

Control

Control Concept

The chromatographic equipment of an analytical laboratory usually comprises instruments from different manufacturers and of various generations. Depending on whether this heterogeneous instrument pool can be controlled via a PC or not, it is called a controlled or a non-controlled system.

Non-controlled system

In non-controlled systems, individual instruments are operated manually. The data system only records the data. For this, two conditions must be fulfilled:

- The injection time is communicated to the data system by connecting the **Inject** contact of the injection valve with a ➢*Remote Input* of the system. This guarantees time synchronization between sample start and recording time.
- Detector data is transferred to the data system in digital or analog form (serial interface or ➢*A/D Converter*).

Controlled System

Controlling a system makes high demands on adaptability of a modern chromatography data system, as operation of individual components must be easy and thus **device-independent**. That is, input and representation of a specific control command (for example the pump flow) is always performed in the same way, regardless of whether the instrument is by manufacturer X or Y.

The Dionex Chromatography Management System enables this by the **Chromatography BIOS** and the available **Device Drivers**. The advantages of the uniform user interface are obvious:

- Short training time for inexperienced users.
- Uniform, device-independent operation: the same commands are used for all systems.
- Chromatographic methods can usually be transferred from one system to another. This requires the availability of corresponding device functions on both systems.
- Clear, uniform documentation.

In principle, there are two ways to control a chromatography system. For details, see the topics below:

Control (Direct)

Control (Programmed)

Control (Direct)

Direct control means the immediate and interactive operation of individual instruments and device functions via a **Control Panel**. Observe the following requirements:

- The data system must be extended by one of the **Options of the Dionex Chromatography Management System**.
- Correct installation and configuration of the controlled instruments and device drivers via the **Server Configuration**.
- Establishment of an intact connection between the PC and the chromatography server.
- Establishment of an intact connection between the chromatography server and the Chromatography system via a **Serial Interface**, **DX-LAN**, or other interface (GPIB, USB).

For an overview of executable system and instrument commands, see the topics below:

System Commands

Dionex Pumps

Controlling Pumps without Separate Device Driver

Dionex Autosamplers

Dionex Detectors

Dionex DX-120 Ion Chromatograph

Dionex Column Oven STH585

Optimum support for all functions is ensured for Dionex instruments. Information on support for third-party instruments is included in the **Installation Instructions**.

For a list of the third-party instruments that are currently supported, see **Installing and Controlling Third-Party Instruments**.

System Commands

System control comprises all commands that concern the entire chromatographic process or the entire system. The commands are available both, via **Command** in the **Control** menu and via the **F8** key in **Commands** view of the PGM editor. In addition, some of them are available on the toolbar as well.

Abort Sample	Stop data acquisition and sample; continue the ➢*Batch* with the next sample
⇒*Abort Batch*:	Stop data acquisition and batch processing
⇒*StopFlow*:	Stop pump flow, interrupt data acquisition, stop batch processing
⇒*Hold*:	Freeze running gradient program, interrupt data acquisition, hold batch processing
⇒*Continue*	Continue all functions in hold mode
⇒*Acquisition On/Off*	Start / terminate data acquisition

Via the **Sound** command, you can select the frequency and the length of a sound to be heard at a specified time.

Dionex Pumps

For controlling HPLC and IC pumps, the following commands are available to the user:

⇒*Flow*	Change flow rate
⇒*Pressure Limits*	Set pressure limits

In addition, the following commands are available for controlling gradient pumps (M480, P580, GP40/GP50, and GS50):

⇒*%A, %B, %C, %D*	Change solvent composition, determine gradient course

The commands can be given either directly (toolbar and menu bar or control) or as part of a ➢*Program* (programmable button).

They enable delivery of a specific liquid volume of defined composition as well as starting and holding the pump. The pump is automatically held as soon as the upper or lower pressure limits are exceeded. Changing the flow rate creates a ➢*Flow Gradient*, changing the solvent composition creates a ➢*% Gradient*. Flow and % gradients can be realized simultaneously (!).

☞ ***Tip***: Dionex GP40/GP50, IP20/IP25, IC20/IC25, GS50, and IS25 pumps do not deliver flow gradient ramps. Instead, changing the flow rate creates a step change; that is, flow rate changes are made immediately, not gradually over time. Also, see **How to ...: Device Control Pump Commands** for additional information.

Dionex Pumps M480 and P580

The Dionex Pumps M480 and P580 support the automatic precompression control, i.e., the pumps are capable of adjusting to the compressibility of commonly used solvents. Optionally, the commands **Learn** and **Freeze** can be used for extending the P580 precompression control to unknown solvent types.

Important specifications (subject to technical alterations) of the Dionex Pump P580 are:

	P580
Operating principle:	Available models include the isocratic model P580A, the quaternary low pressure gradient system P580A LPG, and the binary high pressure gradient system P580 HPG.
Flow range:	1 - 10000 µl/min in 1 µl increments
Pressure range:	1 - 500 bar
Flow accuracy:	0.1% or 0.5 µl
Gradient accuracy:	1% absolute from set value between 250 and 2000µl (P580A LPG)
	0.2% absolute from set value or 0.5 µl per branch (P580A HPG)
Pressure pulsation:	0.5 bar or 0.5%

For the user, it is irrelevant whether the system is a ➢*Low-Pressure Gradient System* or a ➢*High-Pressure Gradient System*. Command input is identical.

Caution: Chromatography pumps are high-precision instruments! Dry operation or crystallization of buffer solutions within the fluidic system must be avoided. These problems occur especially when the pump flow is stopped while the detector lamp is still switched on. The flow cell heats up, and the solvent evaporates. Depositions of substances can result, e.g., salt in a buffer solution.

Dionex Pumps GP40/GP50, IP20/IP25, IC20/IC25, GS50, and IS25

In addition to the general pump commands, the following commands are available for controlling the isocratic or gradient pumps listed above:

On	Turn on the pump motor
Off	Turn off the pump motor
Prime	Prime the pump

For pump operating specifications, refer to the individual pump operator's manuals.

Also, see **Controlling Pumps without Separate Device Driver**

Controlling Pumps without Separate Device Driver

In addition to the device drivers for **Dionex Pumps**, the Dionex Chromatography Management System offers many drivers for controlling third-party pumps. (For an overview on the different manufacturers whose devices can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments** in the Installation section.

Besides, pumps can be controlled for which separate device drivers or serial interfaces are not available (e.g., the former Gynkotek pump M300). Depending on the type of pump to be controlled, the following plug-in boards are available:

1. "Dionex Pump DA Converter (12 Bit)" (for *voltage-controlled* pumps) or
2. "Dionex Pump Control Board" (**Pump Control Board**) (for *frequency-controlled* pumps).

For installation information, see the following topics in the Installation section:

Installing the Dionex 12-Bit DAC Board

Installing the Pump Control Board

In addition, the respective device driver **DAC Pumps** (for *voltage-controlled* pumps) and **Pump Control Board Pump(s)** (for *frequency-controlled* pumps) must be installed (see **How to ...: Actions in the Server Configuration** **Changing the Server Configuration**).

The following control commands are available for voltage-controlled pumps (**DAC pumps**):

⇒*Flow*:	Changes the flow rate
⇒*%A, %B, %C, %D*:	Changes the solvent composition, determines the course of the gradient

With frequency-controlled pumps (**Pump Control Board Pump(s)**), a reset can be performed in addition.

Dionex Autosamplers

Automatic sample injection using a modern ➢*Autosampler* offers several advantages:

- Comfortable processing of large sample batches
- Reproducible and verifiable dosing precision
- Loss-free and bubble-free injection of the sample

In spite of the vast scope of performance, only the "simple" commands **Inject**, **Position**, and **Volume** are required for automatic control of the Dionex Autosamplers:

Simple Commands

⇒*Inject*	Inject sample
⇒*Position*:	Vial Position
⇒*Volume*:	Volume to inject

For information on the individual autosamplers and their respective specifications, see the following topics:

Dionex Autosamplers GINA 50 and GINA 160

Dionex Autosampler ASI-100 / ASI-100T

Dionex Autosampler AS50

Dionex Autosamplers GINA 50 and GINA 160

Beyond the simple commands (see **Dionex Autosamplers**), the Dionex Autosamplers GINA 50 and GINA 160 offer additional commands enabling further functions. These include multiple suck operations (**Suck**) from one sample, washing the sample loop (**Wash**), moving the sample needle (**NeedleUp** for GINA 50, **Needle** for GINA 160), or cooling the sample vials.

The following commands are available:

Special Commands

⇒*NeedleUp*	Move needle
Load	Switching the internal sample valve without moving the needle (also, see NeedleUp)
⇒*Wash*:	Wash
Segment:	Draw an air volume (command available for GINA 160 only)
⇒*Suck*:	General: Suck liquid quantity (special for GINA 50: position = 100 means suck air segment from an imaginary "air vial")
⇒*Dispense*:	General: Dispense sucked liquid quantity (special for GINA 50: Position = 101 means dispense sucked volume in needle seat)
TempCtrl	This command activates the temperature control of the Dionex Autosampler GINA 50T. This sampler is capable of controlling the rack temperature and, thus, the sample temperature within a 15°C range. At room temperature (20°C), maximum sample cooling is to 5°C above zero.

The GINA 50 Autosampler offers the following specifications (subject to technical alterations):

	GINA 50
Operating principle:	Sample loop valve with inline principle (also see ➢*Autosampler*)
Sample capacity:	50 plus 1 standard or 80 minivials
Dosing volume:	1 - 250 µl with standard syringe
Reproducibility:	<0.3% at 10 µl with standard syringe
Sample loss:	None
Flush volume:	None

For information on how to use the commands in practical operation, see **How to ...: Device Control Autosampler Commands (GINA 50)**.

Dionex Autosamplers ASI-100 / ASI-100T

For a basic description of the Dionex Autosamplers including the simple commands, see **Dionex Autosamplers**. Beyond this, the Dionex Autosampler ASI-100/ASI-100T (ASI-100T = with temperature control) provides many commands for controlling all functions an autosampler can possibly control, among others drawing a sample repeatedly (= Draw), mixing different samples (= Mix), or washing the needle (= Wash). You can specify these commands in more detail via the vial whose contents shall be mixed (= Mix Subject) or the volume to be used for the **Draw**, **Dispense**, and **Mix** (= MixVolume) commands.

Special commands:

Command/ Property	Description
BlueSegment	Select the segment type that is used in the blue segment. Available types are: Analytical - Semiprep - Mini - Eppendorf.
Busy	Indicates whether the sampler is busy (working) or idle (comp. Ready).
⇒*Connect*	Connects the device to the data system, enables computer control (comp. Connected, Disconnect).
Connected	Indicates whether the device is connected to the data system, i.e. under computer control (comp. Connect, Disconnect).
CoolingPower (ASI-100T only)	Indicates the cooling power (for diagnosis purposes only).
Disconnect	Disconnects the device from the data system, enables manual control from the device's front panel (comp. Connected, Connect).
⇒*Dispense*	Dispenses the previously drawn volume.
DispSpeed	Specify the speed with which the contents of the syringe shall be dispensed.
DownSpeed	Specify the speed with which the needle moves down.
⇒*Draw*	Draws the specified volume.
DrawSpeed	Specify the speed for filling the syringe.
ExternalMSV	State of the external valve.
FirmwareDownload	Triggers download of device firmware appropriate for this driver.
FirmwareVersion	Indicates the sampler's firmware version.
GreenSegment	Select the segment type that is used in the green segment. Available types are: Analytical - Semiprep - Mini - Eppendorf.
HeatSinkTemperature (ASI-100T only)	Indicates the heat sink temperature (read only).

Command/ Property	Description
⇒*Inject*	Injects a sample.
InjectCounter	Number of injections.
InjectMode	Inject Mode. if set to **Normal**, the sampler draws the specified volume from the specified position and injects. If set to **Mix**, the sampler injects whatever volume is left in the syringe after preceding draw/dispense operations.
InjectWaitTime	Period between the issuing of the command by the data system and the acknowledgement of the sampler.
Input1, *2, 3 or 4*	State of the digital inputs 1, 2, 3, or 4.
Internal MSV	State of the internal motorized switching valve.
Mix	From the position that is determined via the parameter **MixSubject**, the syringe draws and dispenses the volume that is determined via the parameter **MixVolume**. If **MixVial** is selected as **Mix Subject**, the parameter **MixVial** must be specified as well. The parameter **MixRepeat** indicates the number of replicates during mixing.
MixHeight	Needle height for draw, dispense and mix operations, specify how deep the needle will dip into the vial for mixing.
MixRepeat	Repeat count for draw, dispense, and mix operations for mixing.
MixSpeed	Syringe speed for draw and dispense operations for mixing.
MixSubject	Specify the subject to be used for draw, dispense, and mix operations. The following subjects are available: MixVial, SampleVial, WashVial, Air, ReagentAVial, ReagentBVial, ReagentCVial, ReagentDVial. If **Air** is specified as mix subject, air is drawn in. During **Dispense,** the needle moves into the needle port and is dispensed there.
MixVial	Specify the vial position if **MixVial** is selected as **MixSubject** (comp. MixSubject).
MixVolume	Volume to be used for the **Draw**, **Dispense**, and **Mix**.
Msv2ToInject	Switches the external valve to **Inject**.
Msv2ToLoad	Switches the external valve to **Load**.
MsvToInject	Switches the injection valve to **Inject**.
MsvToLoad	Switches the injection valve to **Load**.
NeedleSealCounter	Needle seal wear.
⇒*Position*	The sample's position on the tablet.
RadialSpeed	The speed of the radial needle movement.
Ready	Sampler ready flag, true when sampler is idle (comp. Busy).
ReagentACapacity	Specify how often the volume can be drawn from the vial with reagent A (reagent B, C, and D, respectively).
ReagentAVial	Position of the reagent A (reagent B, C, and D, respectively) vial - is used only if **ReagentAVial** is selected as **MixSubject** (comp. MixSubject).

Command/ Property	Description
RedSegment	Select the segment type that is used in the red segment. Available types are: Analytical - Semiprep - Mini - Eppendorf.
Relay1*, 2, 3 or 4*	The following commands are available: **State** (indicates or sets the state of the relay), **Duration** (when set, the relay's state toggles after the specified time), **On** (turns the relay on), and **Off** (turns the relay off).
Relay3Enabled	Relay3 mode. If set to **Yes**, the relay can be controlled by the data system. If set to **No**, the sampler controls the relay and the relay indicates, whether the sampler is operable.
Relay4Enabled	Relay 4 mode. If set to **Yes**, the relay can be controlled by the data system. If set to **No**, the relay is controlled by the sampler and indicates injection.
Reset	Resets the sampler to its initial conditions, as attained after power-up.
SampleHeight	Indicates the height at which the sample is drawn, measured from the vial bottom to the needle tip.
SerialNumber	Indicates the sampler's serial number.
State	Indicates that the sampler has injected.
Syringe	Indicates the volume of the syringe that is installed in the sampler.
SyringeCounter	Indicates the number of syringe movements.
SyringeDelay	Specify the time the needle shall remain in the vial after loading.
⇒*Temperature* (ASI-100T only)	Defines the set temperature of the sampler's tray and hence of the sample. Opening the command tree shows the following commands: **Value** (= actual temperature, read-only), **Nominal** (= set temperature), **UpperLimit**,and **Lower Limit**. With **UpperLimit** and **LowerLimit**, the system aborts the batch and starts emergency handling if the nominal temperature is outside these limits.
TemperatureControl (ASI-100T only)	The following settings are available: **On** (= cooling/heating enabled), **Off** (= cooling/heating disabled) and **Fixed** (= diagnosis setting only which should not be used by the end user) (comp. Nominal, Value, HeatSinkTemperature, CoolingPower).
Test	Moves the needle to the specified vial. If no vial is specified, MixSubject is used (comp. MixSubject).
TrayDetection	Turns tray detection (including manual interference monitoring) on or off. With enabled tray detection, a home run is executed when the tray is mounted. If, with disabled tray detection, the tray was removed, a self-test must be performed when the tray is mounted again. This is to ensure that the sample is injected from the correct position.
UpSpeed	The speed used to move the needle up.
⇒*Volume*	Injection volume.

Command/ Property	Description
⇒*Wash*	The internal MSV is switched to **Load**, if necessary. The volume specified under **WashVolume** is drawn from the position specified under **WashVial** and dispensed into the needle port/waste. The parameters **WashSpeed** and **WashHeight** are also considered.
WashHeight	Wash height = distance between the bottom of the wash vial and the needle tip (= the depth with which the needle will dip into the vial).
WashSpeed	The speed with which the syringe draws the wash volume.
WashVial	Position of the wash vial.
WashVialVolume	Total volume of the wash vial.
WashVolume	Specify the volume to be drawn from the wash vial.

The ASI-100/ASI-100T samplers offer the following specifications (subject to technical alterations):

	ASI-100/ASI-100T
Principle:	Sample loop valve with in-line split-loop principle (please also refer to ➢*Autosampler*)
Sample capacity:	Depending on the used segment type Semiprep: 63 vials at 4 ml (to be filled with 2 ml only!), Analytical: 117 vials at 1.8 ml (to be filled with 1.2 ml!) Mini: 192 vials at 1.2 ml, (to be filled with 0.6 ml only!) Eppendorf: 66 vials at 2 ml (to be filled with 1 ml!) or at 1.5 ml (to be filled with 0.5 ml only!)
Injection volume:	0.1 - 250 µl with standard syringe and the corresponding sample loop
Reproducibility:	< 0.3% at 5 µl with standard syringe, typically < 1% at 1 µl
Sample loss:	None
Flush volume:	None
Temperature Control	In the range of 4 - 45°C (39.2 - 113°F) cooling: 18°C (64.4F) from ambient heating: 35°C (95°F) from ambient

Note: All inputs of the ASI-100/ASI-100T are also available as CM-Input ports, i.e., other device drivers can use them as well (e.g., Remote Inject).

For information on how to use the commands in practical operation, see **How to ...: Device Control Autosampler Commands (ASI-100/ASI-100T)**.

Dionex Autosamplers AS50

For a basic description of the Dionex Autosamplers including the simple commands, see **Dionex Autosamplers**). Beyond this, the Dionex AS50 Autosampler provides many additional commands for controlling autosampler functions, such as flushing the liquid lines (**Flush**), moving the needle arm to the home position (**Home**), and preparing the sample before injection (**Pipet**, **Mix**, **Dilute**, etc.). The following commands are available:

Special Commands

➢*Cycle*	Set time between injections
Flush	Flush inject port
Home	Move needle arm to home position
Prime	Prime liquid lines
Stop	Stop current process
➢*Syringe Speed*	Set syringe speed

Special Commands for Sample Preparation

➢*Pipet*	Move sample between vials
➢*Mix*	Mix vial contents
➢*Delay*	Pause sample preparation
➢*Flush (SP)*	Flush inject port during sample preparation
➢*Needle Height*	Position needle above vial bottom

The following commands are only available if the AS50 is equipped with the sample prep option:

➢*Dilute*	Dilute sample with reagent
➢*Dispense*	Dispense reagent to a vial

The following command is only available if the AS50 is equipped with a thermal compartment:

➢*Column Temperature*	Sets the temperature of the thermal compartment

The following command is only available if the AS50 is equipped with the sample temperature control option:

➢*Tray Temperature*	Sets the temperature of the sample tray.

For information on how to use the commands in practical operation, see **How to ...: Device Control Autosampler Commands (AS50)**.

Dionex Detectors

The following "simple" commands and functions for representing the recorded data are available for all detectors, even if they supply analog signals via the A/D converter.

Simple Commands

⇒*AcqOn/Off*	Start/stop data acquisition
⇒*Autozero*	Automatic autozero
➢*AutoAutoscale*	Axis/scaling adjustment
⇒*Step*	Step width adjustment
⇒*Average*	Average between datapoints

For information on the special commands available for the individual detectors and their respective specifications, see the following topics:

Dionex UV/PDA Detectors UVD 160S/320S and UVD 170S/340S

Dionex Photodiode Array Detector PDA-100

Dionex Absorbance Detectors AD20/AD25

Dionex Fluorescence Detectors RF1002/RF2000

Dionex Electrochemical Detectors CD20/CD25/CD25A, ED40/ED50/ED50A, and IC20/IC25/IC25A

Dionex UV/PDA Detectors UVD 160S/320S and UVD 170S/340S

In addition to the "simple" commands available for all detectors (see **Dionex Detectors**), "special" control commands are also supported if the detector is connected to a server PC via an appropriate interface.

Special Commands

⇒*Lamp on/off*	UV lamp on/off
⇒*Wavelength*	Wavelength setting
⇒*Bandwidth*	Bandwidth setting
⇒*Reference Wavelength*	Reference wavelength setting
⇒*Reference Bandwidth*	Reference bandwidth setting
⇒*Bunch Width*	Photodiode signal averaging
CheckWavelength	This performs a wavelength check on the UVD170S and the 340S via the ➢*Holmium-Oxide Filter*.
LampIntensity	States the lamp intensity at 254 nm in counts/seconds. The value can be used as a comparison value to determine how much the lamp intensity decreased. This requires that the value be first measured when the lamp is new.

The Dionex Photodiode Array Detectors UVD 170S and UVD 340S are controllable in remote operation, i.e., all commands listed above can be executed via the data system. The detectors offer the following specifications (subject to technical alterations):

	UVD 170S	**UVD 340S**
Operating principle:	➢*UV Detector*	➢*Photodiode Array Detectors*
Wavelength range ([nm])	200 -595	200 -595
Wavelength accuracy ([nm])	± 0.75 (UV), ± 1.5 (visible)	± 0.75 (UV), ± 1.5 (visible)
Light source	Deuterium lamp	Deuterium lamp
Spectral resolution ([nm])	1.9 (variable up to 400nm)	
Pixel resolution ([nm])	1.9 nm (UV), 3.3 (visible)	1.9 (UV), 3.3 (visible)
Noise (AU peak/peak) (254nm/16nm/1 sec))	$<\pm 0.4 \times 10^{-5}$	$<\pm 0.4 \times 10^{-5}$
Drift (AU/h (254nm/1.9nm/1 sec))	$<5 \times 10^{-4}$	$<5 \times 10^{-4}$

Note: For the UVD 340/170, a voltage offset (in millivolt) can be defined via a registry key on the 16-Bit DAC board for the analog output of the detector signal. The offset values for all 16-Bit DAC channels of the CM server are identical.

Enter the respective offset in millivolt into the registry key:

Example for 100 millivolt (hexadecimal entry):
[HKEY_LOCAL_MACHINE\Software\Dionex\Chromeleon\drivers\UVD340]
"DAC Offset"=dword:00000064

Dionex Photodiode Array Detector PDA-100

In addition to the "simple" commands available for all detectors (see **Dionex Detectors**), the PDA-100 detector provides the following "special" control commands.

Special Commands

⇒*Wavelength*	Wavelength setting
⇒*Bandwidth*	Bandwidth setting
⇒*Reference Wavelength*	Reference wavelength setting
⇒*Reference Bandwidth*	Reference bandwidth setting
⇒*Bunch Width*	Photodiode signal averaging
➢*Recorder Range*	Set the range of a full-scale recorder response
➢*Offset Level*	Offset the analog output signal
➢*Rise Time*	Set how quickly the detector responds to a change in signal
➢*Data Collection Rate*	Set the rate at which the data system collects digital data points from the detector
➢*UV Lamp*	Switch the UV lamp off and on
➢*Visible Lamp*	Switch the visible lamp off and on
UV Lamp Age	Report (or reset) the number of hours the UV lamp has been on
Visible Lamp Age	Report (or reset) the number of hours the visible lamp has been on
Leak Detector Calibration	Perform the leak detector calibration
Leak Detector Test	Perform a test of the leak detector
Wavelength Calibration	Perform a wavelength calibration.
Wavelength Verification	Perform a wavelength verification via the ➢*Holmium-Oxide Filter*
Serial Number	Report the detector serial number
➢*TTL Input Mode*	Set the TTL input signal mode

The commands can be given either directly (➢*Toolbar*, menu bar, or ➢*Control*), as part of a ➢*Program*, or via a programmable button).

The following are important specifications (subject to technical alteration) of the Dionex PDA-100 detector:

	PDA-100
Operating principle:	➢*Photodiode Array Detectors*
Wavelength range ([nm])	190 - 800
Wavelength accuracy ([nm])	±1
Light sources	Deuterium lamp (30 W) for UV spectra
	Tungsten lamp (15 W) for visible spectra
Pixel resolution ([nm])	0.7
Noise	±10 µAU; 2 sec rise time, 254 nm, 4 nm bandwidth
	±10 µAU; 2 sec rise time, 520 nm, 10 nm bandwidth
Drift (µAU/h)	<500 (after warm-up)
Linearity (AU)	>2

Dionex Absorbance Detectors AD20/AD25

In addition to the "simple" commands available for all detectors (see **Dionex Detectors**), Dionex absorbance detectors provide the following "special" control and analog output commands.

Special Commands

➢*Data Collection Rate*	Set the rate at which the data system collects digital data points from the detector
⇒*Wavelength*	Wavelength setting
➢*UV Lamp*	Switch the UV lamp to Off, Low, or High (AD20 detector), or Off or On (AD25 detector)
➢*Visible Lamp*	Switch the visible lamp to Off, Low, or High (AD20 detector), or Off or On (AD25 detector)

Analog Output Commands

➢*Full Scale*	Set the full-scale analog out voltage
➢*Offset Level*	Offset the analog output signal
➢*Polarity*	Switch the analog output polarity (+/-)
➢*Recorder Range*	Set the range of a full-scale recorder response

➢*Rise Time* Set how quickly the detector responds to a change in signal

Dionex Fluorescence Detectors RF1002/RF2000

In addition to the commands available for various detector types, such as **Step**, **Average**, **Autozero** (see **Dionex Detectors**), controllable fluorescence detectors allow modifying the **Emission** and **Excitation** wavelengths.

➢*Emission* Modifying the measuring wavelength
➢*Excitation* Modifying the excitation wavelength

These parameters are supported by the Dionex Fluorescence Detector RF1002 and the successor model RF2000. The model RF2000 also enables the Scan mode. For details, see *Scanning* in the Online Help.

Caution: For connecting the Dionex RF1002 and RF2000 Detectors, the following must be strictly noted:

Pin Assignment

Different pin assignments are required for the RF1002 and for the RF2000! The connecting cables (Dionex part no. 8914.0106 for the RF1002 connecting cable and Dionex part no. 8914.0115 for the RF2000 connecting cable) must be configured as follows:

PC		**RF1002**
9-Pin Sub-D-Connector (female)		**(9-Pin Sub-D-Connector (male)**
2	----------	2
3	----------	3
5	----------	**5**
4 on 6		
7 on 8		

PC		**RF2000**
9-Pin Sub-D-Connector (female)		**9-Pin Sub-D-Connector (male)**
2	----------	2
3	----------	3
5	----------	**7**
4 on 6		
7 on 8		

Settings on the Instrument RF2000 (also see RF2000 Manual)

The communications parameters (9600 baud, 7 data bits, no parity, 1 stop bit; handshake: OFF) are set as follows:

- Press the **func** key (or the keys **shift** + **func**) until **RS232C** is shown in the display. Confirm by pressing **ENTER**.
- Press the **func** key until **BAUD** appears in the display. Press **6** for 9600 BAUD. Press **ENTER**.
- Press the **func** key until **DATA BITS** appears in the display. Press **7** for 7 Data Bits. Press **ENTER**.
- Press the **func** key until **PARITY** appears in the display. Press **0** for No Parity. Press **ENTER**.
- Press the **func** key until **STOP BIT** appears in the display. Press **1** for 1 Stop Bit. Press **ENTER**.

Proceed as follows to connect the RF2000 with your PC:

- Press the keys **shift** + **func**, until **RS232C** appears again in the display. Press **ENTER**.
- **CONNECT** will be displayed. Confirm by pressing **ENTER**.

Specifying a handshake is not required. The detector is now working in remote operation. The keyboard of the instrument is now locked.

Note: To release the keyboard lock, press <SHIFT> and <CE> for a minimum of 3 seconds.

Dionex Electrochemical Detectors CD20/CD25/CD25A, ED40/ED50/ED50A, and IC20/IC25/IC25A

In addition to the "simple" commands available for all detectors (see **Dionex Detectors**), Dionex electrochemical detectors provide special commands. **Data Collection Rate** and the analog output commands are available for all Dionex electrochemical detectors in any operating mode. Other special commands depend on the selected operating mode.

➢*Data Collection Rate* Set the rate at which the data system collects digital data points from the detector

Analog Output Commands (All Modes)

➢*Full Scale*	Set the full-scale analog out voltage
➢*Offset Level*	Offset the analog output signal
➢*Polarity*	Switch the analog output polarity (+/-)
➢*Recorder Range*	Set the range of a full-scale recorder response
➢*Rise Time*	Set how quickly the detector responds to a change in signal

Special Commands (Conductivity Mode)

The following commands are available for conductivity detectors (CD20/CD25/CD25A, ED40/ED50/ED50A, or IC20/IC25/IC25A):

DS3 Temperature	Set the ➢*DS3* temperature
Current	Set the current supplied to the SRS or AES
➢*Temperature Compensation*	Set the temperature compensation factor, which is used to stabilize conductivity readings

In addition, the following commands are available for CD25A, ED50A, and IC25A detectors:

Suppressor Type	Select the installed ➢*Suppressor*
Eluent Concentration	Specify the concentration of the eluent(s); this command is enabled only if an AES suppressor is installed

Special Commands (DC Amperometry Mode)

The following commands are available for the ED40/ED50/ED50A detectors in DC amperometry mode:

Cell	Turn the cell on and off
➢*DC Voltage*	Set the voltage applied to the cell
Electrode	Select the type of electrode installed

Special Commands (Integrated Amperometry Mode)

The following commands are available for the ED40/ED50/ED50A detectors in integrated amperometry mode:

Cell	Turn the cell on and off
Electrode	Select the type of electrode installed
➢*Waveform*	Program a waveform (a plot of potential vs. time)

Dionex DX-120 Ion Chromatograph

The following commands are available for direct control of DX-120 operating functions:

Controlled AC	Switches the AC power outlet on the DX-120 rear panel on and off. This provides on off control of an external accessory connected to the outlet. See the DX-120 operator's manual for cabling instructions.
Column	If the DX-120 is in ➢*Column Mode*, the **Column** command sets the flow path to column A or column B.
Eluent	If the DX-120 is in ➢*Eluent Mode*, the **Eluent** command selects the eluent reservoir (A or B).
➢*Data Collection Rate*	Set the rate at which the data system collects digital data points from the detector.
Eluent Pressure	Turns the pressure to the eluent reservoir(s) on and off.
Pressure Unit	Selects the units of pressure to use (psi or MPa).
Pump	Turns the pump on and off.
SRS	Turns the current supplied to the ➢*Self-Regenerating Suppressor* (SRS) on and off.

Dionex Column Oven STH585

The following commands are available for controlling the operating functions of the STH585 Column Oven:

Connect	Connects the unit to the column thermostat (also see ⇒*Connect/Disconnect*)).
Connected	Indicates whether the unit is connected to the data system, i.e. under control (also see Connect, Disconnect).
Disconnect	Disconnects the unit from the column oven (also see Connect, Connected).
LowerLimit	Upper temperature limit (range: 5 - 85°C)
UpperLimit	Lower temperature limit (range: 5 - 85°C)
Temperature	Nominal temperature, the temperature must be set within the current limits, otherwise the command will not be executed.

The column oven's technical specification is as follows (subject to technical alterations):

	STH585
Temperature range	5 - 85°C
Temperature accuracy	± 0,5°C
Temperature stability	± 0,15°C (measured in a 25 cm test column)
Temperature change	2 - 3°C/min.
Nominal voltage	100 - 230 V AC
Rated Frequency	47 - 63 Hz
Power Consumption	max. 100 W

General Commands

Independent from the installed instruments, the following general commands are available.

⇒*Branch*	Terminates currently active ➢*Program* and starts another one
⇒*Log*	Logs device variable values in the Audit Trail (**Protocol Data**)
⇒*Message*	Displays a message to the user and interrupts the program until the message is clicked.
⇒*Protocol*	Logs any message in the ➢*Audit Trail*
⇒*Wait*:	Interrupts the program until a certain condition is fulfilled.
⇒*Delay*	Especially with trigger commands, execution of the next program command is delayed for the specified time.
⇒*Trigger*	Freezes a running gradient program, stops data acquisition, stops sample processing.
⇒*EndTrigger*	Continues all processes in hold mode.
⇒*End*	Starts / stops data acquisition.

Control (Programmed)

Instead of immediately executing a command as in the case of **Direct Control**, commands can be written using a specific syntax in the ➢*PGM File* and can be executed later.

With this type of control, not only the command itself but the time of execution (relative to the time of injection) must be determined.

If several commands are added to a sequence, and if the command sequence contains an ⇒*Inject* and an ⇒*AcqOn/Off* command, this is referred to as (control) ➢*Program*. To view the program, open the **Commands** view of the PGM editor.

When starting the program, all contained commands are executed precisely at the defined time. The same conditions apply as for the direct control.

For further details, see the topics below:

Control Program

Program Syntax

Program Wizard

Control Program

The control program includes a list of time-precise ⇒*Control Commands*, the actual control program (often just referred to as ➢*Program*) put together by the user. The aim is the automatic and repeated execution of specific routine tasks such as automated sample processing or conditioning a column by rinsing with various solvents. Monitoring certain parameters or limits, or triggering reactions when these limits are exceeded, can also be performed via a program.

A program is created either manually or automatically with the help of a ➢*Wizard*, the **Program Wizard**. All user entries are converted automatically in commands that can be read by the data system. Even new users are thus able to create operative programs.

Independently of whether the program was created manually or automatically, the complete program is always saved as a normal text file. Users familiar with the command syntax can therefore change existing programs at any time.

To edit an existing program, open the program by double-clicking the program name in the Browser. This action opens the **Commands** view of the PGM editor, the actual program editor.

Caution: The steps described below are only possible if the PGM file - analogous to a control panel - is connected to a ➢*Timebase*. As this is only possible when the server is active, you must first start the server via the ➢*Monitor Program* of the Dionex Chromatography Management System.

If the PGM file is connected correctly with a timebase, the edit box (F8 box) will offer exactly the commands required for controlling the instruments on this timebase.

If the PGM file and the timebase were not correctly connected, you will recognize this by the gray coloring of the program lines. It is now possible to edit the PGM file manually, but not via the F8 edit box.

Editing a Program Line

- Position the cursor in the line to edit and press the F8 key.
- The Dionex Chromatography Management System opens the **Commands** edit box (**F8** box) that allows editing the program lines.
- Press **OK** to complete the input, press **OK & Prev** or **OK & Next** to change the command in the previous or next line.

Inserting a New Program Line

- Position the cursor in an empty line or generate one by pressing Enter at the end of a line.
- Press the F8 key.
- Create a command line.

Proceed as follows:

- Choose the instrument (in the following called **Device**) for which you want to edit an instruction. A device can be any instrument of a timebase, but also an installed channel, a relay, a remote input, or the system itself. The icon icon represents a device. Click the preceding **+** character to see details.
- Each device has its own **commands** ( ) and/or **properties** (, , ,).

- As soon as you select a command or a property, further edit fields and a short help text (**Help**) will appear in addition to the retention time field.
- Enter the retention time at which to execute the command.
- Assign the required value (e.g., a number) or a status (e.g., **On**) to the command / property.
- Press **OK** to complete the input, press **OK & Prev** or **OK & Next** to change the previous or the next program line.
- Repeat the input procedure until the PGM file is complete.

Manual Input

Each program can be edited directly, if the corresponding program syntax is known. In this case, the user is responsible for the correct input.

- Perform the **Check** command from the **Control** menu to check the syntax.
- Perform the **Sort On Retention Time** command from the **Control** menu to sort all commands based on ascending retention times.

Input Result

The created command in inserted in the program. To facilitate orientation within a program, commands are displayed in black, triggers in blue, and comments in green print.

The input procedure via the F8 key prevents entering invalid command syntax. If The Dionex Chromatography Management System finds an unknown or wrong syntax, the corresponding line is displayed in red print.

- Via F4/Shift+F4, you can browse through the errors to correct wrong input.

After a short period, new users will be able to create clever and efficient programs. An example is the control of a fraction collector depending on the signal height *and* flank slope of a peak.

For further details, see **Control (Programmed)**:

Program Syntax

Program Wizard

For practical tips, see **How to ...:**

Actions in the PGM Editor **Creating a Program**

Device Control **Extending a Program**

Program Syntax

For uniform operation by different users, ⇒*Control Commands* are always entered in English. The commands of a ➢*Program* are based on the following pattern:

```
Retention Time     DeviceName.Command
```

or

```
Retention Time     DeviceName.Property      =    Value
```

If you are not familiar with the program syntax, use the **Program Wizard** (see the following topic) that guides you through program creation.

Note: The syntax of the commands differs from the syntax of the GynkoSoft data system! For information, see **How to ....: Actions in the PGM Editor Differences from GynkoSoft**.

When opening "old" GynkoSoft program files, the commands used are automatically converted into the syntax of the Dionex Chromatography Management System. If a command cannot be converted, a corresponding comment will be included in a separate comment line.

Time Value (Retention Time)

The time value is entered at the beginning of the control command. It determines when the command is to be executed. The information is entered in ➢*Industry Minutes*, for example,

```
2.500
```

This input is optional. If no time is entered, the time specified in the previous program line will be used.

Device

Devices are all instruments, channels, relays, or remote inputs that are available in the current timebase. They can be recognized in the F8 dialog box by the device symbol (). Each **Device** has a number of commands and/or properties.

As various instruments can have the same commands or properties, adding the device name in front of the command makes a distinction. The syntax is as follows:

```
Retention Time     DeviceName.Command
```

or

```
Retention Time     DeviceName.Property              =    Value
```

If no confusion with other commands or properties is possible, the device name can be omitted (e.g., the **Flow** command when only one single pump is installed). The syntax is:

```
Retention Time     Flow                             =    Value
```

Command

Commands are represented in the F8 edit box by an exclamation mark (). If a command can be clearly assigned to an instrument, the name is sufficient for identification:

```
2.500    NeedleUp
```

The ⇒*NeedleUp* command exists for the Dionex Autosampler GINA 50, only. In this case, the device name can be omitted. This is in contrast to:

```
2.500    UV_VIS_1.AcqOn
```

The ⇒*AcqOn* command by itself is not unique (if there is more than one channel in the system). To address one specific channel, the channel name must be added to the command.

In addition, commands can be extended by additional parameters, for example:

```
2.500    ⇒Inject          Position = 20, Volume = 30  or
2.500    Relay1.On        Duration = 20
```

The possible command extensions are predefined as well as their order. They are listed in the F8 edit box. As no confusions are possible here, the following syntax is also valid:

```
2.500    Inject           20, 30                    or
2.500    Relay1.On        20
```

Device-Independent Control Commands

If a command cannot be assigned to a **Device**, it is listed in the F8 edit box by itself. This applies to the commands ⇒*Branch*, ⇒*Log*, ⇒*Message*, ⇒*Protocol*, ⇒*Wait*, ⇒*Delay*, ⇒*Trigger*, ⇒*EndTrigger* and ⇒*End*.

For further details, see **How to ...: Device Control**

Trigger Commands

Mixed Commands

Property

Properties are distinguished by their value. Values predefined by the system (e.g., On, Off, Auto etc.) are represented in the F8 edit box by an I/0-symbol (). Freely selectable values are indicated by the -symbol. A command string is also considered a property (), e.g.:

```
2.500    UV.Lamp                = On              or
2.500    UV_VIS_1.Wavelength    = 300
2.500    %A.Equate              = "%A"
```

If a property gives an actual value (e.g., Pressure (bar), %A (%), Signal (mAU) etc.), this is indicated by a separate symbol (). Properties in connection with the actual value are subordinate to it. For example, the Dionex Chromatography Management System enables the output of the current system pressure (pressure) and the definition of an upper and lower

pressure limit (UpperLimit and LowerLimit). Assigning a solvent name is via the same method (%B, Value, Equate). The corresponding syntax is:

```
2.500    pressure.UpperLimit     = 350
2.500    pressure.LowerLimit     = 20
2.500    %B.Value                = 30
2.500    %B.Equate               = "Methanol"
```

Here the same applies: if the syntax is not clear, the device name must precede the command or property, e.g.:

```
2.500    UV_VIS_1.Signal.UpperLimit     = 500
```

Text, Names

Before, after, or between individual commands, comments on the program or individual commands can be included. The comment lines are started by a semicolon ";."

```
;        The following program ...
```

Text that is displayed on the screen because of a command and is then included in the Audit Trail, as is the case of the commands **Protocol**, **Message,** or **Equate**, must be placed in quotation marks.

```
2.500    Protocol      "Test program"
```

If these commands are entered via the F8 edit box, the quotation marks are added automatically.

Program Wizard

The Program Wizard facilitates creating a ➢*Program*. To start the Program Wizard, select **New** from the **File** menu. Then, select **Program File**.

In single steps, the complete necessary information is collected to generate a basic program. Each step consists of a template in which the user enters or selects data. Depending on the installation, different steps are required. With a typical HPLC timebase, the Program Wizard offers the following steps:

Step 1: Selecting a ➢*Timebase*

Step 2: Selecting the temperature settings (if supported)

Step 3: Selecting a flow system

Step 4: Determining a gradient profile (option)

Step 5: Determining channels and duration of the data acquisition

Step 6: Determining signal parameters for the individual channels

Step 7: Completing the Program Wizard

From the information entered in Steps 1 to 6, the Dionex Chromatography Management System creates an operable program by adding the ⇒*Inject* and ⇒*End* commands. This file is displayed in the PGM editor window.

Pressing F8 opens a dialog box that allows you to edit the program after closing the Wizard even if you are not familiar with the program syntax. Users familiar with the  **Program Syntax** (Control (Programmed) topic), can freely modify or extend the created file directly via the keyboard. Then, the ➢*PGM File* is saved using the **Save as** command of the **File** menu.

Data

Data: Overview

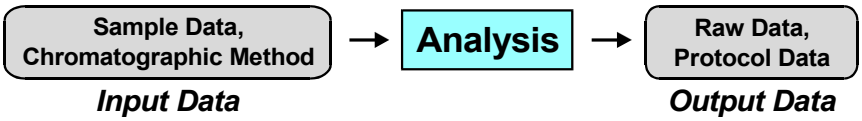
Input Data

For the analysis of a sample and for documentation and archiving purposes, various types of input data are required, which the user must determine or enter before starting the analysis.

These include e.g. the sample name, weight, injection volume, chromatographic conditions (solvent, flow, detection wavelength, connected devices, etc.), as well as the run time. A distinction is made between:

- Data describing a sample (➢*Sample Data*),
- Data describing a sequence (➢*Sequence Data*, usually entered automatically), and
- Data describing the chromatographic treatment of a sample (➢*Chromatographic Methods*).

The user input data serves as the basis for the analytical process.



Output Data

The data recorded during analysis is referred to as output data. Output data includes:

- Data provided by the analysis process itself (analysis and ➢*Raw Data*)
- Protocol data on the analysis (➢*Audit Trail*).

Due to this variety of data types, systematic data organization, and **Data Storage** is especially important.

Datasource

The term ➢*Datasource* is used for the top level of the directory structure displayed in the ➢*Browser*. The Browser is also the tool for handling datasources. Each datasource is based on a separate database. When setting up a datasource, a path to an existing database is entered or a new database is created.

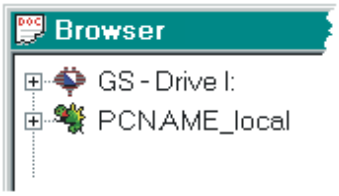
- Choose the **Datasources** command of the **File** menu to set up a datasource. For detailed information on the required steps, see **How to ...: Actions in the Browser Setting up a Datasource**.

The Browser indicates only the name of the *datasource*, not the name of the underlying *database*. The type and number of the datasources visible to the user determine the data that can be accessed. This simplified representation offers the following advantages:

- Data is always accessed in the same way. The user does not have to worry about the data's actual storage location in the network. Entering the path is not necessary. The location is specified when the datasource is created.
- Each user can take advantage of a database without having to deal with special database programs.

Database Formats of a Datasource

The Dionex Chromatography Management System supports several database formats. In addition to the most frequently used Access database format (mdb container), the data system's ➢*ODBC Capability* enables handling SQL ("Structured Query Language") or database formats such as ORACLE and SQL servers. "Old" GynkoSoft directories ("drives") and third-party data can be displayed as if they were datasources with an underlying database. GynkoSoft and the datasources of the Dionex Chromatography Management System are easily recognized by their different symbols (see figure).



GynkoSoft - Datasource
local CHROMELEON datasource

When installing the Dionex Chromatography Management System, a default datasource is created automatically on each client PC. Its name is derived from the computer name (assigned during the installation under Windows installation) and the addition **Local**. This guarantees that each user has a separate datasource in which "personal" results and data are stored. For single systems and for users that do not have additional access rights within a network, this is the only possibility for data storage. Raw data of each manually performed analysis is stored here. Therefore, do not delete the datasource <PCNAME_LOCAL>!

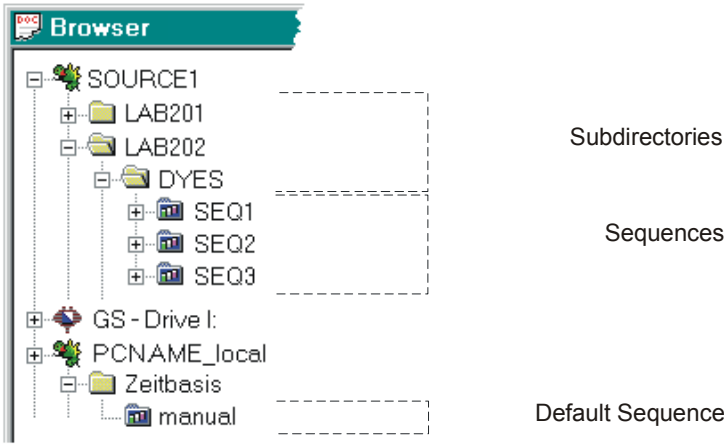
Directory Structure of a Datasource

Each datasource can be equipped with any number of hierarchically organized subdirectories via the **File / New Directory** commands. The result is a data tree similar to the MSDOS data tree.

Caution: Do not use special characters (e.g. umlaut) for new directory names or sequences, as this may cause problems in Novell networks!

Caution: Actions performed in the Browser, e.g. creating datasources or directories, require complex operations below the user interface and cannot be compared to or performed by the Windows Explorer! The representation of directories and data also differs considerably from the Explorer.

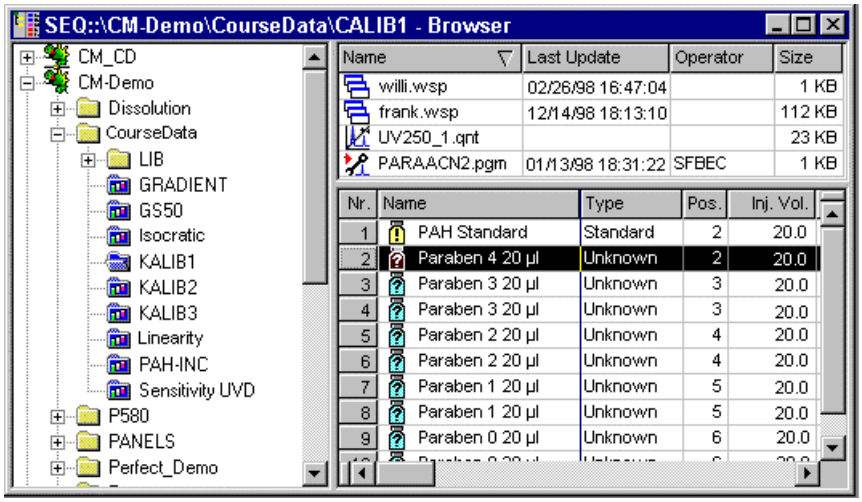
The following illustration shows three example datasources as well as their different directory structures.



Below the datasource **SOURCE1**, the user created the subdirectories LAB201, LAB202, and DYES. The **DYES** directory offers the ➢*Sequences* **SEQ1**, **SEQ2**, and **SEQ3**.

The default datasource **PCNAME_local** has a subdirectory with the name of the timebase installed on this computer, in which there is the default sequence **manual**.

When a sequence is selected, its "inner life" is visible in the right-hand Browser window. The three parts of the Browser window are displayed: the file structure (control programs ( ), quantification methods ( ), report templates, etc.), the sequence information, the samples (standard samples ( ), and unknown samples ( ), etc.). The presentation is described in the **Browser** section. For information on the functions and significance of sequences, see the **Samples and Sequences** section and the **Sample List (Sequence Table)** topic.



Subdirectories, sequences, and chromatographic methods can be moved via **Drag & Drop** within a datasource, but also between datasources of different types. This copy process can also change the underlying database! If you want to actually move a sample, note that the original sample must be deleted in the Browser after the copy process.

Caution: **Drag & Drop** operations can be executed exclusively via the ➢*Browser*. Actions outside of the Dionex Chromatography Management System, e.g. in the Windows Explorer, will result in data losses!

Locking Datasources, Directories, and Sequences

To protect data and results, the Dionex Chromatography Management System offers the possibility to lock datasources, directories, or sequences. If the **Locked** status is enabled, it is not possible to modify the corresponding object. This also applies to all objects below the locked one. If, for example, a datasource is locked, all contained directories and sequences are also locked. Locked items can be recognized in the Browser by the red lock on the icon (/ /).

To lock an object proceed as follows:

- Select the object in the Browser.
- Choose the **Properties** command via the context menu and activate the **Locked** check box in the edit box.

Repeat these steps to undo the operation.

Note: Locking and sharing objects are subject to the **Access Control** and can only be performed by users who have the corresponding privilege.

In addition to locking datasources and directories via the **Locked** check box, access to these items can be controlled by adding them to or removing them from ➢*Access Groups*.

- Select the object in the Browser.
- Choose the **Properties** command via the context menu, and define the Access group assignment via the **Add** and **Remove** buttons.

Access to datasources and directories is only possible for users who are members of an A-group listed in the **Access Groups**.

Data Acquisition, Sensitivity, and Detection Limit

Even the best method of **Data Storage** is only as good as the quality of the stored data. Therefore, data acquisition plays a very important role.

Data acquisition starts with the quality of the used detector, it comprises all components participating in the data flow and is concluded with processing the data in the data system.

The best results are obtained with a detector that is capable of communicating digital signals via a **Serial RS232 Interface**. Detectors that supply analog signals have to rely on precise conversion of the signals. The product range available from Dionex includes an extremely sensitive and low-noise A/D converter. The A/D converter guarantees highest precision with minimum noise.

The detection limit, i.e. the lowest concentration that is just distinguishable from zero (➢*Blank Run Sample*), is reached when the signal to noise ratio is smaller than 2.5. The signal height of a peak is than less than 3 times the signal ➢*Noise*. The lower the noise during analysis, the lower the detection limits. In contrast to sensitivity, the detection limit depends on the instruments used. Sensitivity is the smallest difference in substance concentration resulting from the method itself, i.e. by the slope of the calibration curve.

Data Acquisition with Detectors without Separate Drivers

In addition to the device drivers for Dionex detectors, the Dionex Chromatography Management System offers many drivers to control third-party detectors. (For an overview on the different manufacturers whose devices can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**

In addition, detectors for which separate device drivers are not available can acquire data. Please use the driver **Integrator Driver**.

For information on how to install the device drivers, see **How to ...: Actions in the Server Configuration** **Changing the Server Configuration**

Data Storage

For fast and efficient access to specific data, intelligent storage, and organization of the complete data is very important. The Dionex Chromatography Management System solves this problem by storing data and files in different locations. Databases and sequence directory are available for this purpose. Both are part of the **Datasource**.

Storage in a Database

Data that can be compared across sequences is stored and managed in a relational, ➢*ODBC*-capable database. This applies to the entire ➢*Sample* and ➢*Sequence Data*. The advantage of this type of data management is not only the comfortable integration in other applications such as Excel, Access, dBase, etc., but also the efficient searching and sorting capabilities.

A ➢*Query* allows finding all samples processed on a certain day, created by a certain user and/or carrying a certain name.

Storage with the Sequence

The entire data describing the chromatographic treatment of a sample or data recorded during the analysis is stored in a ➢*Sequence*. This includes control files (➢*PGM File*) and evaluation parameters (QNT method), but also the entire raw and protocol data (see **Raw Data Storage**).

History (File History)

- Select a datasource in the **Browser** and activate the **Enable Modification History** options from the **Properties** of the context menu.

When the ➢*History* **Mode** is activated, the Dionex Chromatography Management System prompts the user for a comment on the modification or operation before saving any modified object. This allows documenting all performed modifications together with the user name and the object name. In combination with the **Copy**, **Create**, and **Save as** commands, the comment is entered automatically.

Objects can be samples, sequences or datasources, ➢*Control Panels*, ➢*Report Definition Files* (RDFs), ➢*PGM Files* and/or ➢*QNT* files and modified chromatograms.

- Select a datasource or a single directory and perform the **Show History** command of the context menu to see all objects that were modified and that received a comment.

Depending on the filter you use, the Dionex Chromatography Management System will show a list of all objects that were modified within a certain period and/or by a certain operator.

- Select an object from the list and press the **Details** button to view information on an object.

The comment entered by a user when storing an object can be modified later by the same user (and only by this user). The user must have the corresponding modification privilege as a member of a ➢*Privilege* group. Enabling and disabling the History Mode is also via the corresponding privilege.

Data Export

The Dionex Chromatography Management System offers various options for data export to enable communication with other programs:

1. You can export report pages from the ➢*Browser* with the **Batch Report** command of the **File** menu. Clicking the **Export** checkbox opens the dialog box **Batch Setup** where you can export the respective report pages in five different formats:
   a) ANDI/Chromatography - ➢*AIA* (*.cdf)

b) ASCII text format (*.txt)

c) Excel file format (*.xls)

d) Adobe Acrobat file format (*.pdf)

e) Archive format (*.cmb) of the Dionex Chromatography Management System

2. A modified version of the **Batch Setup** dialog box can be opened in the **Printer Layout**. This box offers the same functionality as the box that is opened in the Browser.
3. In addition, raw data can be exported in the AIA format from the Browser via the **Export/Backup** command under **ANDI/Chromatography (AIA)** (Also, see **Raw Data Export**)

If you wish to send data of the Dionex Chromatography Management System to another laboratory e.g. via e-mail, we recommend executing a **Backup** first and transmitting the compressed data in the archive format of the Dionex Chromatography Management System.

Backup

To avoid unforeseen data losses that can occur for example due to a defective hard disk, we recommend to regularly backup the saved data on a different data medium using the **Backup** command in the **File** menu of the ➢*Browser* (see **Actions in the Browser** **Creating Backup Files**).

Backup data is compressed, i.e. "packed" and stored in a different location. For security reasons (GLP does not allow modification of backup data), direct access to the data is not possible. The data must be "unpacked" via the **Restore** command in the **File** menu of the Browser (see **Actions in the Browser** **Restoring Backup Files**).

The backup logs each single file that is copied and issues warnings if errors occur. The directory structure is maintained.

Raw Data

All analog or digital values measured by a detector and stored digitally on the PC are referred to as raw data. Raw data only exists for those signals or channels that were selected by the user before the analysis!

The extent and the precision of the stored raw data depend on the selected ➢*Sampling Rate* or ⇒*Step*.

For further details, see

Raw Data Storage

Raw Data Compression

Raw Data Storage

Raw data storage refers to saving the signals received from a detector in digital form. Other important data is also stored, e.g. analysis time, signal unit, number of data points etc.

If a detector is only supplied with an analog output, the data must be converted into digital signals. The A/D converter performs this task.

Storage Procedure

With conventional data systems, an analog value is digitized at a fixed time interval, e.g. a digital value of defined accuracy is stored every second. The number of stored values per second is normally referred to as the ➢*Sampling Rate*. The inverse of the sampling rate (the time interval between two data points) is referred to as ⇒*Step*.

The higher the sampling rate, i.e. the smaller the step, the more data points are stored, and the more exactly the original signal can be restored from the stored data. However, a higher sampling rate has a higher memory requirement. The Dionex Chromatography Management System solves this problem by the step setting **step=auto**. This type of storage requires high algorithmic resources in real time (!), which is justified by the following advantages:

- Raw data files are as small as possible, as fewer data points would result in a loss of precision! If an analysis requires a conventional step width of 0.5 seconds, your Dionex Chromatography Management System can typically acquire such chromatograms with an *average* step width (= chromatogram length divided by the number of data points) of 2

seconds. The compression factor of 4:1 is thus achieved, making optimum use of the available storage capacity.

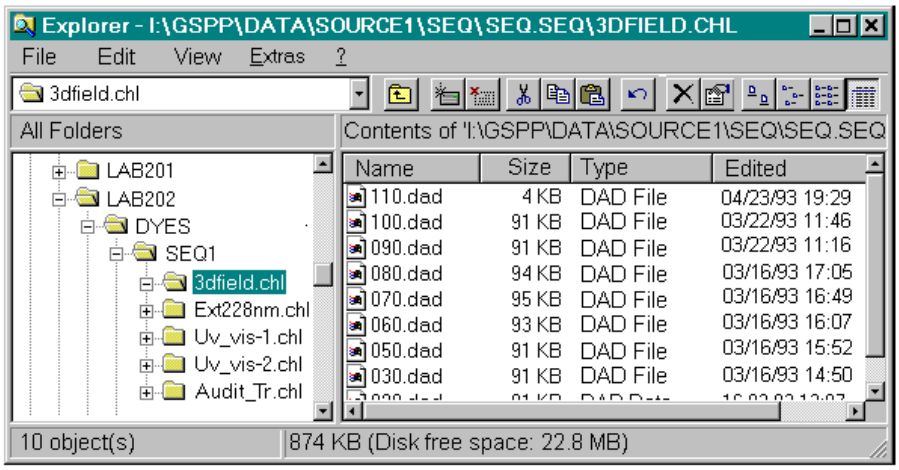
- Despite this minimal file size, maximum integration accuracy is ensured for the given chromatographic conditions, as the continuous signal is approximated to the optimum. Generally, more data points are stored below peaks than with conventional acquisition methods.
- The processing speed, e.g. for peak detection, re-integration, graphical output etc. is significantly higher due to the reduced number of data points.

Storage Location

Raw data is stored in the directory of the current sequence. For each channel that is specified during the installation of the Dionex Chromatography Management System, a separate subdirectory is created. In addition, a protocol data directory is created. The directories are not visible in the Browser.

The reason for this is: the Dionex Chromatography Management System manages the entire raw data automatically. At no time, the user must access the raw data directly.

Viewing this type of data is only possible via the Windows Explorer provided the datasources are not locked. As, however, the datasource names are not displayed in the browser, you must follow the path to the corresponding sequence directory (see figure).



In this example, the channels **3dfield**, **Ext228nm**. **Uv_vis-1**, and **Uv_vis-2** were defined. The protocol data directory **Audit_Tr** was added. If a directory is expanded, the raw data of the corresponding channel is visible.

A separate raw data file is created for each sample in a sequence, for which raw data of a specific channel was recorded.

Caution: Do not modify these directories! Operations outside of the Dionex Chromatography Management System are not permitted! Therefore, we recommend that you protect your datasources to prevent that they are accessed via the Windows Explorer. In the file or context menus of the browser, activate the **Protect Data Set Directory** option on the **Properties** tab of the respective datasource

Raw Data Compression

Storing raw data automatically compresses the data. For the signal value, this is achieved by storing the difference to the next data point instead of storing each data point. Only from time to time, the actual value is stored. This way, the compression is increased by 50%. This effect is especially noticeable in the case of ➢*3D-Fields*.

The size of the raw data file of a 3D-field increases with the number of recorded data points. These depend on the ➢*Optical Resolution* of the detector, the field size (area between the upper and lower limit of the 3D-field) as well as the selected ➢*Sampling Rate*.

At a sampling rate of e.g. two spectra per second (step = 0.5) and an optical resolution of 2nm, this means that 2 x 60 x 70 = 8400 data points per minute must be recorded for the UV range from 200 to 340nm. As each absorption value is recorded with an accuracy of 25bits, a hard disk storage capacity of m x (N+1) x 4 = 70 x ((2x60)+1) x 4 = 33.88kByte per minute is required. The storage requirement for the 3D-field of a "normal" (20-minute) chromatogram is thus 0.678 MByte!

However, by skillful data compression procedures, it is possible to reduce the required storage capacity by approx. 50-60%. This is possible by completely storing approx. each eighth spectrum. Of all other spectra, only the difference to the previous one is stored and is re-calculated, when needed. This procedure is a good compromise between optimum data compression and the required time for restoring a 3D-field.

Note: The compression procedure is not destructive, i.e. the complete data is stored. The 3D-field thus contains the complete information provided by the detector. The data can be restored at any time.

Furthermore, there are three ways to minimize storage capacity requirements:

- Limit the wavelength range to the necessary range.
- Reduce the sampling rate (step) so that no more than 10 to 20 spectra are below the narrowest peak, or select an automatic sampling rate (step).
- Use the possibilities of the ⇒*Diode Bunching*.

Restoring a Chromatogram from Raw Data

When restoring a chromatogram from the raw data, equidistant data points are joined with straight lines. A diagram "resembling" the recorded analog signal is thus created.

Clearly, the resemblance (and thus the precision of integration) is increased with an increasing sampling rate. However, a higher sampling rate requires more storage capacity. When using a fixed sampling rate, the sampling rate must be set so that a minimum of 10 datapoints is stored during the smallest peak in order to integrate the smallest peaks of a chromatogram (generally the

earlier peaks) with the same precision as the larger peaks. This results, however, in huge data volumes especially in the case of wide peaks and long baseline sections.

Using a dynamic sampling rate can solve this problem. The Dionex Chromatography Management System is capable of continuously optimizing the sampling rate during an analysis, i.e. few data points are stored during baseline sections, whereas many are stored below peaks. The local sampling rate is set according to the actual information volume such that the deviation between the resulting diagram and the actual analog signal is never greater (or smaller) than the actual noise component of the signal. This method ensures that neither too many nor too few data points are stored, but always the optimum. The ⇒*Step* values vary between 0.01 and 5 seconds (sampling rate: 0.2 to 100 Hz).

Raw Data Export

The Dionex Chromatography Management System supports exporting raw data by conversion into ➢*AIA* and ASCII formats. In addition, raw data can be exported as a ➢*Backup* file (*.cmb). Use the **Export / Backup** option from the **File** menu to export as an AIA or backup file.

Format	Description
AIA Cat. 2	Samples and peak variables are stored in the AIA format.
AIA Cat. 1+2	In addition to samples and peak variables, the raw data of a chromatogram (each stored data point) is stored in the AIA format.
Dionex Chromatography Management System backup (*.cmb):	All data of a ➢*Sequence* or a ➢*Datasource* are stored in the cmb format.
ASCII	Raw data may be exported in the ASCII format as well. Use the command **Batch Report** from the **File** or context menu. Click **Export** in the dialog box and then select the **ASCII** export format. All raw data from the channels selected for the actual sequence are stored in the ASCII format.

☞ ***Tip***: If you intend to export raw data to other applications or other computers, it may be necessary to use a fixed ⇒*Step* (= equidistant raw data storage) instead of a dynamic step.

It is also possible to export data sheets of the report in different formats (see **Data Export**).

Raw Data Import

Importing the following raw data is possible:

- ➢*AIA* data (*.txt)
- GynkoSoft data
- ➢*LIMS*/➢*Worklist* data (*.wle)
- PeakNet (up to version 5.2) data
- Files in the archive format (*.cmb) of the Dionex Chromatography Management System

In the **File** menu of the Browser, choose **Import / Restore** and the corresponding option. Use **Import** to import any of the above raw data. Use ➢*Restore* to import ➢*Backup* data of the Dionex Chromatography Management System.

In addition, it is possible to install databases from third-party chromatography data systems. Proceed as follows:

- Open the Browser and choose the **Datasource** command from the **File** menu.
- Follow the instructions described under: **How to ...: Actions in the Browser Connecting a Database.**

For details on importing PeakNet 5.2 or earlier data files, see **How to ...: Actions in the Browser Importing PeakNet (Release 4.5 through 5.2) Data Files**.

Raw Data Storage in Case of Power-Failure

The raw data of a sample interrupted by a power failure is not lost, as a raw data autosave is performed continuously during sample processing. The autosave ensures that the raw data is stored on the hard disk in short intervals. The user can reduce the time intervals to approx. 30 seconds. In the case of a power failure, the maximum data loss is thus 30 seconds.

If a power failure interrupts the automatic sample batch, the ➢*Power-Failure Protection* and the power-failure handling ensure that processing is continued

at the same position after starting the system anew. In addition, you can run a power-failure program before to reset the system to a defined state.

If processing is interrupted by warnings or error messages, it is possible to react with an appropriate ➢*Emergency Program*. The system is then in a defined state that is recorded in the ➢*Audit Trail*.

For information on how to develop appropriate programs for both cases, see:

How to ...: Actions in the PGM Editor:

Creating an Emergency Program

Creating a Power-Failure Program

Protocol Data (Audit Trail)

In addition to raw data, the Dionex Chromatography Management System also records the data of the **Audit Trail** (protocol data storage). The following information is included:

- Commands from a control file
- Manually executed commands
- Commands activated by a trigger condition
- Error messages
- Start of sample processing
- New start of the Dionex Chromatography Management System after booting the computer

Each item is stored with the current time. Furthermore, the current program time is added to information during recording of data and processing a sample batch, respectively.

Storage is continuous over a whole workday as well as for the duration of processing a single file. That is why the following distinction is made:

Daily Protocol

Sample Protocol

Audit Trails can be displayed either from the Browser (as daily or sample protocols) or as audit trail control in the control panel. To select extent and type of the display, a display filter (**Normal**, **Advanced**, **Expert**, and **Error**, or **Warning**, respectively) can be chosen by means of the context menu (right mouse click). The display options **Advanced** and **Expert** can only be used for audit trails created with version 4.0 or higher of the Dionex Chromatography Management System.

Daily Protocol

The daily protocol stores the entire GLP relevant data that is related to the status of a specific timebase. This information is displayed in the **Audit Trail Control** of the control panel.

When starting the ➢*Server* of the Dionex Chromatography Management System, the **AUDIT** directory is created in the server datasource below the timebase. The server saves the daily protocol in this directory. The daily protocol receives the current date as the file name (e.g. '19980527.slg' for the daily protocol of May 27, 1998). A new file will be created for each day.

On the right section of the Browser window, the daily protocols are displayed together with their names and the time of their last change. Double-clicking opens the file and shows its content in a separate window. The display corresponds to the audit trail control of the control panels and a printout of the display is possible as well.

In the Browser, you can copy and delete daily audit trails. For both actions, the corresponding user rights are defined in the user mode of the Dionex Chromatography Management System.

Note: In contrast to the GynkoSoft data system, the daily protocol is not overwritten by the protocol of the following day. As the Dionex Chromatography Management System generates a new file for each daily protocol, old protocols that are no longer required should be deleted from time to time.

Sample Protocol

The sample protocol contains the entire audit trail data of the corresponding sample. The sample protocol is part of each default report.

- Display a report in any method window and select the worksheet **Audit Trail** to view the Audit Trail data of the current sample.

The sample protocol can be activated via the **Browser**. Open the context menu of the sample in the Browser. Via **Open**, open a box and then open the sample protocol via **Audit Trail**.

Samples and Sequences

Sample Preparation

Sample preparation is a major part of the chromatographic analysis. It can include simple procedures as weighing, solving, and diluting a sample, as well as more complicated physical (filtration, centrifugation etc.) and chemical separation procedures (liquid-liquid-extraction, fixed phase extraction). Generally, the careful performance contributes substantially to the quality and the reproducibility of chromatographic separations.

Furthermore, the Dionex Chromatography Management System offers two correction factors (➢*Sample Weight* and ➢*Dilution Factor*) that allow using the "approximate weight" as well as defining dilution steps and can thus be used to consider the sample preparation when evaluating the data.

Sample Processing

Sample processing includes three major steps:

- Sample definition (single samples and sequence / batch)
- Analytical procedure (manual or automatic control)
- Evaluation (methods and reports)

The performance of each step primarily depends on the used methods and the available instruments. The working environment could range from a fully automatic sample laboratory with large quantities of samples to single-user applications in a research lab. Easy and quick analysis procedures may be the focus in the first case, while special methods and parameters for peak recognition may have priority in the latter case. Thus, it is not surprising that functions crucial to one group of users may be irrelevant to others.

Consider these facts, when information is presented from different viewpoints in the following sections.

Sample Definition

In the Dionex Chromatography Management System, the term **sample** has a more specific meaning than in normal colloquial use.

Each injection is defined as an individual "sample"!

Multiple injections from the same sample vial under similar conditions are considered several samples.

Defining a sample means the process of determining how much of a substance is injected from which vial and under which conditions, and which evaluation parameters are used. A distinction is made between a single sample and a sample series.

Single Sample

A sample can be analyzed individually by entering all required information and user commands via the keyboard or the mouse.

The user selects the **Inject** command, enters the volume to inject, and performs the injection via a hand-operated valve. If an ➢*Autosampler* is available, the user determines the sample location with the ⇒*Inject* command. Then, data acquisition is started (via the ➢*AcqOn/Off* command). When the end of the sample is reached, the user terminates data acquisition (**Acq Off** command) and specifies where to save the acquired data.

The recorded data is temporarily saved to the **manual** sequence of the default datasource of the system. In network operation, this datasource is designated with the computer name of the user in the network.

As soon as the user terminates data acquisition, the user is prompted to select the final storage location for the temporarily saved data.

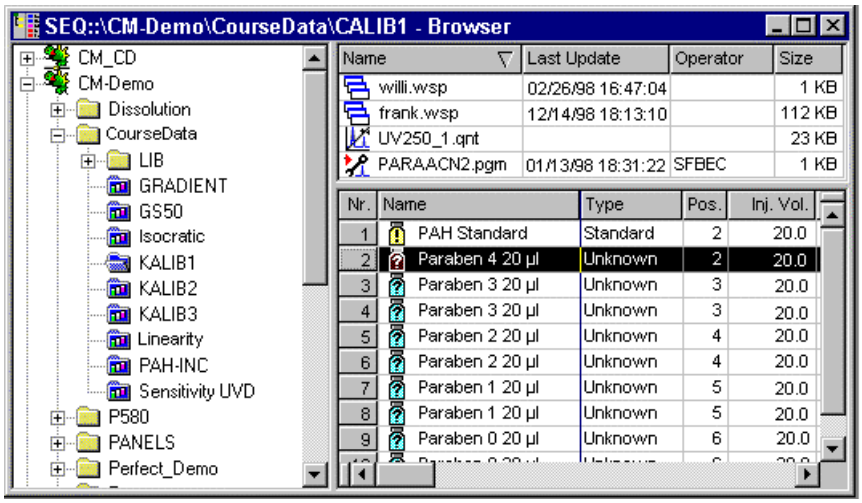
Sequence / Batch

If several samples are to be processed successively, they are included in a sample list (sequence table), together with the instrument control and evaluation information. The samples are then processed by starting automatic ➢*Batch Processing*.

For details on how to create a sample list, see  **Sample List (Sequence Table**).

Sample List (Sequence Table)

The sample list (sequence) is part of the **Browser**. It appears on the lower right window section as soon as a ➢*Sequence* is selected, and it is "read" line by line. One line corresponds to one sample.



A sample is characterized by various column entries. The entries are managed in a database and are referred to as ➢*Sample Data*. A short explanation of each column is displayed upon pressing the F1 key.

The user has to create the list of samples to be processed with the characteristic sample data before each analysis. There are various options:

- Select a cell with the mouse, then change the cell input via the keyboard.
- Select a cell with the mouse, press F8 to open an edit dialog box facilitating data input.
- Open a similar, existing sequence table and modify the input.
- Automatically generate a sequence table via the **Sequence Wizard**.

Having entered all relevant information, the sample list is saved under a unique name using the **Save as** command in the **File** menu.

In addition to "real" sample data, e.g. the sample name, the injection volume, the vial, and the sample type (**unknown** or **standard**), especially the **Program**

File and **Method** columns are important for the analysis procedure. Entries here refer to specific ➢*Chromatographic Methods* determining the performance of the analysis. These include programs (**Control Program**) required for fully automatic control of analytical instruments as well as evaluation instructions (**Overview: Quantification Method**) determining the integration and calibration.

The number of samples per sequence is not limited, but it should exceed 100 only in exceptional cases. The fewer samples are added to a sequence, i.e. the more sequences are created, the faster single samples can be accessed and the easier it is for the user to keep track of the processed samples. Criteria for combining several samples in one sequence could be, for example, the same analysis conditions, the same origin, the samples of the same day etc.

For detailed information on how to create a sample list, see **How to ...: Actions in the Browser Creating a Sample List (Sequence Table**).

Sequence Wizard

The Sequence ➢*Wizard* helps you to quickly create a basic sample list consisting of analysis and standard samples. The **Sequence Wizard** is opened via the **File/New** command in the Browser. Creating a ➢*Sequence* is performed in five easy steps (for further information see links below to the respective topics in the Online Help):

- Step 1: Selecting the timebase
- Step 2: Generating the analysis samples
- Step 3: Generating the standard samples
- Step 4: Determining the ➢*PGM File* and the analysis method
- Step 5: Saving the sequence and assigning a name

Also, see the Online Help for a detailed description of the mentioned steps .

Each step is performed in a separate input screen. Press one of the two arrow buttons (<Back, Next>) to browse through the input screens.

Press the <Finish> button in the fifth step to save the sequence and close the wizard.

Caution: Do not use special characters (e.g. umlaut) for new directory names or sequences, as this may cause problems in Novell

networks!

Note: In future versions of the Dionex Chromatography Management System, including validation and/or blank run samples with the **Sequence Wizard** will also be possible.

Automatic Batch Operation (Online Batch)

The enormous technical complexity of modern chromatography systems, the resulting high purchasing costs and the constantly increasing number of samples in analysis laboratories make continuous operation even outside of regular working hours a necessity. Thanks to ➢*Autosamplers*, very efficient PCs, and modern data systems, this has become routine. The user merely provides "replenishment."

When the actual sample preparation is completed, the chromatographic conditions of processing, the samples to be processed and in which order must be communicated to the data system. This is performed in the sequence table. The result is stored as a ➢*Sequence*.

Independently processing one or several sequences is known as ➢*Batch Processing*. To start processing, the following steps are required:

Starting the Automatic Batch

After data input is completed, the analytical process can be started in an online batch.

- Open a control panel and choose the Edit command from the Batch menu.
- Enter the names of the sequences containing the samples to be analyzed.
- Perform a ➢*Ready Check*.
- Start the analysis process by pressing the **Start** button.

Processing the Automatic Batch

As soon as the online batch is started, all samples of the sequence with the status **single** or **multiple** are analyzed successively. If a sequence contains a sufficient number of samples, sample processing "around the clock" is possible.

Instead of including all samples in one sequence, they can be distributed on several sequences. Accordingly, more sequences are then entered in the batch dialog (max. 16).

This list can be considered a batch; it is also referred to as online sample batch or online batch. The order of the sequences determines the order of processing, i.e. when starting the batch process, samples 1 to n of the first sequence, then samples 1 to n of the second sequence are analyzed.

Saving the Results

The results of the online batch are saved with the individual samples.

Sample Evaluation

In spite of largely automated work processes and intelligent pre-settings, it is within the responsibility of each user to set the framework conditions of sample evaluation.

Calculations

As in the case of sample processing, which is performed based on a program (➢*PGM File*) previously created and included in the Sample List, the analysis results are calculated based on the evaluation method indicated in the Sample List. The method itself is created in the **QNT Editor**.

Result Output

The result of sample processing can be represented in graphics and tables, either on the screen or in a printed output. The Dionex Chromatography Management System provides method windows for generating this output. In the **Printer Layout**, templates can be defined for standardized presentations of the sample results.

For a list and detailed description of available method windows, see **Data Reprocessing**.

Electronic Signature

During the last decades, quality assurance and ➢*GLP* have become increasingly important with the data verification being one of the key aspects. Especially ➢*Raw Data* must not be modified later. In addition, the results,

which have been generated from the raw data, should not be modified without asking once they have been accepted. Contrary to the data system, this can be achieved with a printout in part, only.

If the ➢*CmUser* mode is activated, the electronic signature allows you to sign the results from your raw data that is important within the scope of quality assurance and GLP. In this way, you can sign and save ➢*Sequence* reports that have been accepted as correct so that the current state of your results is "frozen".

Note: Electronic signature is available for user databases only that were created with a CmUser program version 6.10 or higher. Update your database if an error message notifies you that electronic signature will not be possible.

Electronic signature includes three steps:

- Submit
- Review
- Approve

Typically, the report will be signed and **submitted** by the user who created it. Having **reviewed** the report, the laboratory manager will sign it. Finally, the quality assurance manager can **approve** the results.

For information how to electronically sign reports see **How to ...: Actions in the Browser Signing Sequences Electronically**.

Theory of Calibration

Calibration: Overview

The signal of an HPLC Detector is suitable for quantitative determination if it is proportional to the concentration of a substance in the flow cell. This characteristic is for example offered by the absorption supplied within the range of validity of the Lambert-Beer law by a UV detector.

The corresponding proportionality constant does not only depend on the chemical quality of the substance in question, but also on the physical properties of the used detector. For UV detectors these are, above all, the optical wavelength and the spectral bandwidth. As integration programs can only determine the area (and height, respectively) below a peak, conversion into absolute amount or concentration units is only possible if a *calibration* was executed before the analysis.

For details, see the topics below:

Principle

Calibration Types (Linear)

Calibration Types (Non-linear)

Using the Calibration Curve

Calculating the Calibration Curve

Standard Methods (External / Internal / ...)

Evaluation with Various Standard Methods

Implementation

At the end of a calibration, the Dionex Chromatography Management System creates calibration curves from the available calibration points for each calibrated substance. Representing and evaluating the curves is performed in the method window

Calibration Curve

Principle

The principle of the calibration is based on that one or several samples of known composition are analyzed by chromatography and a conversion factor amount (or concentration)/ area is calculated from the detected areas below the individual peaks and the known amounts or concentrations. This factor can then be used to multiply the area of the respective peak of an unknown sample. The result is the corresponding amount of the substance (or concentration of the substance). However, this simple method will work only,

- if the relation between amount and area is strictly linear (i.e. if, e.g. for UV detectors, the Lambert Beer Law is applicable) and
- if the area zero equals the amount zero, i.e. the calibration line leads through the origin (no offset).

If the detector signal S is proportional to the concentration (K) of a dissolved substance, the proportionality factor c1 applies:

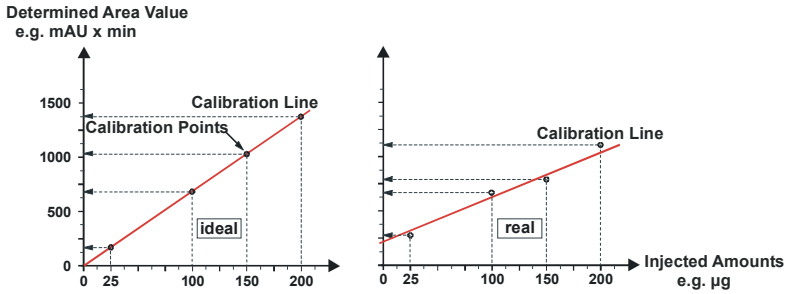
$$S = c1 * K$$

Under certain conditions, the area F(x) corresponding to a certain amount (x) is proportional to the contained amount.

$$F(x) = c1 * x$$

If a sample of the substance A of known concentration (the standard / calibration sample) is analyzed chromatographically, the result is a specific ratio between the injected amount and the determined area value. The result can be graphically presented by entering the value pair in an amount / area diagram. In this diagram, each injection corresponds to one ➢*Calibration Point*.

Ideally, all calibration points are located on a straight line, and there is a direct ratio between the amount and the determined area. The "conversion factor" corresponds to the slope of the calibration line (left fig. "ideal").



During each calibration, deviations from the ideal behavior might occur which are above all caused by weight and/or dilution errors. This causes scattering of calibration points. Therefore, the Gaussian method of the least squares (see **Calculating the Calibration Curve**) is used to calculate a regression line. This line is defined as the best approximation to the existing calibration points and, usually, it does not go through the origin (right fig. "real").

If the various calibration points are not located on a straight line, but show a parabola or exponential shape, the slope of the curve and the distance to the zero point (**offset**) describe the corresponding (approximate) curve (**calibration curve**). The basic mathematical function is referred to as ➢*Calibration Function*; the coefficients are the calibration coefficients.

By selecting the ⇒*Calibration Type* peak table variable, the user decides whether a linear or a non-linear calibration curve is calculated from the existing calibration points. The following distinction can be made:

Calibration Types (Linear)

Calibration Types (Non-linear)

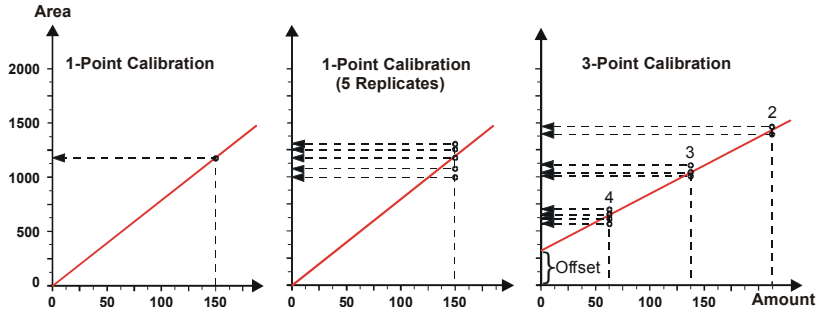
Calibration Types (Linear)

If one calibration sample of a standard substance is analyzed for calibration only, the user enters exactly one concentration value in the first ⇒*Amount* column of the peak table. The result is exactly one ➢*Calibration Point*. Connecting the calibration point with the origin then forms the calibration curve.

It is described by the function derived from the Lambert Beer law:

$$F(x) = c_1 * x$$

The slope of the line corresponds to the proportionality factor c1 (left partial fig.). C1 is also called RF value.



If one calibration sample is analyzed several times, several points can be entered in the amount/area diagram. The points of one concentration are called **replicates**. With an increasing number of available replicates, the impact of imprecision decreases after averaging. In spite of several replicates, only one amount/area ratio is determined. This is referred to as **multi-point calibration on one calibration level** (in the middle of the partial fig.).

The result is better secured if several concentrations are measured instead of one. Of course, several replicates can be used per concentration. As a result, calibration points at different concentrations are received in addition to the replicates of one concentration. This is called a **multiple point calibration on several levels** (e.g. 3-level calibration (see right partial fig.)). The calibration curve does not necessarily have to go through the origin. The linear ➢*Calibration Function* is therefore corrected by an offset.

$$F(x) = c_0 + c_1 * x$$

Caution: The decision whether a calibration type differing from the **linear** default is physically sensible, is within the responsibility of the user, not the data system!

Calibration Types (Non-linear)

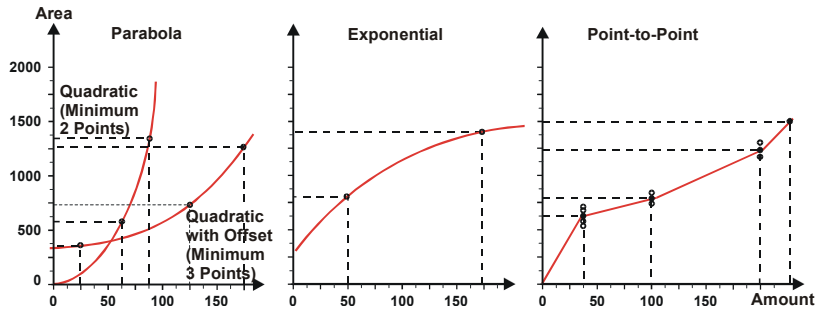
In (the more general) case of a non-linear calibration, further terms are added to the linear ➢*Calibration Function*.

Parabola-shaped curves are described as follows:

$$F(x) = c_1 * x + c_2 * x^2 \qquad \text{(Quadratic)}$$

$$F(x) = c_0 + c_1 * x + c_2 * x^2 \qquad \text{(Quadratic with offset)}$$

To calculate curves of this type, a minimum of two (quadratic) or three (quadratic with offset) calibration samples must be available (left partial).



The power function is described as follows:

$$F(x) = c_0 * x^{c_1}$$

To calculate curves of this type, a minimum of two calibration samples must be available (right partial fig.).

If none of the above described functions can be applied to the available ➢*Calibration Points*, the calibration curve can be described as a polygon, i.e. a linear interpolation between two adjacent calibration points (**Point to Point**). If several replicates of one calibration level are available, these are averaged before interpolation.

Caution: The decision whether a calibration type differing from the **linear** default is physically sensible, is within the responsibility of the user!

Caution: A large number of replicates increases the precision and the reliability of the curve at this point (on the calibration level), but is not decisive for the entire curve. The more calibration levels are examined, i.e., the more standards of different concentrations are measured, and the more precise is the area/amount allocation for a larger range. To be exact, the calibration is valid for the range of the calibration samples only and not beyond it.

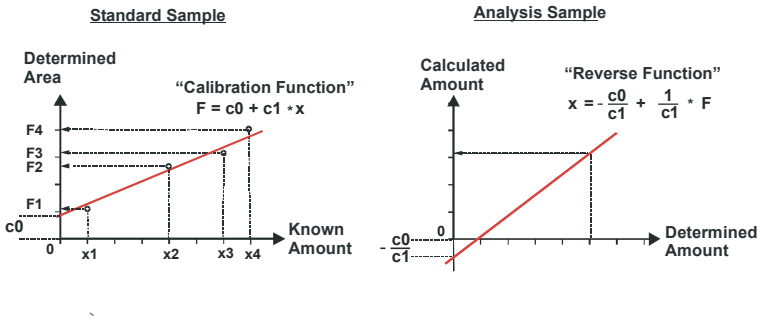
Using the Calibration Curve

If the calibration coefficients are known, the amount value can be calculated for any area value by inserting the coefficients in the formula of the respective calibration type.

Within the range of the curve that is covered by the calibration points it is possible to convert any peak area into the corresponding amount. This is shown in the following example:

Standard Sample

The user enters the amounts (x1 to x4) of the different standard samples and determines the ➢*Calibration Function* by selecting the calibration type (here: linear with offset). Depending on the selected integration type, area values (F1 - F4) are established from the detected peaks. One area and one substance amount value form one calibration point. The positions of the calibration points determine the curve that the Dionex Chromatography Management System calculates with an approximate method. The final course of the calibration curve is determined by the calibration coefficients (here: c0, c1).



Unknown Sample (Analysis Sample)

In the case of an unknown sample, the previously calculated calibration coefficient and one or several area values are known. The area value is now a known parameter and is thus drawn in x-direction. In the diagram, the two axes must be exchanged for one another. As a result, the calibration function must be converted in its inverse function. This is also performed by the data system. Now, the amount can be calculated by inserting the calibration coefficients and area values.

Furthermore, the exclusion of outliers, the different weighting of calibration points, and the formation of "averaged" calibration points from one calibration level, offer additional ways of calculating the calibration curve.

Calculating the Calibration Curve

Calculation of the calibration curve (➢*Calibration Function*) is based on the method of least squares. With a given calibration type (linear, linear with offset,...), the parameters of the calibration curve F(a), i.e. c0, c1, and c2 are determined so that the sum of the squared distances of all measured points becomes negligible. For this purpose, the following optimization problem is solved:

$$\sum_{i=1}^{n} w_i * (x_i - F(a_i))^2 \rightarrow \min$$

(xi- F(ai)) refers to the distance of the xi-value from the calibration curve F(a), wi is the selected weighting (see ➢*Weights*, e.g. wi=1, wi=1/Amount or wi=1/Amount^2) and xi is the actual value.

Standard Methods

Calibrations can be based on an external or ➢*Internal Standard ("ISTD")*. **External standard** means that there is a separate standard sample. Using an **internal standard** means adding the standard to the unknown sample. This can be either before (**External/Internal**) or after (**Internal**) sample preparation.

Standard	Description
external	= Default setting. Calibration is via one or several standard samples. Via the amount values entered in the **Amount** column, a ratio is established between the area and the amount. On this basis, the amount in samples of unknown concentration is determined via the peak area. With an increasing number of different amounts, the area/amount ratio (=calibration curve) can be determined more exactly. If different amounts are obtained by diluting the original substance, a ➢*Dilution Series* is resulting. The amount of each concentration is entered in a separate amount column in the corresponding line of the peak table. If the calibration is performed with a single standard sample by injecting different volumes (**Var.InjectVol.**), only the amount of the original sample is stored in an amount column. The remaining amount values (for the different injection volumes) are calculated by the data system.
internal/ external	As ➢*Internal Standard ("ISTD")* choose a substance with a retention time behavior similar to the behavior of the substances to be analyzed. Before the sample preparation, an internal standard is added to all samples (unknown and standard samples) in exactly the same amount so that the concentration is identical in all samples. For example, diluting the sample or performing a pre-column derivatization later will change the concentration of the internal standard. During calibration, the internal standard and the substances to be determined are calibrated.
internal	In the pure internal standard method, calculation is via area and amount ratios instead of absolute areas and amounts. For this procedure, it is necessary to inject a constant amount of the ➢*Internal Standard ("ISTD")*, i.e. the internal standard is added before the sample preparation. In a dilution series, the standard does not have to be diluted (**Const. Internal Standard**). Due to the equivalent amount of added internal standard, the same ISTD result should be achieved for all samples. Forming the ratio of ISTD values allows drawing conclusions about the precision of the analysis and calculating the actual result. Due to the intense experimental procedure, this type of calibration is rarely used in HPLC.

For examples of the different standard methods, see **How to ...: Actions in the QNT Editor Calibration**.

Evaluation with Various Standard Methods

The following describes how the Dionex Chromatography Management System calculates calibration points which form the basis for any calibration function F. Please note that there are differences depending on the selected standard methods (External, Internal/External (with/without Var.ISTD), Internal (with/without Var.ISTD)).

For evaluating unknown samples, i.e. calculating the ⇒*Amount* values, the inverted form of the corresponding ➢*Calibration Function* F is used (=inverted function A). This means that the c0, c1, and c2 calibration coefficients form function A that is inverted for amount calculation. The result is F.

'External' Evaluation:

Calibration:

- Y(i,k) = RESPONSE(i,k)
- X(i,k) = AMOUNT_NOMINAL(i,k) ∗ (WEIGHT(k)/DILFAC(k)) ∗ (INJECTVOL(k)/REFINJECT)

Evaluation: Calculation of the Amount peak variable for peak i in the sample x

- AMOUNT(i,x) = F(RESPONSE(i,x)) ∗ (DILFAC(x)/WEIGHT(x)) ∗ RSP-FACTOR(i)

Description: see below.

'Internal' Evaluation:

Calibration:

- Y(i,k) = 100 ∗ (RESPONSE(i,k)/RESPONSE(ISTD,k)
- X(i,k) = AMOUNT_NOMINAL(i,k) ∗ (WEIGHT(k)/DILFAC(k))

Evaluation: Calculation of the Amount peak variable for peak i in the sample x

- AMOUNT(i,x) = F(100 ∗ (RESPONSE(i,x)/RESPONSE(ISTD,x)) ∗ (DILFAC(x)/WEIGHT(x)) ∗ RSP-FACTOR(i)

The ISTD peak itself will not be evaluated!

Description: see below.

'Internal' Evaluation (with variable ISTD):

Calibration:

- Y(i,k) = AMOUNT_NOMINAL(ISTD) * RESPONSE(i,k)/RESPONSE(ISTD,k)
- X(i,k) = AMOUNT_NOMINAL(i,k) * (WEIGHT(k)/ DILFAC(k)) * (INJECTVOL(k)/REFINJECT)

Evaluation: Calculation of the Amount peak variable for peak i in sample x

- AMOUNT(i,x) = F(AMOUNT_NOMINAL(ISTD) * (RESPONSE(i,x)/RESPONSE(ISTD,x)) * (DILFAC(x)/WEIGHT(x)) * RSP-FACTOR(i)

The ➢*Internal Standard ("ISTD")* peak itself is not evaluated!

Description: see below.

'Internal/External' Evaluation:

Calibration:

'External' calibration, including the ISTD peak! (Also, see 'External')

Evaluation: Calculation of the Amount peak variable for peak i in the sample x

- The ISTD peak itself is evaluated 'Externally'!
- FACTOR_IS(x) = AMOUNT_NOMINAL(ISTD)/AMOUNT(ISTD,x)
- AMOUNT(i,x) = F(RESPONSE(i,x)) * (DILFAC(x)/WEIGHT(x)) * RSP-FACTOR(i) * FACTOR_IS(x)

Description: see below.

'Internal/External' Evaluation (with variable ISTD):

Calibration:

Calibration is 'External', including the ISTD peak! However, the nominal amount for the ISTD peak from the sample list (Sample Amount) is used. The sample weight of the ISTD peak is not considered.

- Y(i,k) = RESPONSE(i,k)
- X(i,k) = AMOUNT_NOMINAL(i,k) * (WEIGHT(k)/DILFAC(k)) * (INJECTVOL(k)/REFINJECT)
- X(ISTD,k) = AMOUNT_NOMINAL(ISTD,k) * (1/DILFAC(k)) * (INJECTVOL(k)/REFINJECT)

Evaluation: Calculation of the Amount peak variable for peak i in the sample x

The ISTD peak itself is evaluated 'Externally', but without Weight correction.

- AMOUNT(ISTD,x) = F(RESPONSE(ISTD,x)) ∗ (DILFAC(x)) ∗ RSP-FACTOR(ISTD)
- FACTOR_IS(x) = AMOUNT_NOMINAL(ISTD,x)/AMOUNT(ISTD,x)
- AMOUNT(i,x) = F(RESPONSE(i,x)) ∗ (DILFAC(x)/WEIGHT(x)) ∗ RSP-FACTOR(i) ∗ FACTOR_IS(x)

Description:

F:	Calibration function
X(i,k):	X-coordinate of a calibration point for peak i for the standard sample k
Y(i,k):	Y-coordinate of a calibration point for peak i for the standard sample k
k:	Calibration sample
x:	Unknown sample (analysis sample)
RESPONSE(i):	Reference variable (Int.Type; i.e. Area, Height, CE-Area) of peak i in a sample
RESPONSE(ISTD):	Reference variable (Int.Type; i.e. Area, Height, CE-Area) of the corresponding ISTD peak of a sample
AMOUNT_NOMINAL(i):	Amount of peak i from the peak table for the standard sample k
AMOUNT_NOMINAL(ISTD):	Amount of the ISTD peak from the sample list (Sample Amount) for the sample k
AMOUNT(ik):	Calculated amount of the peak i for the sample k
WEIGHT:	Sample weight of a sample
DILFAC:	Dilution factor of a sample
INJECTVOL:	Injection volume
REFINJECT:	Injection volume of the first sample in a calibration series
RSP-FACTOR(i):	Response factor of the peak i from the peak table

Implementation

To perform a calibration, user input is required as follows.

Sample List

- The available standard samples are entered in the **Sample List**, similar to unknown samples.
- Input can be automated via the **Sequence Wizard**.
- Then, each sample in the sample list can be converted into a standard sample by assigning the ➢*Sample Type* **STD**. Please note that the position (line number) in the sample list determines the order of processing. If a standard sample is to be injected several times, a separate line for each injection is created in the sample list.
- In the **Method** column, specify the quantification method to be used for evaluating the sample.
- Input in the remaining fields of the sample list is analog to each unknown sample (**Position**, **Injection Volume**, ...).
- For a detailed description of the procedure, see **How to ...: Actions in the Browser Creating a Sample List**.

Quantification Method (QNT Editor)

- Open the worksheet **General** and check the current settings. Define the calibration⇒ *Mode* to be used.
- Enter the names and the retention times of the peaks to be determined on the **Peak Table** sheet. If a processed sample refers to a QNT file with an "empty" peak table, the peak table can be automatically filled with the retention times of the integrated (!) peaks after the analysis by executing the **Autogenerate Peak Table** command. Each peak contains a successively numbered default name.
- Enter the amount values of the standard substances in the amount columns. Determine the standard method, the calibration type, and the integration type for the calibration.
- Determine the standard method, the calibration type, and the integration type to be used for the calibration.
- For a detailed description of the procedure, see **How to ...: Actions in the Browser Creating a Peak Table**.

Validation and System Wellness

Validation

Analysis data from various workstations or laboratories can only be compared if it is possible to determine the quality of the results that were produced with a chromatography system.

Validation (Definition)

The process ensuring that a system and its analysis procedures supply reproducible and reliable results is referred to as validation. This includes procedures guaranteeing the optimum technical condition of instruments (hardware and firmware) and of computers (hardware and software), especially regarding planning, implementing, and documenting a method. Validation is thus an integral part of ➢*Good Laboratory Practice (GLP)*.

When is validation necessary?

Instruments should be validated before bringing them into service and in regular intervals. This especially applies after exchanging wear parts, repairs, or complete replacement of an instrument. Also following a software update, the system must be validated.

Besides, the Data System itself should be validated at least following an update using the ➢*Installation Qualification* and ➢*Operational Qualification*.

➢*Quantification Methods (QNT Methods)* and ➢*PGM Files* should be validated before they are used in daily laboratory procedure. As the quantification method changes when modifying single parameters, validation is also necessary in the daily routine.

The **SST** tab in the ⇒*QNT Editor* allows you to define ➢*System Suitability Tests* for checking whether your quantification method and your program file are suitable for analyzing special samples.

How is validation performed?

At startup, many instruments perform an automatic self-test, ensuring optimum function. For example, automatic spectra calibration via the ➢*Holmium Oxide Filter* is performed on the Dionex Photodiode Array Detector UVD340S after each startup.

First, the focus of an analysis procedure is on **Calibration** as described above in detail. Within the scope of validation checking, calibration is important: The precision, detection limits, dynamic work range, and robustness of a procedure and the involved components are to be determined using ➢*Validation Samples*, ➢*Blank Run Samples*, ➢*Matrix Blank Samples*, averaging, normal distribution, outlier tests, detection of statistical and systematic errors, ➢*Correlation Coefficient*, ➢*Standard Deviation*, ➢*Relative Standard Deviation*, etc. .

The Dionex Chromatography Management System offers numerous options to meet all GLP and validation requirements. See the topics below for details:

Installation Qualification Manager

Log File CMSetup.log

Operational Qualification of the Dionex Chromatography Management System

System Suitability Test (SST)

Further modules are currently under preparation and will be available in future versions of the Dionex Chromatography Management System.

Installation Qualification Manager

The program CMIQ.EXE located in the IQ directory of the Dionex Chromatography Management System is referred to as Installation Qualification Manager. Following each update of the Dionex Chromatography Management System, this program automatically checks the current installation (➢*Installation Qualification*). This check can be started manually as well.

Activating CMIQ.EXE Automatically

After copying all files and completing the Setup, the program is automatically activated. CMIQ.EXE generates an ASCII report that can be read using the Windows Notepad or any other word processor. The report in the file CHKSETUP.log contains information on:

- The system (time, computer name, user name, operating system, processor)
- The Dionex Chromatography Management System (version, Setup date, Setup operator, ➢*Key Codes*, serial number, number of installed ➢*Timebases*, status of installed software modules)
- All copied files (file name and path, file version, date of last modification date, file size in bytes, product version, 32-bit check sum)

The data is compared to the data in a write-protected list (IQDATA.dat) supplied with the Setup. If the lists are identical, successful installation of the Dionex Chromatography Management System is confirmed. As soon as there are differences, the Dionex Chromatography Management System issues a warning or error.

If a warning is displayed, the functionality of the Dionex Chromatography Management System should not be affected. You can start the Dionex Chromatography Management System as usual.

If any problems occur, please contact the Dionex Service. The same applies if the Dionex Chromatography Management System reports an error.

Activating CMIQ.EXE Manually

Especially after installing or updating other software packages, it is possible that specific system files (DLL) used by several programs are overwritten. Thus, they impair the functionality of the Dionex Chromatography Management System.

In this case, it can be useful to open the program outside the Setup routine via the **Installation Qualification** command of the **Qualification** menu.

☞ ***Tip***: For a correct system check of all files all applications must be closed (not just modules of the Dionex Chromatography Management System). Do not forget to close the ➢*Server* and the ➢*Monitor Program* of the Dionex Chromatography Management System.

There are three options:

Check Installation: Checks the files of the current Dionex Chromatography Management System version and the required Windows system files. Type and scope are freely selectable.

- **Normal**: Checks the Setup.
- **Extended**: Compares the installation with the stored status (see Save System Status). The scope of the report is freely selectable.
- **Full**: Checks and reports all files.
- **Short**: Checks all files. The report includes only errors and warnings.

System Information: Generates the system info of your Dionex Chromatography Management System

Save System Status: Saves the current system status.

Use this option to save the names and the versions of all files contained in the Windows System directory and in the BIN directory of the Dionex Chromatography Management System.

If you performed this option once, the saved system status can be used as the basis for the file check (see **Check Installation / Extended**) instead of the IQDATA list.

Log File CMSETUP.LOG

The entire information on the system and the operations performed by the Setup is logged in the file **CmSetup.log**. The file is first saved to the Windows installation root directory and is moved to the main directory of the Dionex Chromatography Management System after successful completion of the Setup.

This file includes the information by whom and when the installation was performed, which files were copied and which files did other files with the same name replace. The latter is especially important to find out which default reports or ➢*Control Panels* were replaced.

Operational Qualification of the Dionex Chromatography Management System

Within the scope of the Instrument ➢*Operational Qualification*, it is important to prove the functionality of your instruments. The purpose of the Dionex Chromatography Management System OQ is to prove that the software functions according to its operating specification in your specific working environment. The software regenerates data from special files and reevaluates them. These newly calculated results are then compared to the data generated by the manufacturer.

Select the **Chromeleon OQ** or **PeakNet OQ** option in the **Qualification** menu to start the operational qualification of the Dionex Chromatography Management System from the ➢*Client*. A ➢*Wizard* guides you through the process so that the OQ runs almost automatically. Below please find the steps that must be performed:

- Establish a connection to the local ➢*Server* PC.
- If the server is running and a process is active, the user will be prompted to terminate the current process. Otherwise the qualification cannot be performed. If the server is running and no process is active, the server will be stopped.
- Load the server configuration CM_OQ.CFG which is required for the OQ:

  Dionex P580 LPG (➢*Demo Mode*)

  Dionex GINA 50 (demo mode)

  Dionex UVD 340S (demo mode: read).

- The demo mode allows you to simulate all program commands that are available for the selected instruments. Besides, special files are available for the UV detector from which new raw data are generated. Depending on the set measuring parameters the data provided in the demo files are processed in the same way as the data acquired from a real sample.
- Restart the local CM server with the new configuration CM_OQ.CFG being loaded.
- Select the source directory that holds the sequence template CM_OQ.seg and specify the target directory for saving the OQ results. Afterwards start the OQ, which will now run automatically.
- The seven samples of the sequence will be processed. The resulting raw data are evaluated with the ➢*Report Template* CM_OQ.rdf. The results can be printed automatically. If you did not select the option to print the results automatically when specifying the target directory for saving the results on the respective page of the wizard, the report can be printed via the function **Batch Report** in the **File** menu of the browser. This ensures that all pages are updated.
- Finally, the wizard will stop the server and reload the configuration that was used before the OQ was started.

For further information, see the following topics:

Preconditions for the Chromeleon/Peaknet OQ

Documenting the Chromeleon/PeakNet OQ

For performing the operational qualification of the Dionex Chromatography Management System, see

How to ...: Actions in the Browser Performing the Chromeleon/PeakNet OQ

Preconditions for the Chromeleon/PeakNet OQ

The operational qualification of the Dionex Chromatography Management System can be performed both, for pure ➢*Client* PCs and for ➢*Server* PCs. Connect the ➢*Datasource* which is available on the CD to the Client. You can either use the original datasource from the CD or a copy saved on any drive.

The logged on user must have the right to start and stop the server of the Dionex Chromatography Management System and to start its client. Without having those rights, he cannot perform the operational qualification of the Dionex Chromatography Management System automatically using the wizard. (User rights are assigned via the membership of the user in the respective ➢*Privilege* group. For further information on access rights see the CmUser Online Help if this program is installed on your PC.)

If the logged on user does not have the right to start and stop the server of the Dionex Chromatography Management System, he must at least be entitled to define its configuration and to start its client. For information on how to proceed, see **How to ...: Actions in the Browser Performing the Chromeleon/PeakNet OQ Manually**.

If the logged on user is not allowed to define the configuration of the Server, he cannot perform the operational qualification of the Dionex Chromatography Management System.

For further information regarding the operational qualification of the Dionex Chromatography Management System, see

Operational Qualification of the Dionex Chromatography Management System

Documenting the Chromeleon/Peaknet OQ

For performing the operational qualification of the Dionex Chromatography Management System automatically, see

How to ...: Actions in the Browser Performing the Chromeleon / PeakNet OQ Automatically.

Documenting the Chromeleon/PeakNet OQ

The Report (Printer Layout) CM_OQ.RDF contains nine pages:

1. Current_Formula
2. Current_CM
3. Reference_CM
4. Reference_CM_vs_Current_CM
5. Current_Formula_vs_Current_CM
6. General_Information
7. Report_Formula
8. Report_CM
9. Difference_Report

If the report is printed automatically or via the batch report, pages 6 to 8 will be output. All other pages are for calculation purposes only, but can be printed as well.

Two different tests will be performed: 1. The results of the calibration parameter test are indicated on page 7 **Report_Formula**. 2. The results of the function test are given on page 8 **Report_CM**.

Test 1: On the first page, **Current_Formula**, all parameters required for a ⇒*Calibration Type* are calculated (Calibration Type: Linear with Offset, ⇒*Integration Type*: Area, Standard Method: External, ⇒*Calibration Mode*: Total). Some calibration coefficients are calculated with the ➢*Functions* of the ➢*Report Publisher*. The fifth page, **Current_Formula_vs_Current_CM**, compares the ➢*Calibration Coefficients* that resulted from the calculations in the Dionex Chromatography Management System to those resulting from the calculation with the documented formulas. **TRUE** is indicated if the values correspond to each other within the limits of the comparison format described on the ninth page, **Difference_Report**. Otherwise, **FALSE** will be given. The above is performed for each substance. The results of the comparisons are transferred to the seventh page, **Report_Formula**, where **TRUE** is replaced by **Ok** and **FALSE** by **Deviation**. The whole test is evaluated either as "passed" (there is no deviation for any of the variables) or as "failed" (there is a deviation for at least one variable).

Test 2: On the second page, **Current_CM**, the measured values are evaluated with the functions implemented in Dionex Chromatography Management

System. The third page, **Reference_CM**, shows the numerical values that were calculated by the manufacturer during the validation of the respective version. On the fourth page, **Reference_CM_vs_Current_CM**, the newly evaluated parameters are compared to the values received from the manufacturer. The used comparison format is described on the ninth page, **Difference_Report**. **TRUE** is indicated if both values correspond to each other within the limits of the comparison format. Otherwise "FALSE" is given. The above is performed for each sample. On the eighth page, **Report_CM**, each parameter is given only once. If the fourth page, **Reference_CM_vs_Current_CM**, shows **TRUE** for all samples, the respective parameter is **Ok**. In all other cases, **Deviation** will be indicated. Again, the result of the whole test is either "passed" (there is no deviation for any of the variables) or "failed" (there is a deviation for at least one variable).

The sixth page, **General Information**, provides information on the used version as well as on the computer and the user names.

For further information on the operational qualification of the Dionex Chromatography Management System, see

 **Operational Qualification of the Dionex Chromatography Management System**

 **Preconditions for the Chromeleon/PeakNet OQ**

For performing the operational qualification of the Dionex Chromatography Management System, see

How to ...: Actions in the Browser  **Performing the Chromeleon / PeakNet OQ**

System Suitability Test (SST)

Checking whether the quantification method and the ➢*PGM File* are suitable for analyzing special samples is by defining ➢*System Suitability Tests (SSTs)* on the **SST** tab in the ⇒*QNT Editor*. (For further details, see **How to ...: Actions in the QNT Editor Defining the System Suitability Test**.)

The System Suitability Test can already be performed during chromatogram recording. The corresponding QNT method needs to be available in the sample list (in the Browser). Defining **Abort Batch** as **Fail Action** allows aborting the sample ➢*Batch* automatically if a test condition is not met.

System Wellness: Overview

What is System Wellness?

System Wellness monitors the overall "health" of a chromatographic system. It provides built-in diagnostic and calibration features that help prevent unscheduled system shutdowns and assure reliable operation of system devices. Calibration and diagnostic commands are available from Wellness control panels and Help topics are provided for performing the various tasks.

Supported Devices

For System Wellness support, a device must be connected to the Dionex Chromatography Management System via the DX-LAN and it must have a version of ➢*Moduleware* installed that supports System Wellness. The following devices are supported:

Device	Moduleware Version Required
IC Pumps	
GP40 / IP20	3.46 (or higher)
GP50 / IP25	3.46 (or higher)
GS50 / IS25	1.00 (or higher)

Device	Moduleware Version Required
Detectors	
AD25	1.02 (or higher)
CD20 / ED40	3.05 (or higher)
CD25 / ED50	1.05 (or higher)
CD25A/ED50A	1.00 (or higher)
PDA-100	1.04 (or higher)
➢*Autosampler*	
AS50	1.05 (or higher)
➢*Eluent Generator*	
EG40	2.23 (or higher)
System Modules	
IC20	3.08 (or higher)
IC25	1.04 (or higher)
IC25A	1.00 (or higher)

System Wellness Features

- System Wellness control panels, which allow easy access to diagnostic and calibration commands and data
- Download of current, previous, or factory calibration data
- Leak detector testing and calibration
- Wavelength verification and calibration for UV and PDA detectors
- Cell calibration for conductivity detectors
- pH calibration for amperometry detectors
- Pressure offset and degas calibration for pumps
- Flow rate calibration for pumps

For instructions on setting up and using System Wellness features, see

How to ...: Actions in the Browser System Wellness

Data Reprocessing

Definition: Data Reprocessing

Data reprocessing is the presentation of raw data under various aspects. This includes the simple display of an integrated chromatogram, peak purity analysis, representation of calibration curves, or searching single spectra in a spectra library.

Each operation is displayed in a separate window. Opening a **partial method** is also mentioned in this context. Each partial method is intended for one specific task and has its own window arrangement and menu structure. The Dionex Chromatography Management System features the following partial methods that are described in separate chapters:

- **Integration**
- **Calibration**
- **Printer Layout**
- **Peak Purity Analysis**
- **Spectra Library**

In addition, the **Quantification Method (QNT Editor)** that is required for evaluating a sequence can be considered part of data reprocessing. The reason for this is as simple as sensible:

If the detection and peak table parameters chosen in the QNT method prove to be inappropriate after the analysis, the parameters can be changed without requiring a new analysis of the corresponding samples.

All modifications are immediately and globally effective, i.e. modified variables are immediately re-calculated. The new values are displayed on the screen.

If the modified quantification method is saved, the results of all samples using this method will be adjusted.

Caution: The automatic offline batch necessary in the data system "GynkoSoft" is no longer required! The entire data is *always* updated and displayed.

QNT Editor

Quantification Method (QNT Editor): Overview

In the Dionex Chromatography Management System, all instructions and parameters representing the basis of calculation for the sample evaluation are included in the Quantification Method (QNT file). This refers for example to the following questions:

- Below which height, width, or area a peak will be ignored?
- Which course has the baseline?
- Which peaks are classified as ➢*Riders*?
- What is the ⇒*Amount* of the standard samples?
- Which ➢*Calibration Function* is used for creating a calibration curve?
- Which peaks are identified by name?

Before the actual analysis, these evaluation parameters are defined in the Quantification method (QNT file).

- Select **File / New / Method File** to generate a new QNT file.
- Alternatively, select a sequence in the Browser and double-click the corresponding QNT file to open it.
- To open the QNT editor from a method file, click the **QNT Editor** icon on the toolbar. This allows you to view the QNT file data of the current sample.

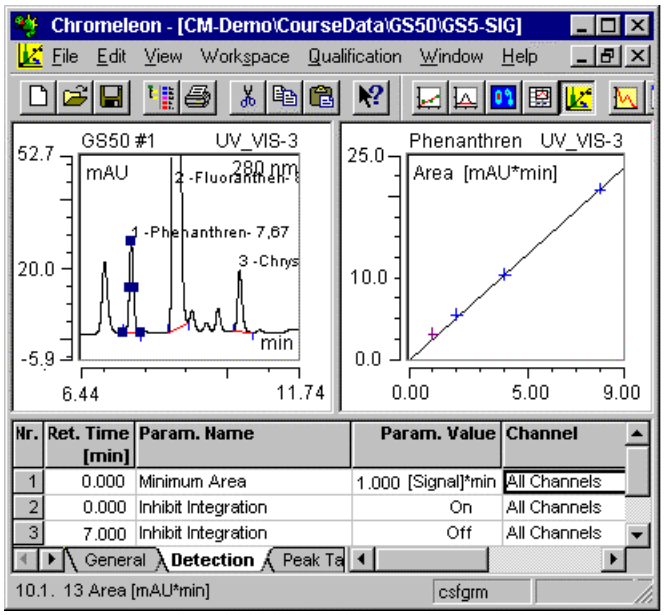
The QNT editor is divided in two window sections. The upper section serves for information purposes. To create a QNT file, use the lower window section, only.

Upper Window Pane

The upper section serves to display additional plots:

- Choose **Show Chromatogram** or **Show Calibration Curve** from the **View** menu to enable or disable the display of the chromatogram and/or the calibration curve.
- Press the F4 key/Shift+F4 or choose the **Next / Previous Chromatogram** option (in the **File** menu) to toggle between the chromatograms of the individual samples.
- Choose **Show Spectra** to enable or disable the display of the spectrum of a single peak.

Of course, representation is only possible for chromatograms, spectra, and calibration curves of samples that were already analyzed.



Lower Window Pane

The lower window pane serves to determine the evaluation parameters.

- By selecting a specific tab in the lower left corner, a worksheet is opened, similar to Microsoft Excel.
- The user can freely select the names of the worksheets. Double-click the corresponding name, and enter a new name in the edit dialog box.

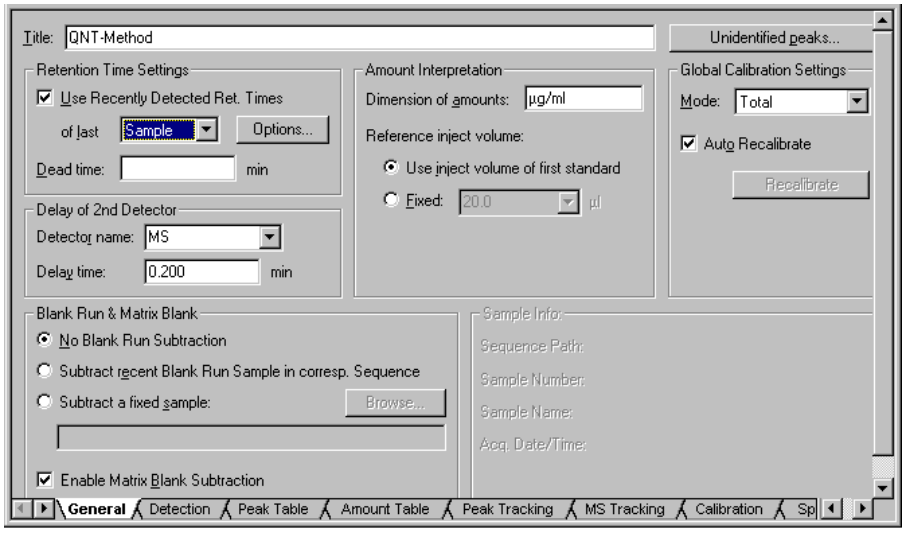
Below it is assumed that the default names have not been modified. The following worksheets described below are available:

General
Detection
Peak Table, Amount Table, Peak Tracking, and MS Tracking
Calibration
Spectra Library Screening
System Suitability Test
Mass Spectra (MS)

☞ ***Tip***: These topics describe the structure and functions of the individual worksheets. For detailed information on how to enter data, see **How to ...: Actions in the QNT Editor** section.

General

The sheet contains global settings for the worksheets **Peak Table** ("Retention Time Settings"), **Amount Table** ("Amount Interpretation"), and **Calibration** ("Global Calibration Settings"). Use the **Title** field to enter a name for the current QNT file. The name appears in the Browser and can be included in a Report when printing data of the QNT editor. The **Unidentified Peaks** button allows you to determine how to quantify unidentified peaks.



Retention Time Settings

- Select the check box **Use Recently Detected Ret. Times**, if the ⇒*Retention Time* of the preceding sample should be used when identifying a peak via a retention time window (⇒*Window*). You can also use the retention time of the last standard. The button **Option** provides further options. (For details see ⇒*Use Recently Detected Retention Time*). This function allows the system to automatically react to changing retention times, e.g. due to column trends. If the option is disabled, the actually determined retention time listed in the peak table is used for identifying the peak.
- Enter the ⇒*Dead Time* in the field **Dead Time**. This time is used for calculating the ➢*Capacity Factor* k' and the ⇒*Kovats Indexes*.

Delay of 2nd Detector

- Select the name of the second detector in the Detector Name field.
- Enter the delay time in the ⇒*Delay Time* field (also, see **Defining the QNT Method for Several Detectors**).

Amount Interpretation

- For documentation purposes (exclusively), the physical dimension (amount or concentration) that is used for the amount values can be included in the field ⇒*Dimension of Amounts*. Amount values are not automatically converted into concentration values or vice versa.
- In addition, the reference injection volume is defined on this page. Either select the injection volume of the first standard (**Use inject volume of first standard**) or enter any volume via **Fixed**.

Global Calibration Settings

- Use the **Mode** field to determine how and based on which ⇒*Calibration Mode* the samples of a sequence are calibrated. This allows, for example, calibrating certain samples as a group or including calibration samples for samples that are analyzed later.
- When **Auto Recalibrate** is activated, each modification within a chromatogram (e.g. moving peak delimiters) results in an automatic recalculation of the ➢*Calibration Coefficient* as well as all derived calibration data. If you deactivate **Auto Recalibrate** in your peak table so that the c0, c1, and/or c2 columns are included, re-calibration is preformed by pressing the **Calibrate** button. Nevertheless, the corresponding values can be entered manually as well.

Blank Run & Matrix Blank

Use the section **Blank Run Subtraction** on the **General** sheet of the QNT editor to determine whether the absorption values of a ➢*Blank Run Sample* are considered (= subtracted) in the sample evaluation (= ➢*Blank Run Subtraction*). You can also subtract the results of a single ➢*Matrix Blank Sample*.

- Select **No Blank Run Subtraction** if no correction is to be performed.
- Select **Subtract Recent Blank Run Sample in Corresponding Sequence** to use a finished blank run sample of the current sequence for the subtraction. The chromatogram of the blank run sample is subtracted point by point from the current chromatogram.
- Select **Subtract a Fixed Sample** to perform the correction with any sample. Choose **Browse** to search for the sample.
- **Enable Matrix Blank Subtraction** activates the subtraction of matrix blank samples. Contrary to the other options the resulting peak areas or peak heights are subtracted.

Detection Parameters (Detection)

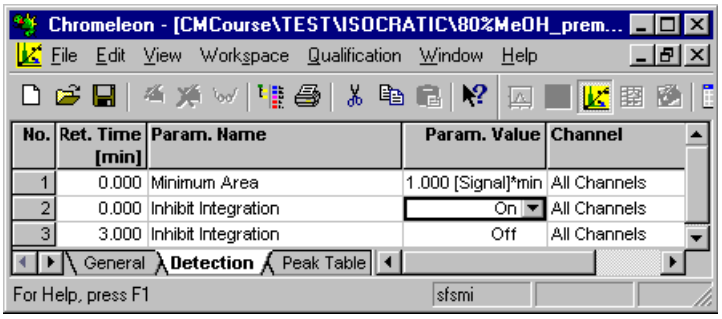
Detection parameters serve e.g. to recognize, classify and suppress peaks as well as to determine the baseline.

The default values are normally suitable for optimum integration of 90% of all recorded chromatograms.

In critical cases, e.g. with wavelength switching, the user can improve the integration results by modifying the parameters.

Detection parameters are time-dependent. Each parameter can be activated, deactivated, or changed in its value at a specific time. The time when the parameter shall change, the parameter name and its value are entered in the corresponding column of the first line. It is possible to change a parameter several times in succession.

Detection parameters are defined in the QNT editor. You can either enter them in the table of the **Detection** tab or define them graphically in the chromatogram.



In the example above, integration is inhibited (command: ⇒*Inhibit Integration*) at the time t = 0.000 (**On**). After three minutes (t = 3.000), integration is activated again (**Off**). It is also stipulated that peaks with a minimum area of 1 x [Signal] *min only are recognized as peaks.

The last defined value of each parameter is valid until the sample run is completed. After that, the parameters assume their preset (default) values.

The ➢*Channel* column indicates whether the settings are valid for a specific channel (as in this example) or for all channels.

For further details and examples of possible detection parameter modifications, see **How to ...: Actions in the QNT Editor Defining Detection Parameters** and ⇒*Detection Parameters (Overview)*.

Peak Table, Amount Table, Peak Tracking, and MS Tracking

The peak table contains all parameters required for identifying a peak and to determine the amounts of the substances serving as standards. The peak table contains 26 columns (the **Amount**, **C0**, **C1**, and **C2** columns are duplicated according to the number of different standards) and is therefore spread over three tabs: **Peak Table**, **Amount Table**, and **Peak Tracking**. Individual columns and whole pages can be faded in and out.

Creating the peak table is usually performed manually, i.e. the user enters the names and retention times of the expected peaks. Peaks that serve as standards must be labeled accordingly in the ⇒*Standard* column. The (known) concentration of a standard is included as ⇒*Amount* value in the Amount column of the table. The values form the basis for any type of calibration.

Via the **Autogenerate Peak table** command of the **Edit** menu, it is possible to automate the creation of the peak table. Two different types are available. If **Enumerate peaks of current chromatogram** is selected, the system includes all peaks integrated (!) in the current sample in the peak table. As peak name, a combination of sequence name and consecutive number is assigned.

When reference spectra were found via **Spectra Library Screening**, you can also use these for automatic peak table creation. Choose the type **Use Spectra Library Screening results**. In both cases, the values for the **Retention Time** and **Window** columns are recalculated. Default settings are used for all other entries (see **How to ...: Actions in the QNT Editor Autogenerating the Peak Table' by Including Library Screening Results**).

Caution: All previous entries are overwritten and lost when saving the peak table or the QNT file!

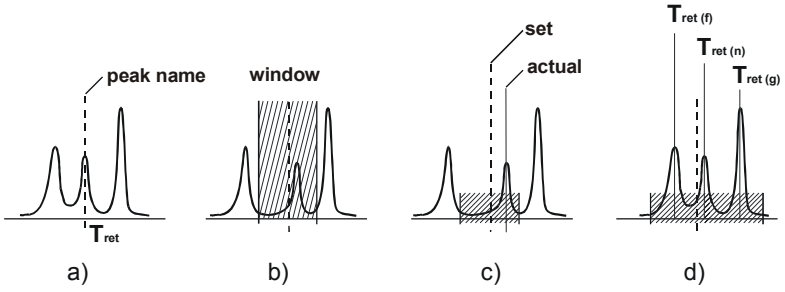
For detailed instructions, see **How to ...: Actions in the QNT Editor Creating a Peak Table**

Peak Identification / Peak Tracking and MS Tracking

Peak identification refers to the following procedure: a previously unknown peak is recognized due to peak-specific properties (e.g. the retention time or its UV spectrum) and is then labeled with a characteristic substance name.

Most frequently, peaks are identified via their **retention time**. If the user knows the exact retention time of a peak, the retention time is entered together with the **Substance name** in the corresponding columns of the peak table. If a peak is detected at the specified time, the name is automatically assigned (Fig. a).

Even if there are retention time fluctuations or neighboring peaks, identification is possible. This is enabled by a tolerance range defined via the ⇒*Window* peak table parameter (fig. b). If a peak is detected within the tolerance range, it is identified, even if the *set* (nominal) and the *actual* retention time do not match exactly (fig. c). If several peaks are detected within this range, the data system identifies the *"greatest,"* the *"first"* or the *"nearest"* peak, depending on the selected extension for the **window** parameter (fig. d).



The retention time value previously entered in the peak table is corrected accordingly!

Another method to identify peaks is offered by the **UV spectrum**. For identification purposes you can either use the **Spectrum** only or the spectrum and the retention time (**Spectrum and time**). A photodiode array detector (e.g. Dionex UVD 320S or UVD 340S) is required for this elegant and very reliable method. The substance spectrum is recorded for each peak and is compared to the spectra in a library based on certain criteria (see **How to ...: Actions in the QNT Editor** **Peak Tracking**). If the spectra match, the peak is identified.

If you use an aQa ➢*Mass Spectrometer*, peaks can also be identified based on ➢*Mass Spectra*. Mass spectra present a very reliable method for peak identification. The **MS Tracking** tab allows you to select different options as

described under **How to ...: Actions in the QNT Editor** **Identifying Peaks via Their Mass Spectra (MS Tracking)**.

Calibration / Amount Table

In a calibration, the peak area of a known amount is determined. Then, the result is used for calculating the amount of an unknown sample via the area/amount ratio.

For this method, not only the peaks serving as standard substances and the amount of the corresponding standard samples are required, but also a mathematical procedure that determines how a generally valid ratio is established from the area/amount of few standard samples.

This is performed via the **Amount**, **Standard**, **Cal.Type**, and **Integration Type** columns in the **Amount Table**. For a detailed description of the columns and instructions on the input required for the columns, see **How to ...: Actions in the QNT Editor** **Creating a Peak Table**.

☞ ***Tip***: Background information on calibration is available in the chapter **Calibration**.

Calibration Settings (Calibration)

In the simplest case of a chromatographic analysis, first one or several standard samples and then the unknown samples are analyzed. All samples of a sequence are evaluated based on the same standard samples. If the quality of the column changes between processing the first and the last sample, this will not be considered.

Therefore, the Dionex Chromatography Management System allows evaluating samples via specific patterns or based on any selected standard samples. This is determined via the ⇒*Calibration Mode* on the **General** sheet of the **QNT Editor**.

The **Calibration** sheet indicates which standard samples will be used for evaluating the current sample of a sequence. When changing from the current sample to another one via F4 or SHIFT+F4, the list of the displayed standard samples is updated again.

If you notice that a specific standard sample falsifies your calibration results, you can deactivate this sample in the **Enabled** column. The standard sample is then excluded from the calculation. The corresponding calibration points are then highlighted in the curve by a different color.

Spectra Library Screening

To identify substances, spectra can be compared to library spectra. The spectra search can be performed via the **Spectra Library Screening** sheet of the **QNT Editor**.

For details on how to perform spectra library screening, see **How to ...: Actions in the QNT Editor Spectra Library Screening**.

System Suitability Test

The aim and objective of the ➢*System Suitability Test (SST)* is to ensure that the operational conditions required for a specific measurement are achieved. Specify the conditions for the SST on the **SST** tab in the QNT Editor.

For details on how to perform System Suitability Testing, see **How to …: Actions in the QNT Editor / Defining the System Suitability Test**.

Mass Spectra (MS, MS Tracking)

Acquiring mass spectra with your Dionex Chromatography Management System is possible provided a Finnigan aQa ➢*Mass Spectrometer* mass is installed. For further information on how to install the spectrometer and acquire data, see **How to ...: Actions Related to the aQa-MS**.

In HPLC MS, mass spectra especially serve for peak identification. Using mass spectra for identifying substances is via the **MS Tracking** tab. For details, see **How to ...: Actions in the QNT Editor Identifying Peaks via Their Mass Spectra**.

As MS chromatograms normally show heavy noise ➢*Mass Spectra* need to be processed before being used. On the **MS** tab, define the number of single peak spectra to be averaged. Also, define how many background spectra shall be aggregated into a total background spectrum that is then subtracted from the averaged peak spectrum.

For details, see **How to ...: Actions in the QNT Editor Processing Mass Spectra**

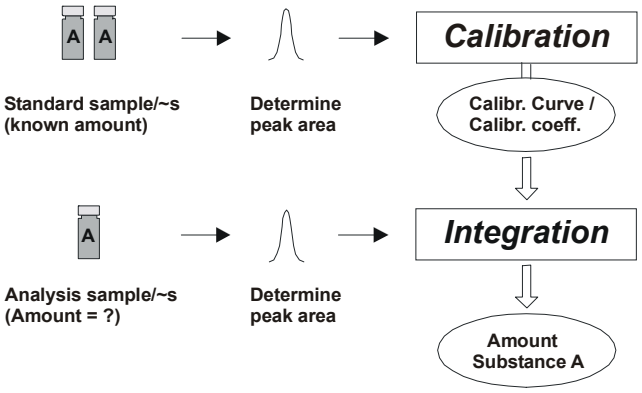
Integration

Overview: Integration

The chromatographic process of converting peak areas below peaks in amount or concentration values is referred to as integration.

The integration is performed based on the **Calibration**. It supplies a calibration curve and a ➢*Calibration Coefficient*.

Inserting the calibration coefficients in the ➢*Formula for Amount Calculation* supplies the amount concentration in a single peak area. The data system automatically performs this process for all peaks it "finds."



How many peaks are detected and whether at least part of these peaks can be identified, depends on the **Quantification Method (QNT File)** specified for each sample before the analysis.

The results of the area calculation and peak identification processes are represented graphically (chromatogram) and as a table (Report) in the window of the partial method **Integration**.

For further details and features, see the following topics:

Opening a Sample
Operation
Manual Re-Integration
Chromatogram Comparison
Data Smoothing
Peak Ratio
Spectra Plot
Mass Spectra Plot

Opening a Sample

Opening a sample automatically opens the integration method window and displays the sample chromatogram. There are three options:

- Select a sample via the **Open** command of the **File** menu, or
- Double-click a sample of a specific sequence in the ➢*Browser*, or
- Select a sample in the Browser and select a channel of the sample via the **Open** command of the context menu (right mouse button).

Usually, you will open samples that have been completely processed. However, samples can be opened as well while being analyzed, i.e., while being in **Running** ⇒*Status*. A certain amount of data must have already been acquired in a running sample. Depending on the ⇒*Step* and other detector settings the sample must have run for up to several minutes. A running sample can be opened either

- From the Browser (via different options - see above) or
- From a ➢*Control Panel* via the **Integrate** command of the **View** menu.

Operation

Modifying the Appearance

Each displayed chromatogram can be changed by enabling/disabling the display of various elements and by modifying them.

- Double-click a peak to see its **Peak Properties**.
- Draw a frame around the section of the chromatogram you want to view enlarged.
- Select the **Decoration ...** command in the context menu (right mouse click) to modify the window background, the different axes, the layout of individual peaks as well as the color, shape, and size of their captions.
- Activate the **Spectra Tool** command in the context menu (or press the corresponding icon in the *Integration Toolbar* (topic available in the Online Help only)) to view the spectrum from the chromatogram at the time t. As soon as the spectrum symbol is added to the mouse cursor, clicking any position will extract a spectrum that is displayed in the **Spectra Plot** window (if the corresponding data exists). A minimized representation of the spectrum itself is displayed in the integration window. Repeat the operation while pressing the SHIFT key to overlay single spectra. Alternatively, choose the **Overlay Spectra** command in the context menu. **Hide Time Spectra** will remove overlaid spectra again.

Opening Additional Window Sections

Using one of the following commands displays further window sections:

- Perform the **Split Zoom** command from the **View** menu to split the window. By drawing a frame, you can zoom a section of the window. The upper half of the window shows the entire chromatogram and the frame, the lower half displays the zoomed section. Use the mouse to move and position the frame in the upper window section. This mode is recognized by the shape of the mouse cursor (✣). Of course, a new frame can be drawn any time.
- Select the **Report** command from the **View** menu to display the integration report (see **Integration/Integration Report**).
- Choose the **Show Spectra** command from the **View** menu to display the peak spectrum of the currently selected peak (see **Integration/Spectra Plot**).

- Compare two chromatograms by enabling the display of an additional chromatogram (see **Integration/Chromatogram Comparison**).

Manual Re-Integration

The Dionex Chromatography Management System largely automates sample integration. In special cases, the user may prefer to perform manual modifications. The Dionex Chromatography Management System therefore allows manually moving peak delimiters, inserting, and deleting peaks, or modifying the baseline, etc.

If the **Automatic Tool** is selected via the context menu, these alterations are possible directly in the chromatogram. The shape of the mouse pointer indicates the performed operation.

	Move left / right peak delimiter
	Change baseline point (left / right / center)
	Move baseline point (left/right/center)
	Move
	Move baseline segment
	Move ⇒*Detection Parameter*
	Insert peak
	Zoom out an area
	Display spectrum
	Operation not possible

Use the individual commands such as **Baseline Tool**, **Insert Peak Tool**, or **Zoom Tool**, if you only need a specific scope of functions. For details on the possible operations see

How to ...: Actions in the Chromatogram **Manual Re-Integration**.

Tip: If manual modifications are performed, the numeric result can be seen when displaying the **Integration Report**.

Chromatogram Comparison

When comparing two or more samples or chromatograms, comparing their numerical results would be the most exact method. However, overlaying the chromatograms is in many cases sufficient. This is performed via the chromatogram comparison.

What can be compared?

Chromatogram comparison always compares individual channels. Whether these channels are from the same or from different samples, is irrelevant. The number of simultaneously displayed chromatograms in the Dionex Chromatography Management System is theoretically not limited.

As the presentation becomes confusing with an increasing number of displayed chromatograms, the Dionex Chromatography Management System prompts the user to confirm whether to display more than 20 chromatograms. This prevents the display of chromatograms due to an operator error and a resulting decrease in system performance.

How are chromatograms compared and displayed?

A comparison is performed by displaying the chromatograms in the integration window. One chromatogram represents the currently active chromatogram. It is selected with the mouse. It can be recognized by the displayed additional information (decoration etc.). The names of all represented chromatograms are listed above the window. The currently active chromatogram is marked by a different color. Click the name of any chromatogram to select it as the active chromatogram.

The presentation of the window and the active chromatogram is controlled via **Decoration** of context menu.

How do I select the chromatograms or channels to be compared?

There are various ways to select one or several chromatograms.

- Select one or several samples in the Browser and drag them into an open integration window. The Dionex Chromatography Management System automatically attempts to load the ➢*Channel* of the current sample. If this is not possible, e.g. because the channel does not exist, the default channel is loaded. The default channel is the first channel in the list when opening a sample (**Open** command of the context menu in the Browser).
- Choose the **Add Overlay ...** command from the **File** menu to display a specific channel of any sample in an opened integration window.
- To compare all channels of a single sample choose the command **Open / All Channels**.
- Choose the **Compare** command to compare a specific channel in several selected samples.
- Perform a query to specifically compare samples with certain properties.

- Click the **Next Chromatogram** icon () while holding down the CTRL key to additionally display the chromatogram of the next sample.
- Click the **Previous Chromatogram** icon () while holding down the CTRL key to additionally display the chromatogram of the previous sample.
- Click the **Next Channel** icon () while holding the CTRL key to additionally display the next channel of the same sample.
- Click the **Previous Channel** icon () while holding the CTRL key to additionally display the previous channel of the same sample.

For details on selecting chromatograms / channels to be compared, see **How to ...: Actions in the Chromatogram**  **Performing a Chromatogram Comparison**.

Placing chromatograms and channels in relation to each other

The appearance of a chromatogram is determined considerably by external influences such as flow rate, solvent, column quality, detector amplification etc.

As these conditions cannot be modified later, other possibilities must be found to perform the comparison as exact as possible. This is achieved by adapting the position and the size of a chromatogram to match another. The Dionex Chromatography Management System offers several options:

- Chromatograms can be assigned an offset in x- and y-direction
- Chromatograms can be time-normalized, i.e. they can be overlaid at a specific retention time
- Peak height can be normalized, i.e. the height of a specific peak can be adjusted
- Chromatograms can be stretched and compressed
- Chromatograms can be subtracted from each other

For the active chromatogram, the **Decoration** command is chosen via the context menu. The settings are entered via the **Comparison** dialog.

For further details, see **How to ...: Actions in the Chromatogram**  **Performing a Chromatogram Comparison**.

Data Smoothing

Data smoothing applies a digital filter to sample data to reduce signal noise and helps improve chromatogram appearance and reproducibility of peak baselines. Data smoothing is performed in the integration window (for MS chromatograms, data smoothing is defined in the ➢*PGM File* or during ➢*Mass Trace* extraction.) After smoothing, the smoothed chromatogram is displayed overlaid over the original chromatogram. The original sample data file is **not** altered and the smoothed data file is stored separately.

Filter Types

The **Savitzky-Golay** filter smoothes to least-squares fit, using a weighting function based on second-degree and third degree polynomials. Savitzky-Golay smoothing is useful for reducing high-frequency noise of a data set that is continuous (such as a chromatogram) without significantly degrading the underlying signal.

The **Moving Average** (= **Boxcar**) filter is a simple algorithm that produces a set of output values in which each output value is equal to the average of n points centered around the corresponding input value, where n represents the filter size. Because the Moving Average filter equally weights each point, its ability to discriminate between noise and signal is limited.

The **Olympic** filter is very similar to the Moving Average filter, except that the maximum and minimum points of each input data set are rejected before the average is calculated. This provides better rejection of impulse noise (spikes) than the moving average filter.

In addition, the **Gaussian** filter is available for acquiring MS chromatograms and extracting a mass trace (in the Mass Spectra window). This filter applies the Gaussian distribution for chromatogram smoothing.

Filter Size

Filter size is the number of input data points used to generate each output data point. The filter size is an odd number between 5 and 999. Use a narrow filter size if desired peaks are narrow, and a wider filter size for wider peaks. As a rule of thumb, select a filter size that approximately equals the peak's half width. Note that too narrow a filter results in insufficient smoothing while too wide a filter can lead to distorted data.

☞ ***Tip***: Distortion of data during data smoothing mainly affects the peak height. Therefore, it is generally better to evaluate smoothed chromatograms by area rather than height.

Iterations

If a filter is applied several times, by far the highest smoothing result (>95%) is achieved when the filter is applied the first time. Thus, normally a single smoothing step is sufficient. However, applying a narrower filter multiple times often provides improved noise reduction without the signal degradation that can occur when using a wider filter size. This requires additional processing time, however, so a wider filter size may be preferable if its results are acceptable.

For additional details, see **How to ...: Actions in the Chromatogram** **Performing Data Smoothing**.

For MS Chromatograms, see **How to ...: Actions Related to the aQa MS** **Extracting Mass Traces Afterwards**.

Peak Ratio

If the baseline-corrected signals of two channels (of the same sample!) are related to each other, a rectangular curve results. This curve is referred to as peak ratio. It is based on the observation that the ratio between two detector signals must be constant, as according to the Lambert-Beer law the detector signal (S) must always be proportional (c1) to the concentration (K) of a dissolved substance.

$$S = c1xK$$

If the quotient q is formed of the two channels, the substance concentration K is canceled out. The quotient now only depends on the ratio of the two wavelengths, not the time.

$$q = \frac{S1}{S2} = \frac{c1(\lambda 1)}{c2(\lambda 2)}$$

If q is entered against the time, the (theoretical) result for each peak of the sample is a horizontal line of the height c1(λ1)/c1(λ2).

The width of the rectangle is determined by the baseline and the ⇒*Peak Purity Threshold* parameter. The ratio formation is only performed where both (!) peaks have a baseline and where both (!) peaks have intensity above the defined peak purity threshold. The range to be actually overlaid (= width of the rectangle) is thus the intersection of the baseline and Peak Purity Threshold condition. The default Peak Purity Threshold value is 10% of the peak maximum and can be changed in the QNT editor.

The rectangle heights of two adjacent peaks differ if the corresponding peaks have different spectra and if the two wavelengths are selected so that the absorption quotient is significantly different.

Consider the following limitations and requirements:

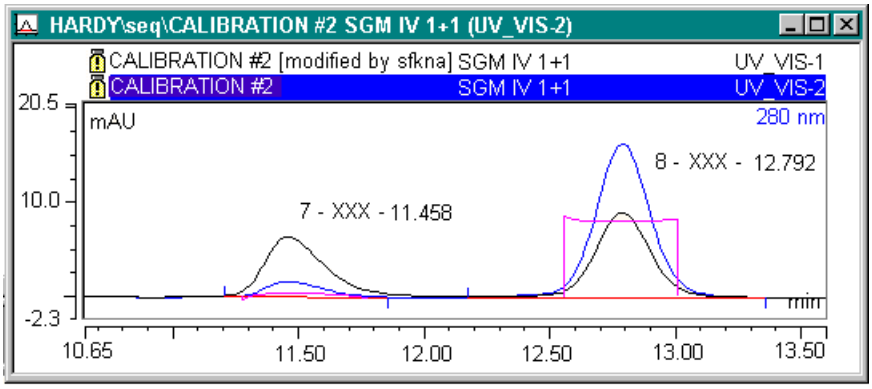
- The detector may not drift.
- The correlation only applies to the linear range of the Lambert-Beer law (<2000 mAU).
- The solvent composition may not be altered (isocratic conditions).
- The solvent only slightly contributes to the absorption. The baseline correction allows eliminating the solvent absorption.

Note: A peak ratio can only be formed with the signals of the same detector.

Forming the Peak Ratio

- Within the integration window, overlay two channels of the same sample (e.g. by clicking the **Next/previous channel** icon while holding down the CTRL key).
- Use the **Decoration** command of the context menu to open the dialog **Chromatogram Decoration**.
- Activate the check box **Peak Ratio** under **Peak Decoration**.

In the integration window, a rectangle curve in a different color should appear in any place where two peaks are overlaid in addition to the two chromatograms.



Result

A regular rectangle shape, as shown at 12.70min in the illustration, *can* serve as a criterion for evaluating the peak purity. The more the curve deviates from the rectangle shape, the higher the probability that the overlaid peaks do not originate from the same substance. If the rectangle slightly overshoots on the right or on the left, this is tolerable due to the lower signal intensity at the peak start and the peak end.

To express the result of the peak ratio numerically, the *Peak Ratio Mean Value* and *RSD Peak Ratio* report variables are available (in the Online Help only).

Spectra Plot

Overview

The **Spectra Plot** enables the display of UV spectra. The prerequisite for the spectra plot is the availability of the corresponding raw data. Raw data is generated by recording a 3D field with a ➢*Photodiode Array Detector*. The spectra plot can be opened from the **Integration** method.

- Open the Spectra Plot window via either the **Show Spectra** command of the **View** menu or the  button.

The representation of a spectrum in the **Spectra Plot** is usually (height) normalized, i.e., the height of the spectrum is represented in percent and thus independent of the concentration (also, see ➢*Normalization*). As a default, this normalization is by the greatest relative maximum within the spectrum.

Normalization allows objectively comparing two spectra of different concentrations. If spectra of the same peak, but from different peak heights are overlaid, these will generally coincide despite the differences in concentration.

- Use the **Decorations** command from the **View** or context menu to determine via the **Frame & Axes** tab which type of normalization should be applied to the spectrum.

The normalized spectra representation allows performing the following tasks:

- Comparing two spectra (e.g. a standard and a sample)
- Determining the number and position of minima and maxima
- Selecting an appropriate type of normalization
- Verifying the linearity of the Lambert-Beer law
- Deciding: Baseline correction Yes/No
- Determining exact integration limits by checking peak purity at various wavelengths and peak heights
- Identifying components

Displaying Spectra of one Peak

- In the chromatogram window, select the peak for which to display the peak spectrum (= spectrum in the peak maximum).

- If several peak heights were activated below **Peak Spectra** in the **Decoration** dialog of the **Spectra Plot** window, the spectra from different peak heights are displayed simultaneously when clicking the peak.

Displaying any Spectra of a Chromatogram

Perform the following steps to extract any spectra of a chromatogram via mouse-click.

- Activate the **Spectra Tool** command in the context menu (or click the corresponding icon on the *Integration Toolbar* (for further information see the respective Online Help topic). The changed mode will be indicated by a spectra symbol that is added to the mouse pointer.
- Click anywhere in the chromatogram to view the corresponding spectrum.
- Repeat the operation while keeping the Shift key depressed to overlay several spectra.

Displaying Spectra of Different Samples

To objectively compare spectra of different samples, proceed as follows:

- Open the **Decoration** dialog box and select the **Peak Spectra** tab.
- Select the **Retention time spectrum of fixed sample** option and navigate to the desired sample in any sequence via the **Browse...** button.
- Alternatively, you may also use the retention time spectrum of the last standard (= **Retention time spectrum of recent standard**), the reference spectrum of the peak table (= **Reference spectrum in corresponding peak table**), or any spectra that was found during library screening (**Spectra library screening result**).

Match Factor, Difference Spectra, and 1st and 2nd Derivative of Spectra

As soon as two or more spectra are represented with the Spectra Plot, a frequent question is the similarity between the various spectra.

This can be expressed by the Match Factor, the formation of difference spectra or by representing the first or second derivative of a spectrum.

- Choose the **Decorations** command from the **View** or context menu and activate the **Show match** check box on the **Label** tab. The Dionex

Chromatography Management System issues a value for each represented spectrum specifying the match degree relative to the main spectrum (0 = no match; 1000 = perfect match).

- On the **Analysis** tab choose whether the difference spectrum or the first or second derivative of a spectrum are displayed in a second window in addition to the actual spectra.

In the case of the match factor and the difference spectrum, the question which spectrum is considered a main spectrum is especially important, as this is the basis of comparison or the basis for all calculations.

Usually, this is the peak spectrum extracted at the retention time. If there is no peak spectrum, a distinction is made between two situations: If the spectra were extracted individually from the chromatogram via spectra tool, the spectrum that is first extracted is the main spectrum. If spectra are automatically extracted at different peak heights (see **Displaying Spectra of one Peak**), the spectrum with the "oldest" retention time is considered the main spectrum. When representing difference spectra, the entry **Difference to ...** indicates the basis of calculation.

Comparing a Spectrum with Spectra of an Existing Spectra Library

To clearly identify a spectrum, it should be compared to a reference spectrum stored in a spectra library.

- Via the context menu, perform the **Library Search** command to start the comparison. The window of the method **Spectra Library** lists all library spectra that have a minimum similarity with the (normalized) spectrum. For details on performing the library search, see **How to ...: Actions in the UV Spectra and Mass Spectra Starting a UV Spectra Search**.

If the Spectra Plot window contains more than one starting spectrum, the Dionex Chromatography Management System always uses the spectrum that is displayed first for the comparison with library spectra.

Mass Spectra Plot

General

The Mass Spectra Plot enables the display of ➢*Mass Spectra*. The prerequisite for opening the mass spectra plot is the availability of the corresponding raw

data that were recorded by a ➢*Mass Spectrometer*. The mass spectra plot can be opened from the **Integration** method.

- Open the Spectra Plot windows via either the **Show Mass Spectra** command of the **View** menu or the  button.

The representation of a mass spectrum is height normalized, i.e. the height of the spectrum is represented in percent and thus independent of the concentration (also, see ➢*Normalization*). As a default, this normalization is by the ➢*Base Peak* of the spectrum.

Normalization allows objectively comparing two spectra of different concentrations. If mass spectra of the same peak, but from different peak heights are overlaid, these will generally coincide despite the differences in concentration. Due to their higher information density, mass spectra are displayed in the Dionex Chromatography Management System one below the other, which is contrary to the display of UV spectra that are overlaid.

Displaying Mass Spectra of one Peak

- In the chromatogram window, select the peak for which to display the mass spectrum (= spectrum in the peak maximum).
- If several peak heights were activated below **Peak Spectra** in the **Decoration** dialog of the **Mass Spectra Plot**, the mass spectra from different peak heights are displayed simultaneously when clicking a peak.

Displaying Mass Spectra of Different Samples

To objectively compare mass spectra of different samples, proceed as follows:

- Open the **Decoration** dialog box and select the **Peak Spectra** tab.
- Select the **Retention time spectrum of fixed sample** option and navigate to the desired sample in any sequence via the **Browse...** button.
- Alternatively, you may also use the retention time spectrum of the last standard (= **Retention time spectrum of recent standard**), the reference spectrum of the peak table (= **Reference spectrum in corresponding peak table**), or any spectra that was found during library screening (**Spectra library screening result**).

Report

Report: Overview

The report (or better: screen report - contrary to the printer layout that defines the printout) includes several tables for displaying all relevant data of samples, sequences, datasources, etc. on the screen. The report is saved in the ⇒*Report Definition File* together with the printer layout.

The report is opened via either the **Show Report** command (in the **View** menu) or the  button. Usually, it is displayed in the window of the partial method Integration. Nevertheless, you can have the report displayed in the ⇒*QNT Editor* as well to directly check the effects of changes in the QNT method.

You can add, edit, or extend the individual report tables as required. The following tables are available via the **Insert Report** command of the **Table** menu:

Report Type	Description
Audit Trail	Shows the  Audit Trail.
Calibration History	Documents the course of the calibration.
Calibration Report	Shows the calibration report.
Database Query	Shows the results of a database query.
Detection Parameter Report	Shows the Detection Parameters.
History Report	Shows the ➢History report.
Integration Report	Shows the integration report.
MS Instrument Info Report	Provides information on the ➢Mass Spectrometer.
MS Instrument Method Report	Indicates the MS method.
MS Raw Report	Shows the raw data of the current ➢*Mass Spectrum*.
MS Status Log Report	Indicates the mass spectrometer settings.
MS Tune Data Report	Indicates the tune data of the ➢*Xcalibur* raw data file.
Peak Summary	Shows the peak summary
Program Report	Shows the ⇒*PGM File* for the current sample.
SST Report	Shows the report regarding the ➢*System Suitability Test*

Tip: Using the **Print** command of the **File** menu allows printing the

chromatogram and the report at any time. The pages that have been defined in the printer layout will be printed, also from within a report.

For further details on some of the reports mentioned above, see the following topics:

Integration Report

Calibration Report

Peak Summary Report

History Report

Integration Report

The first page of a report usually is an integration report. The **DEFLTDAD** ⇒*Report Definition File* , for example, includes the following integration report tables:

- Integration
- Peak Purity
- Peak Analysis

Contents

- The integration report contains all relevant numeric data of the current sample such as retention time, peak area and height, amount, peak type, and other ⇒*Peak Variables*.
- The individual columns contain variables of the ⇒*Peak Results* report category. Nevertheless, you can add further columns from other ⇒*Report Categories*.
- If the chromatogram is modified, e.g. by manual re-integration of a peak, this is reflected immediately by the changed report data.

- Via the Windows clipboard, data of the report can be directly integrated in other Windows applications.
- Within the report, the values of different cells are added, subtracted, multiplied, or divided, as is possible in MS Excel. To do so change into the Layout Mode via the **Layout Mode** command of the **Table** menu.

Formatting

You can design your integration report mostly according to your requirements. The necessary commands are available in the context menu or in the **Table** menu.

For further details, see **How to ...:** **Actions in the Report**.

Calibration Report

The calibration report is very similar to the **Integration Report**:

Contents

- Similar to the integration report, the calibration report shows data of the current sample. In the calibration report, however, this data refers to the calibration of the current sample.
- The individual columns contain variables of the ⇒*Peak Calibration* report category. Nevertheless, you can add further columns from other ⇒*Report Categories*.
- The calibration report allows understanding changes made during the calibration (in the QNT method).

For further details, see **How to ...:** **Actions in the Report**.

Peak Summary Report

Commonly used reports (e.g. **Integration Report** and **Calibration Report**) contain data of one sample only. In case of a chromatogram comparison, only the data of the selected, i.e. the current, chromatogram is displayed.

Comparing peak data from different samples is possible via the **Peak Summary** report type.

Sample Selection

- If **one sample** is selected and opened from the Browser, the **Peak Summary** is based on the corresponding ⇒*Sequence*.
- If **several samples** are selected in the Browser, these selected samples only will be part of the Peak Summary.
- If a ➢*Query* is started in the Browser, the search result forms the basis for the Summary. In this way, it is possible to compare peaks from different sequences.

Peak Selection

- Normally, **no peak** is selected in the chromatogram of the sample. The Peak Summary Report therefore contains **no entries**. All fields are marked **n.a.** (not available) or **Div/0** (Division/0). Only when a peak is selected manually within a chromatogram, the Peak Summary Table receives entries. As soon as this is performed, this peak is searched in all previously selected samples. The search result is displayed in the **Summary Report**.
- For each Peak Summary column (!), it is possible to define whether the values of the currently selected (**Selected Peak**) or one specific peak (**Fixed Peak**) are displayed. Access these options by choosing **Column Properties** from the context menu.
- If the currently selected peak is an **identified** peak, i.e. a peak labeled with its name in the peak table, all involved samples are searched for this peak name. The corresponding values of all found peaks are displayed in the Summary.
- If the currently selected peak is a **non-identified** peak, i.e. a peak not labeled with its name in the peak table, a "fixed time window" (± 5% of the detected retention time) is calculated for this peak. All peaks within this time window will be included in the summary. If two or more peaks are detected in the time window, the peak that is nearest to the specified retention time will be selected. If the peak is an identified peak, this will be indicated by **Ambiguous?** in the **Summary** header.

Creating a Summary

- Double-click one of the samples to open the Integration window.

- Display the Report and select the default worksheet **Summary** available in the Dionex Chromatography Management System. It contains a selection of the most important default ⇒*Peak Variables*. For each sample that is part of the Summary, a separate line is reserved in the report.
- If the default Summary Report is not available, a new worksheet can be defined. Proceed as described in: **How to ...: Actions in the Report Adding/Renaming a Worksheet.**

As in all reports, the currently selected sample in the chromatogram window is highlighted in the Summary Table.

History Report

The default ⇒*Report Definition Files* include both, an **Integration Report** and a **Calibration Report** but no history report. However, you can include it without problems (see: **How to ...: Actions in the Report Adding/Renaming a Worksheet**).

Contents

- As default, the history report shows the ➢*History* of the current sample. The **Objects** tab of the **Table Properties** (context menu), however, allows displaying the histories of other objects.
- In addition, you can limit the displayed history as to time and/or certain actions / users.

Formatting

- The entries of the history report can be sorted according to specific details.
- The history mode includes a special layout mode that can be activated on the **Layout** tab.

Special Reports

The default ⇒*Report Definition Files* include both, an **Integration Report** and a **Calibration Report** but none of these special reports. However, you can include them without problems (see: **How to ... Actions in the Report Adding/Renaming a Worksheet)**.

MS-Reports

MS Instrument Info Report	Information on the ➢*Mass Spectrometer*.
MS Instrument Method Report	MS method.
MS Raw Report	Raw data of the current ➢*Mass Spectrum*.
MS Status Log Report	Mass spectrometer settings.
MS Tune Data Report	Tune data of the ➢*Xcalibur* raw data file.

Note: If you do not have the **MS Control** option enabled on your PC, the MS reports will not be displayed in the **Insert Report** dialog.

Other Special Reports

Database Query	Results of a database query.
Detection Parameter Report	Indicates the⇒ *Detection Parameters*.
Program Report	➢*Program* of the current sample.
SST Report	➢*System Suitability Test*.

Note: All MS reports as well as the Database Query report, the Detection Parameter Report, and the Program Report comprise the default columns only; further columns cannot be added.

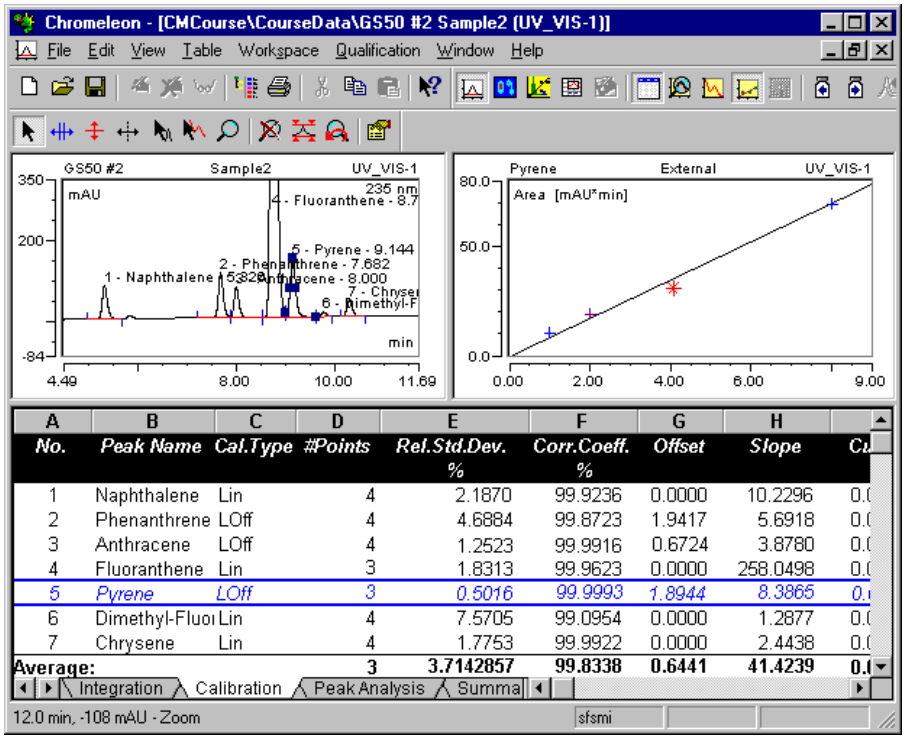
Calibration Curve

Calibration Curve

For evaluating the calibration, the **Calibration Curve** method window is available. Detailed background information on the calibration is included in the  **Theory of Calibration** section.

- Open the window from a different method (e.g. from the **Integration** window) by choosing the **Show Calibration Curve** command from the **View** menu, or
- Click the corresponding icon on the toolbar.

As shown via the methods **QNT Editor** and **Integration**, various window sections can be displayed. Generally, the window arrangement consists of the **Chromatogram**, **Calibration curve**, and **Report** windows.



- Press F4 or Shift+F4 to change to the chromatogram of a different sample. Generally, all chromatograms of a sequence can be thus displayed on after the other.
- In the chromatogram, select the peak for which you want to see the calibration curve. The corresponding peak will be indicated by a different background color.
- The **Calibration** tab of the **Report** window shows the most important calibration data such as the ⇒*Calibration Type*, the number of calibration points, the ➢*Relative Standard Deviation* (Rel.Std.Dev.), the ➢*Correlation Coefficients* as well as the calibration coefficients ➢*Offset*, ➢*Slope*, and ➢*Curve* (Offset c0, Slope c1, Curve c2). In addition, you can view e.g. the ➢*Variance* or the ➢*Standard Deviation* (Std.Dev.).
- Choose the **Decoration** command of the context menu to change the colors and the captions of various window elements.

- Choose the **Column Properties** or **Table Properties** command of the context menu to change the contents and the layout of the table. For further details refer to **How to ...:** **Actions in the Report**.

Note: We would like to point out that the Dionex Chromatography Management System's default division of the report variables in the Integration report, the calibration report and the peak summary is not binding. Each one of the three reports is freely configurable and can be supplied with any variables or renamed as any new report.

Printer Layout

Printer Layout: Overview

The increasing number of samples makes printing analytical results a complex and time-consuming procedure especially because results are not only used on hardcopy but in all types of presentations.

The Dionex Chromatography Management System considers this fact and emphasizes flexible report generation that meets all your requirements. Use the appropriate **Report Template** to produce reports. With each installation of the Dionex Chromatography Management System, the respective DEFAULT report template is stored in the REPORT directory of the Client PC.

- Choose the **Printer Layout** command from the **View** menu to open a new report template.

Note: For further printing options, see **Basic Operation** **Printing**.

Report Template

The report template represents a type of folder for various worksheets. Each sheet describes one or several printed pages (size of the chromatogram, where to position it, columns included in the numerical report, results represented in a chart, what is included in headers and footers).

With an increasing number of worksheets in the report template, the printing possibilities also increase. If, for example, you want to print all samples of one sequence, it may be a good idea to present the results of a calibration sample differently from the unknown samples, and the lines of a PGM file or summary report in yet another way. Specify which sample or file type should be printed and worksheet to be used.

The DEFAULT report template contains the worksheets **Integration**, **Calibration (Curr.Peak)**, **Calibration (Batch)**, **Peak Analysis**, **Summary**, and **Audit Trail**, and, thus, covers all default requirements.

If the report template consists of only one worksheet, it includes a single template. These are used to print a single object such as a ➢*PGM File* or the

result of a single sample. If a single template is used for an entire sequence, *all* samples are printed in the same way.

For details, see the topics below:

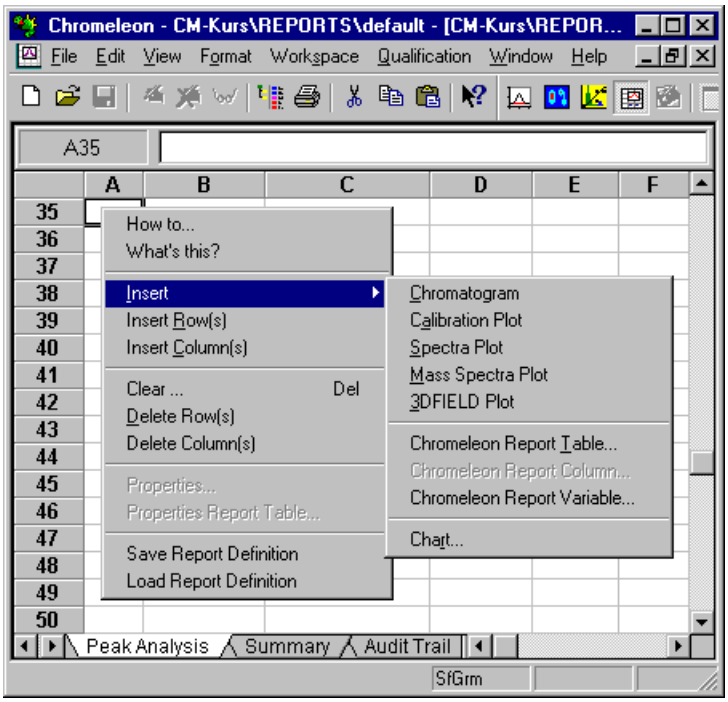
Appearance and Function

Creating Your Own Templates and Worksheets

Printing

Appearance and Function

Important features of a report template are:



- The appearance and the structure of report templates are similar to Microsoft Excel. The functional scope is similar to Excel as well. For entering formulas and for creating diagrams, the ➢*Report Publisher* is required, which is an add-on product to the Dionex Chromatography Management System.

- Toggling between the individual sheets of a report template is by clicking on the tabs on the lower left window corner.
- Double-click a tab to assign a name to it (e.g. **Integration Special**).
- Each sheet consists of a large number of columns (256) and lines (16000).
- Choose **Insert Row(s)/Column(s)** or **Delete Row(s)/Column(s)** to insert columns or to delete columns or lines on the worksheet.
- Single areas or cells of a worksheet can be "filled" using the Windows clipboard or via the **Insert ...** command from the context menu (for details, see **Creating Your Own Templates and Worksheets**).

☞ ***Tip***: Note that you can place several report tables on a worksheet. The tables, however, must be positioned one below the other, not next to each other!

The worksheets that are virtually unrestricted in horizontal and vertical direction, allow creating page layouts larger that one printed page. Depending on the selected page size on the printer, one or several pages are required for printing this type of page layout. The worksheet is divided in many invisible horizontally and/or vertically positioned print pages.

If the user, for example, inserts a chromatogram that does not fit on one page, the rest is printed on a new page.

- Via the **Page Setup** command from the **File** menu, you can specify in which order ("from left to right" or "top to bottom") the printed pages of a worksheet are printed.

Creating Templates and Worksheets

In addition to the included default report templates, the Dionex Chromatography Management System allows you to create your own report templates. Perform the following steps:

- Select the **Printer Layout** command in the **View** menu to change to the **Printer Layout** from your currently selected view. The Dionex Chromatography Management System automatically opens the default report template. Use the **Load Report Definition** command of the context menu to open a specific report template.

Note: If only the default report template is available in your system, save it under a new name via the **Save Report Definition** command. Now you can edit the duplicate as follows:

- Choose **Layout Mode** command from the **Edit** menu to perform manual changes on the report template.
- Choose the worksheet you wish to edit, or insert an additional (empty) worksheet via the **Insert Sheet** command (**Edit** menu).
- Choose **Delete Sheet** (**Edit** menu) to delete a superfluous worksheet.
- Choose **Insert ...** in the context menu to position chromatograms, tables, diagrams, report variables or similar elements on the worksheet.

Caution: Note that you can place several report tables on a worksheet. The tables, however, must be positioned one below the other, not next to each other!

Each element inserted in this way reserves a specific area on the worksheet. If a report template or a single worksheet serves as a print template, these areas are "filled" with the values or graphics of the current sample. It is also possible to determine whether the printed output includes data and chromatograms of all channels of a sample or only of one channel.

Note: In addition to report variables that can be combined to form new functions via the four basic arithmetical operations (plus powers), it is possible to calculate additional functions known from Microsoft Excel. For a list of supported functions, see ➢*Additional Functions* in the Glossary.

For detailed information on creating worksheets and report templates, see **How to ...: Actions in the Printer Layout**.

Printing

From the Printer Layout

The Printer Layout allows printing the created report template at any time.

- Choose **Print** from the **File** menu to start printing.
- Press **Preview** in the **Print** dialog box to preview the layout of the printed output.

The printed output uses the data of the current sample with the layout of the currently opened sheet.

From the Browser

Use the Browser to print larger quantities of data. The Browser allows printing single samples and entire sample series.

- Use the mouse to select the samples to print. If you want to print all samples of one ore several sequences, just select the corresponding sequence(s).
- Perform a ➢*Query* to use samples from several sequences.
- Choose **Batch Report ...** from the context menu and select the **Report Definition** to be used for the printed output. Also, choose the channel to print and specify the printer.

In addition to the results, it is possible to print sample data, i.e., the information in the sample list.

- Open a sample list and choose **Print Table ...** from the context menu.

PPA

PPA: Peak Purity Analysis

Caution: The basic requirement for using the PPA method is the availability of a Dionex ➢*Photodiode Array Detector*. In this case, the data supplied by a detector can be "read" and viewed on any client PC. The most common method to relate chromatograms to spectra is the representation of data in a ➢*3D-field* in the method PPA. The 3D-field is the default view in the **iso-pixel plot** representation.

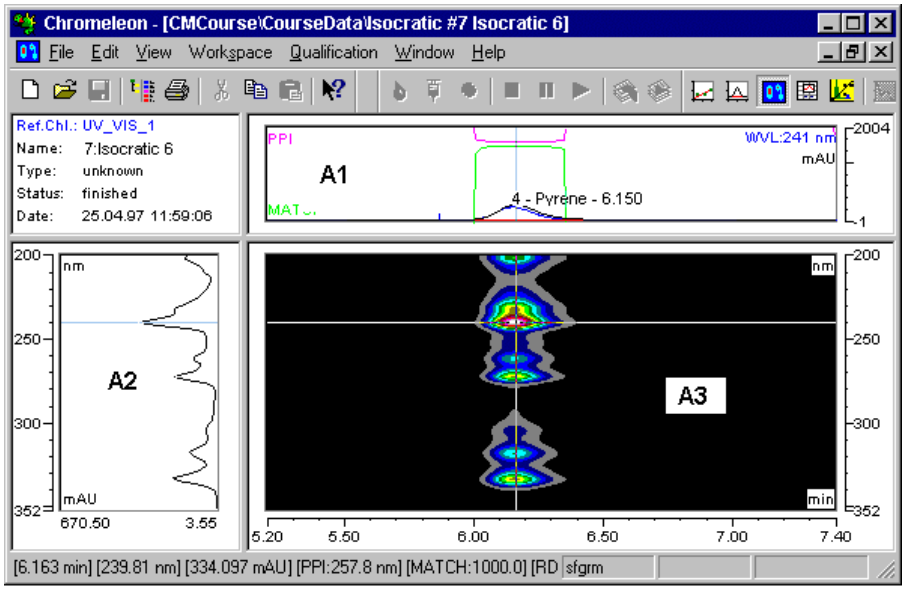
Use one of the following methods to view a sample (for which you have the corresponding 3D-raw data) in the method PPA:

- Select the sample in the Browser and choose the **Open / 3DFIELD** command from the context menu, or
- Change from a different method to the PPA method. Use the icon or the **PPA** command from the **View** menu.

View and Operation

In the default view, the method window is divided in four sections. The 3D-field window (A3) is the most important section. Choose either the **Iso Pixel Plot** or the **3D-Plot** (see ➢*3D-Field Presentation Modes*).

The cross-wires that are freely positioned via the left mouse button or the arrow keys "extract" a chromatogram at a specific wavelength in horizontal orientation from the plot representation. In vertical orientation, a spectrum is extracted at the time t and is displayed above (A1) or next (A2) to the 3D-field (A3). Use the ➢*Zoom* function for a more detailed view.



The display of the window sections A1 and A2 can be enabled or disabled via the **Show Chromatogram** or **Show Spectra** options. Optionally, an additional numeric report (PPA report) can be displayed (**Show Report**). The line of the currently selected peak is highlighted by a different color.

In addition to the context menu commands that allow undoing a **Zoom** operation, restoring the original 3D-field, selecting a different 3D representation, or displaying additional information such as the ➢*PPI Index*, ➢*Match Factor*, etc., there are additional operations that can be executed via the keyboard or a mouse-click.

- Double-clicking in the A3 windows opens the 3D-field Decorations ... dialog box.
- Pressing the right mouse button while the 3D-field is redrawn stops redrawing. This option is useful when the wrong zoom area was chosen.
- Double-clicking the time axis of the window executes the **Full Size** command. In the wavelength scaling, the same operation performs the **Autoscale** command.

- Pressing the CTRL key makes the currently displayed spectrum in the spectra window "permanent," i.e., it is still displayed even when moving the cross-wires. The spectrum extracted via the cross-wires is displayed in addition. If the operation is performed several times, any number of individual spectra can be displayed in the spectra window.
- It is also possible to combine pressing the CTRL key and moving the cross-wires: Position the x-axis of the cross-wires on the required wavelength and press the CTRL key. Then move the y-axis over a peak in the chromatogram. The spectra window now shows all spectra within the covered range. This procedure can be performed for various peaks in a chromatogram. Release the CTRL key between the individual peaks to represent each peak in a different color. For each peak, a number of spectra can thus be displayed.
- If the y-axis of the cross-wires is located on a peak, the peak spectrum (= spectrum in the peak maximum) can be copied to the Windows clipboard via the **Copy** command. From there, the spectrum can be included in the spectra library. For this operation, approximately positioning the y-axis is sufficient.
- Choose one of the **Extract: ...** commands to extract the current chromatogram, the optimum integration path, the current spectrum or the 3D-field data and save the item under a separate name. For a description of the required steps, see **How to ...: Actions in the PPA Window** **Extracting Spectra, Chromatograms, and 3D-Field Data**, and **Selecting the Optimum Integration Path**.

Note: Copying or printing a 3D-plot is more time-consuming than copying or printing the Iso-plot!

- Choose the **Library Search** command from the context menu to search the spectra library for the displayed spectrum. For a detailed description of the required steps, see **How to ...: Actions in the UV Spectra and Mass Spectra** **Starting a UV Spectra Search**.

Function

The PPA method allows the following:

- Peak purity analysis (see **How to ...: Actions in the PPA Window** **Checking Peak Purity**).
- Interactive peak assignment via the spectrum
- Extraction of chromatograms, spectra, and the optimum integration path (see **How to ...: Actions in the PPA Window** **Selecting the Optimum Integration Path**, and **Extracting Spectra, Chromatograms, and 3D-Field Data**).
- Visualization of chromatograms for presentation and archiving purposes
- Evaluation of baseline effects
- Checking the Lambert-Beer linearity range
- Quantitative analysis of overlapping peaks

These methods are completed by various procedures and calculations that enable interpreting or comparing results. These include:

➢*Baseline Correction*

➢*Blank Run Subtraction*

➢*Normalization*

➢*PPI: Peak Purity Index*

➢*PPI: Match Factor*

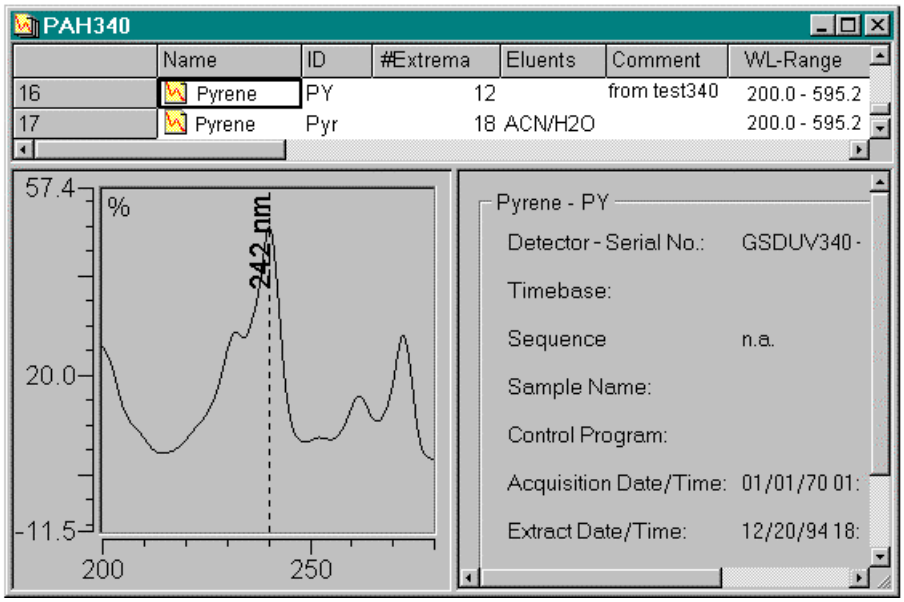
Spectra Library

Overview: Spectra Library

The partial method **Spectra library** enables the comparison of ➢*Normalized* and ➢*baseline-corrected* individual spectra with spectra from various libraries. There are three sections:

Spectra Table

The upper section indicates all spectra contained in a library as well as their data (= ➢*Spectra Criteria*). Double-clicking a column header sorts the list according to the criteria of the selected column (e.g. name, ID, or number of extremes). Select the first column of the table to select the corresponding spectrum.



- As soon as you move the mouse cursor over the first column, the cursor changes to a horizontal arrow. Press the left mouse button to select a spectrum.
- Press and hold the CTRL key to select several spectra.

Spectra Plot

The spectra plot is shown in the lower left window section. It shows the spectra of all substances selected in the spectra table.

- Double-click the window or choose the **Decoration...** command of the context menu to change the spectra representation. For details, see **Spectra Plot** in the **Integration** chapter.

Data Window

The lower right window section of the Spectra Library is reserved for representing the data. It shows important data regarding the spectrum currently selected in the spectra table.

Working with the Spectra Library

The aim of any spectra administration is the identification of an unknown substance based on its UV spectrum. If you have a spectrum of a previously unidentified substance (e.g. in the spectra window of the PPA method), you can start searching various libraries from there.

The Dionex Chromatography Management System compares the curve form of the two spectra (comparison process), calculates a similarity value (evaluation process), and displays similar spectra (hit criterion).

Depending on whether a single spectrum is identified or whether all peaks of a sample were identified, the Dionex Chromatography Management System makes the following distinction:

Hit List

This procedure shows all library spectra that have a certain similarity to the extracted (and normalized) spectrum. For details, see **How to ...: Actions in the UV Spectra and Mass Spectra Starting a UV Spectra Search**.

Peak Tracking

This procedure assigns each peak in a chromatogram the spectrum of a library that matches the spectrum extracted at the peak maximum best.

For further details on the Spectra Library, see the topics below:

Creating a New Library

Comparing Spectra

Creating a New Library

Generating

Choose **File / New** to open a new and empty spectra library by selecting the type **Spectra Library**.

Filling

There are two options for filling a spectra library:

- Copy a spectrum to the Windows clipboard (**Copy**) from the partial methods **How to ...: PPA: Peak Purity Analysis** or **Integration Spectra Plot** and insert it in the opened library via **Paste Spectra**. Or:
- Generate a subset of an existing selection based on specific ➢*Hit Criteria*.

Note: To be able to compare UV spectra with each other, the spectrum and the reference spectrum should be recorded under identical conditions. The best search results are therefore obtained based on spectra that were recorded and saved by the user. It is highly recommended to write down the conditions under which the spectrum is recorded. The notes will be very useful when there are several spectra for the same sample.

Saving

Via the **Save as** command, save an open library under a different name to a directory of your choice. Libraries have the file extension **LIB**.

Comparing Spectra

To compare two spectra with each other, the curve of the normalized spectrum can be compared to those of individual library spectra. In some cases, better results are achieved when the first or second derivations are compared instead of the spectra themselves.

Via the comparison function (see ⇒*Check Derivative*), the user determines the curve form to be used for the comparison.

In the next step, the user determines how the individual curves are compared with each other. This is by selecting one of three mathematical methods (⇒*Match Criterion*).

The combination of comparison function and standard of comparison results in a "similarity value" between 0 and 1000 that expresses the match degree between the search spectrum and various library spectra. The similarity value is known as ➢*Match Factor*. A perfect match has the value 1000.

Depending on the method (hit list or peak tracking), a similarity list is displayed or each peak is assigned the most similar spectrum. Entering a minimum similarity value (threshold) displays only the hits above the threshold.

For a detailed introduction to the required steps in a spectra search, see **How to ...: Actions in the UV Spectra and Mass Spectra Starting a UV Spectra Search.**

Result Presentation in a Hit List

Using the hit list, a similarity list sorted by the match factor and a representation of the original spectrum and the library spectrum with the best match are displayed. Entering a minimum similarity value excludes dissimilar spectra.

Due to the frequently insufficient characteristics of UV spectra, it may be necessary to further limit these hit lists. That is why ➢*Hit Criteria* are available as a further filter. Only the spectra fulfilling the selected criteria will be displayed.

How to ...:

Actions in the Browser

The **Browser** serves to manage, copy, move, and delete chromatographic data and files.

Warning: Its functions are similar to the Windows Explorer. However, do not the confuse Browser window with the Windows Explorer! Do not use the Windows Explorer for operations within the datasource of the Dionex Chromatography Management System.

In addition, the Browser allows creating a sample list, setting up datasources, searching and selecting data in a database. For further details, see:

- **Creating a Sample List (Sequence Table)**
- **Creating User-defined Columns**
- **Setting up a Datasource**
- **Creating SQL Server Databases**
- **Handling Files, Datasources, and the Network**
- **Signing Sequences Electronically**
- **Performing a Query**
- **Performing the Chromeleon/PeakNet OQ**
- **System Wellness**
- **Importing PeakNet Method Files (Release 4.5 Through 5.2)**

Creating a Sample List (Sequence Table)

For creating a **Sample List**, there are the following two possibilities:

1. Manually editing an existing sequence and saving them under a different name
2. Automatically creating a new sequence using the Sequence Wizard

Proceed as follows:

Manually

- Select a sequence in the left pane of the **Browser** whose QNT and ➢*PGM File* you wish to use (probably edited) for the new sequence. Saving the sequence under a different name (**Save as**) creates a new sequence that can now be edited.
- Enter the name and the properties of the standard samples and the unknown samples to be analyzed line by line in the lower right window section. Proceed as follows:
- Click the cell in the table and enter the new value or the name via the keyboard.
- Enter a name for each of the samples to be analyzed in the ⇒*Name* (sample name) column.
- Determine the sample type (**Unknown/Standard/Blank Run/Validate**) via ⇒*Type*.
- Determine the autosampler position and the substance volume via the ⇒*Pos.* (sample position) and ⇒*Inj. Vol.* (injection volume) columns.
- In the ⇒*Program* and ⇒*Method* columns, enter the names of the ➢*Chromatographic Methods* to be used for the analysis.
- Determine via the sample ⇒*Status* (sample status) whether to process a sample once (**Single**) or several times (**Multiple**).
- To analyze two unknown samples (Sample I and II) on the basis of a 2-point calibration the input can be as follows:

	Name	Type	Pos	Inj.Vol	Program	Method	Status
1	STD 1	Standard	1	10.0	Control1	QNT1	Single
2	STD 1	Standard	1	20.0	Control1	QNT1	Single
3	Sample I	Unknown	2	10.0	Control1	QNT1	Single
4	Sample II	Unknown	3	10.0	Control1	QNT1	Single

- Input in the remaining columns, e.g., ⇒*Weight* (sample weight), ⇒*Dil. Factor* (dilution factor) and ⇒*Inj. Date/Time* is not necessary. These special parameters or fields are automatically filled by the system after the analysis.

- If you are not sure which values or names to enter, select the cell and press the **F8 key**. This opens an edit dialog box, in which values and options are listed that are valid. Select the desired value. The cell input is then automatically updated.
- Press the **F1 key** to view further information on the individual columns.
- Select the **F9 key** to fill all subsequent cells of a column with the same input.
- Save the sequence with a new name (**Save as**).
- Check the sequence properties by pressing **Alt** + **Enter**.

Note: It is of course possible to edit an existing sequence. Exception: A currently running sample cannot be edited (the corresponding line in the sample list is indicated by a different color).

Automatically

- Select the **New** item in the **File** menu and select **Sample List**.
- Press **OK** to start the **Sequence Wizard**.
- Follow the instructions from steps 1 to 5 to create a basic sequence structure.
- Press F1 if you require further help.

Also, see **Creating User-defined Columns**

Creating User-defined Columns

In addition to the existing columns, new columns can be created both, in the sample list of the **Browser** and in the peak table of the QNT editor as follows:

1. a) In the Browser sample list: Click the datasource for whose sequences the new columns will be displayed and select **Properties** in the context menu. In the dialog box, open the **User-defined Columns** tab.

b) In the peak table of the QNT editor: Click **Display User-defined Columns ...** under **Columns** in the context or **Edit** menu.

2. Under **Columns**, select **<New user-defined column>** to activate the right part under **Properties**.
3. Under **Name**, type the desired caption for the new column.

Note: When entering the name, keep the following restrictions in mind:

- Use characters, numbers, and the underscore only. The first character must be a letter.
- Do not use the German "Umlaute" and "ß".
- Names starting with **SEQ_** or **SMP_** are not permitted.
- In addition, names that are already used as SQL keywords (e.g., INTEGER), we recommend placing a company prefix before the desired caption (e.g., with DX=Dionex: DX_INTEGER). This avoids collisions with already used SQL keywords. Thus, having the further advantage that user-defined column will be recognized instantly.
- Names of columns that have been deleted in the current 'dialog session', cannot be entered again. Close and open the dialog box, to re-enter these names.

4. Use **Value type**: to define the type for the values in the new column:
   - Integer (whole numbers)
   - Floating point (numbers with a defined number of decimal points)
   - Date
   - Time
   - Date and Time
   - Enumeration (open the combo box to select an item from the list)
   - String (any sequence of characters)
5. Define the dimension for the values in the new column.
6. Depending on the selected type of variable, further specifications can be set for the column.

Note: Due to the restrictions of the operating system, dates can be entered for the period 1/2/1970 - 12/30/2037, only.

7. Use the **Append Column** command to add the new column to the list. Pressing OK appends the new column to the existing ones.

The new column, which was created in the sample list of the Browser, applies to the entire ➢*Datasource*, i.e., it is used for all ➢*Sequences* of the respective datasource.

Tip: Be careful when creating user-defined columns in the Browser sample list. Ensure that you do not assign column names twice in the different datasources and even on different computers that may communicate with each other. Otherwise, unless the column definitions are identical, problems may occur when copying sequences or when **Restoring** backup files.

Setting up a Datasource

All steps connected with the **Datasource** setup are initiated using the **Datasources** command in the **File** menu.

- Open the ➢*Browser* and choose the **Datasources** command from the **File** menu.

The datasource manager lists all Datasources that can be accessed by the Client.

Note: As a minimum, the default datasource (<PC-NAME_LOCAL>) created during the installation of the Dionex Chromatography Management System should be visible here. In case of a local station that is not integrated in a network, the name entered in the operating system under **Control Panel / Network / Identification** is used instead of the computer name. If no identification was entered, the datasource receives the name **DEFAULT_LOCAL**.

The following actions are possible:

Connecting a Database ("Connect")

Disconnecting a Database ("Disconnect")

Creating a New Database ("New")

Note: GynkoSoft data and third-party data are regarded as existing databases to the Dionex Chromatography Management System. To display these data in the Dionex Chromatography Management System; a connection must be available to the corresponding directory (**Connect**). Setup of a new datasource is not required.

Connecting a Database

Accessing data of an existing database is possible only for the client, if a connection is available between the Client and the database.

- Open the ➢*Browser* and choose the **Datasources** command.
- Select the **Connect** button in the datasource manager to establish a connection to a datasource.
- Select the type of the underlying datasource.

Currently, connection is possible to genuine database of the Dionex Chromatography Management System ("Native Chromeleon Datasource"), "old" directories of the GynkoSoft chromatography data system (= "GynkoSoft Drives" as of version 5.xx), standard Microsoft Access databases ("mdb containers"), SQL, and Oracle databases. Support for other formats will be made available in future versions.

Depending on the datasource type, different input is required, e.g.:

- In the case of Access datasources, the mdb container must be specified,
- For GynkoSoft datasources, a directory must be specified, and
- For SQL data sources, the dialog of the ODBC driver will be opened.

Note: If you want to include databases in *SQL* or *ORACLE* formats, see to the information in the corresponding Online Help sections.

Disconnecting a Database

The ➢*Datasource* can be disconnected at any time, if necessary.

- Open the ➢*Browser* and perform the **Datasources** command.
- Select the datasource in the datasource manager and press the **Disconnect** button.

Via this method, a client can be denied access (e.g. by the system administrator) to a specific datasource.

Note: The connection to a datasource can also be terminated via the **Dismount Datasource** command from the context menu. For details on the Mount/Dismount Datasource commands, see **How to ...: Actions in the Browser Locking Datasources on Removable Media**.

Creating a New Database ("New")

The Dionex Chromatography Management System enables setting up a datasource with a new database. The new database is always in the Microsoft **Access** database format (mdb container).

- Open the ➢*Browser* and choose the **Datasources** command from the **File** menu.
- Select **New** to create a new database.
- Enter the name of the new datasource. This name will be displayed in the Browser.
- Enter the path of an empty subdirectory in which to store the database for the new datasource. Use the **Browse** button to search for an empty directory.

Tip: Creating a database is possible only if the selected directory is empty!

- Activate **Common Data Source** if the ➢*Server* of the Dionex Chromatography Management System shall be able to access this datasource. Processing sequences is possible only on datasources with activated Common Data Source setting.

Note: The local datasource is always selected as **Common Data Source**.

- If a datasource is not defined as Common Data Source under Windows NT/Windows 2000, the datasource must be set up for each potential user.

Upon completing the procedure (**OK**), the Dionex Chromatography Management System generates a database called **cm_local.mdb** in the selected directory. Databases with different formats cannot be generated in the Dionex Chromatography Management System but must be created with the respective database software, instead (also, see **Creating an SQL Server Database**).

Creating an MS SQL Server Database

In order to use Microsoft SQL Server as the database management system for a Chromeleon datasource, proceed as follows:

Create the SQL Database via the SQL Enterprise Manager

Create the Folder Structure for Data

Connecting the Dionex Chromatography Management System to the SQL Database

Tip: A similar procedure is followed with the ➢*CmUser* Manager if the user database is to be located on an SQL Server. The third step of the procedure differs in that connection to the database is done through the CmUser Manager application rather than through the Client application of the Dionex Chromatography Management System.

Creating the SQL Database via the SQL Enterprise Manager

☞ ***Tip:*** This guide only provides specific details relevant to the Dionex Chromatography Management System for creating an SQL database. For general instructions on installing MS SQL Server and creating a database, refer to the Microsoft MS SQL Server documentation.

- Create a ➢*Database* through the SQL Enterprise Name using the default settings.
- Give the new database a meaningful name (this will be used in the ODBC connection.
- Assign at least two users to the database -- an administrator and a normal user -- using the SQL login (create specific users for the database).

Administrator

The administrator account is used to set up and manage the database of the Dionex Chromatography Management System, so full privileges should be granted to this account. Essential privileges are those for creating tables and views; all the tables are created at the time the administrator first connects to the database via Dionex Chromatography Management System. (A typical name for the administrator would be CMADMIN.)

Normal User

This is the normal user account that connects to the database via the Dionex Chromatography Management System during normal operation. This account must have the following two privileges for the database of the Dionex Chromatography Management System:

- db_datareader
- db_datawriter

Further privileges are not necessary in order to access the data through the Dionex Chromatography Management System later on. (A typical name for the common user would be CMUSER or simply CM.)

Tip: The SQL login is required to impersonate the user on the database. Once the connection is made, any user can log in to Chromeleon, subject to the access rights and privileges set in the security system of the Dionex Chromatography Management System.

For further information on how to create SQL data sources, see **How to ...: Actions in the Browser**:

Create the Folder Structure for Data

Connecting the Dionex Chromatography Management System to the SQL Database

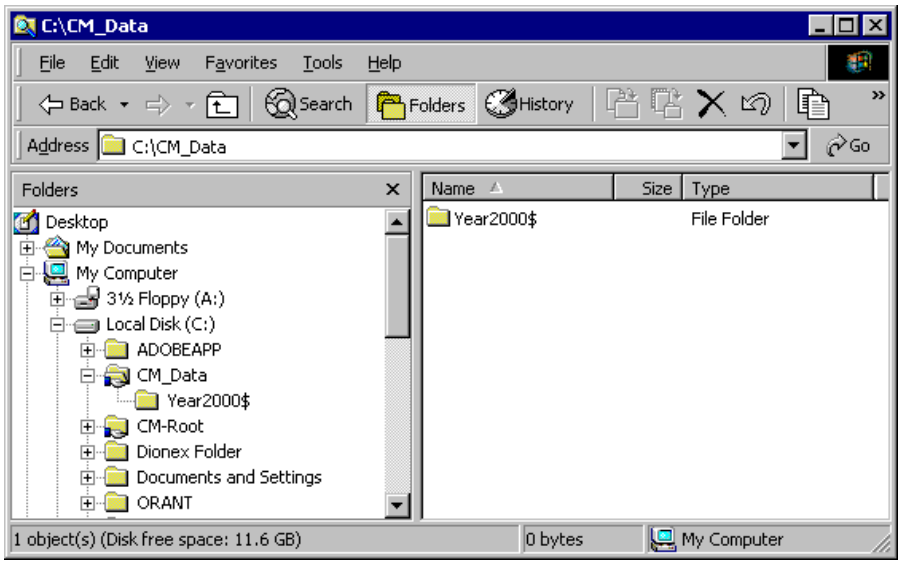
Creating the Folder Structure for Data

The data storage model of the Dionex Chromatography Management System consists of a hierarchical file system that is indexed by a relational database. Before connecting to an SQL ➢*Datasource*, define the location of the parent folder of the file system. This folder does not need to be on the same computer that is running the SQL server application, but keeping them on the same computer makes administration, backup, and archiving easier.

Create a master shared folder for the file system. (This example has this folder on the PC that is hosting the database.) Dionex recommends sharing it as an administrator share that it is not visible in the network. The users need to have **Modify** privileges only. Under this master folder, create a folder in which to store the data. For this folder Modify privileges will be sufficient. Dionex recommends appending the **$** character to the folder name to prevent display of the total path in the status bar and the window title. Example:

Folder structure on the PC **MySQLServer** assuming drive C:

C:\CM_Data\Year2000$



For example, **Year2000$** is a folder in which all data for the year 2000 will be stored.

In this case, the **data set path** entered in the **Connect Data Source** dialog of the Dionex Chromatography Management System will be **\\My SQL-Server\CM_Data$\Year2000$**.

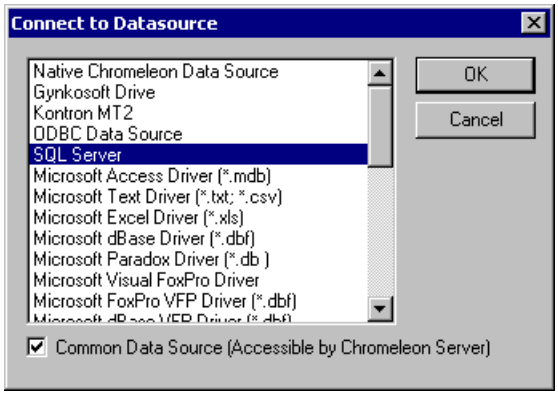
For further information on how to create SQL data sources, see **How to ...: Actions in the Browser**:

Create the SQL Database via the SQL Enterprise Manager

Connecting the Dionex Chromatography Management System to the SQL Database

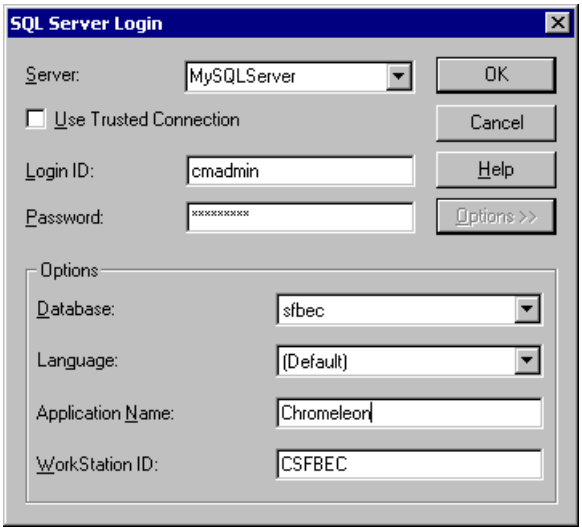
Connecting the Dionex Chromatography Management System to the SQL Database

Log in to the Dionex Chromatography Management System with full administrator privileges at the operating system and application levels. From within Chromeleon, connect to the SQL database via the **Datasources** command of the **File** menu. In the opening dialog box, press **Connect** and from the driver list, choose **SQL Server**. If the instrument ➢*Server* application of the Dionex Chromatography Management System is running on the local machine, and if the application needs to access the ➢*Datasource*, be sure to select the **Common Data Source (Accessible by Chromeleon Server)** check box.

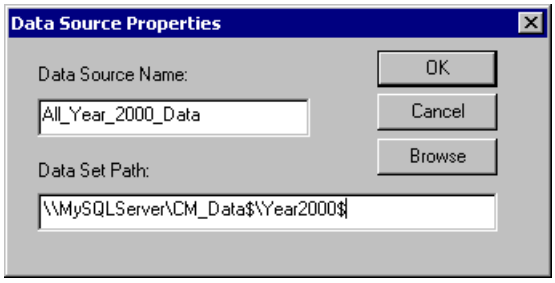


The next dialog prompts for the connection information to the SQL database:

Select the PC that is running the SQL Server application. Log in as administrator to select the database that was created via the SQL Enterprise Manager. Leave the **Application Name** as is (default: Chromeleon):



In the next dialog, enter the name of the data source, as you want it to be displayed in Chromeleon, and specify the data set path:



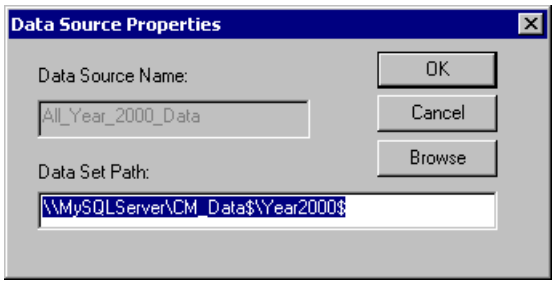
In the example, the datasource will appear in Chromeleon's Browser with the name **All_Year_2000_Data**.

The **Data Set Path** is the path to the shared folder containing the data folder **Year2000$**, as created in the first step of this procedure. Dionex recommends using the UNC naming convention, as shown in the example, so that Chromeleon can find the location of the data automatically if the applications are loaded at system start (boot time). A drive mapping is only applied if a user logs on.

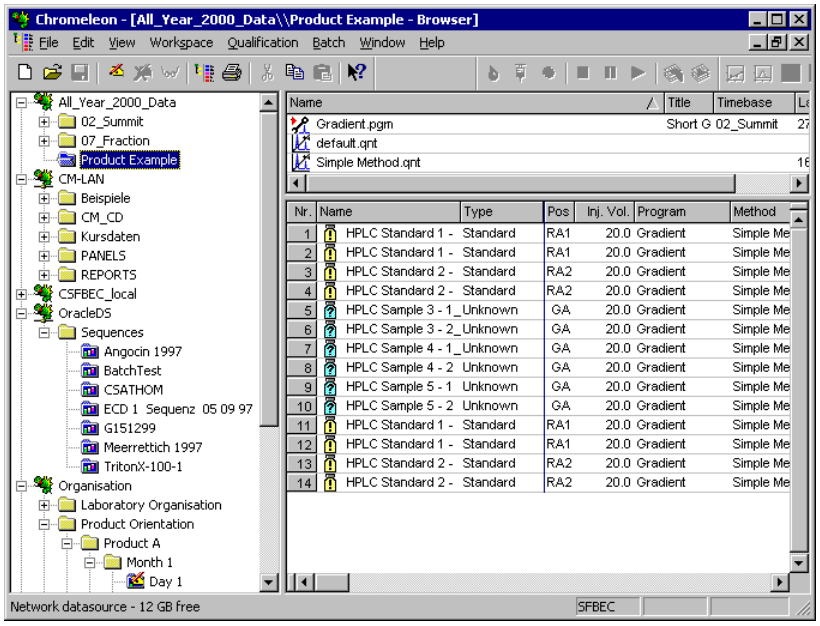
After following the above steps, the new data source is automatically created and configured with all tables except those related to Modification History, which are only created when they are needed. For maximum flexibility, the administrator should create these tables even if they will not be used immediately. To create these tables, select the data source in the folder tree of the Browser, select **Properties** in the **File** menu. Then select Enable **Modification History**, and **OK**. All tables will now be available for the Normal User. (If you do not currently want to maintain a Modification History for the data source, return to the **Properties** dialog and de-select the check box.)

At this point, the administrative setup is complete. Use the Dismount command of the context menu to disconnect the SQL data source, and re-connect as the Normal User. Follow the same procedure as above, but use the Normal User's user name and password.

In the following dialog, the Data Source Name will be grayed out, because the administrator assigned this name. In addition, the Data Set Path will default to the path stored in the data source; do not change this entry.



The connection to the MS SQL Server database is finished. Now, data may be copied from any other data source to the new data source. The example shows several different data sources. On the top is the newly created MS SQL Server data source, followed by a local Microsoft Access data source and a network-based Oracle data source. They look all the same for the user.



Servers and Network Datasources of the Dionex Chromatography Management System

Users often want to store acquired data directly on a central database somewhere in the network. In this case, the server application of the Dionex Chromatography Management System on the local machine needs to have a separate account that is known to the target machine that is hosting the database. It is typically a domain account that is generic to all servers of the Dionex Chromatography Management System in the net. This account must be assigned in the operating system services (Windows NT and Windows 2000 Professional) to the Chromeleon Server service **The Dionex Chromatography Management System under Windows 98 and Windows NT/Windows 2000)**. This account must be made part of the **Chromeleon Operators Group** on the operating system level.

For further information on how to create SQL datasources, see **How to ...: Actions in the Browser**:

Create the SQL Database via the SQL Enterprise Manager

Create the Folder Structure for Data

Handling Files, Datasources, and the Network

When working with your Dionex Chromatography Management System, you will surely collect many data. To handle, store, and save them in the best possible way, the Dionex Chromatography Management System offers different possibilities:

- **Locking Datasources on Removable Media**
- **Locking Datasources, Directories, and Sequences**
- **Repairing a Datasource (ODBC Manager)**
- **Opening Protocol Data ("Audit Trails")**
- **Network Failure / Non-Availability**
- **Creating Backup Files**
- **Restoring Backup Files**

Locking Datasources on Removable Media

In addition to the hard disk of the local PC or a network PC, ➢*Datasources* can be installed on removable media, e.g. on diskette, ZIP or CD-ROM drives.

- Choose the **Mount Datasource** command from the **File** menu and select a drive or search for the datasource via the **Browse** command.

The Dionex Chromatography Management System will automatically show the Windows drive letters of all currently available removable media.

- If the Dionex Chromatography Management System finds an existing datasource on the selected media, this datasource is automatically "connected" and is displayed in the Browser as any other datasource.
- If the Dionex Chromatography Management System does not find a datasource on the selected media, the user can install a new datasource on this drive. The datasource will receive the name of the drive.

Note: Datasources in the Microsoft Access database format can be copied to the removable medium. Simply copy the DATA directory of the local datasource of the respective subdirectory of a network datasource to the corresponding removable medium.

***Caution*:** If a connection is established to a datasource on a removable medium via the **Mount Datasource** command, the corresponding medium (diskette, Zip disk, CD ROM) may not be removed until the connection is correctly terminated via the

context **Dismount Datasource**. **Otherwise, the operating system will crash!** command.

Locking Datasources, Directories, and Sequences

To protect data and results, the Dionex Chromatography Management System offers the possibility to lock ➢*Datasources*, directories, or sequences. If the "Locked" status is enabled, it is not possible to modify the corresponding object. This also applies to all objects below the locked object. If, for example, a datasource is locked, all contained directories and sequences are also locked. Locked items can be recognized in the ➢*Browser* by the changed icon (red lock).

To lock an object proceed as follows:

- Select the object in the Browser.
- Choose the **Properties** command via the context menu and activate the **Locked** check box in the edit box.

Repeat these steps to undo the action.

Note: Locking and sharing objects are subject to the **Access Control** and can only be performed by users with the corresponding privilege.

Apart from locking datasources and directories via the **Locked** check box, access can be controlled by adding them to or removing them from ➢*Access Groups*.

- Select the object in the Browser.
- Choose the **Properties** command via the context menu, define the Access group assignment via the Add, and **Remove** buttons.

Accessing datasources and directories is possible only for users who are members of an A-group listed in the **Access Groups**.

Repairing Datasources (ODBC Manager)

Defective datasources can be repaired via the **Datasource Manager** dialog box that is opened by the **Datasources** command of the **File** menu. Select the defective datasource and press the **Repair** button. Your datasource will be automatically repaired - as far as possible.

Among other functions, the repair function is available via the ODBC Manager as well. Normally no modifications are required in the ODBC Manager. Should you need to perform changes, proceed as follows:

- Press the **ODBC Mgr…** button in the Datasource Manager to open the Windows ➢*ODBC* dialog box of the control panel.

Caution: Modifications to the ODBC Manager should be performed by experienced users only. Otherwise, re-installation of the Dionex Chromatography Management System may be necessary. Loss of data may result!

Opening Protocol Data (Audit Trails)

From the Browser, protocol data, e.g. the **Protocol Data (Audit Trails)** of single days (**Daily Protocols**) as well as of single samples (**Sample Protocols**) can be activated.

In the server ➢*Datasource*, daily protocols are located in the **AUDIT** directory under the corresponding ➢*Timebase*. Double-clicking opens the daily protocols.

To view a sample protocol, select the corresponding sample. Choose **Open** via the context menu (right mouse click) and open the sample protocol via **Audit Trail**. Alternatively, you can view sample protocols in the **Report**. Open the sample by double-clicking and select the **Audit Trail** tab.

Network Failure / Non-Availability

In case of a sudden network failure or crash of the network server

If the network fails during data acquisition, the acquisition will not be interrupted even when being performed on a remote ➢*Server* of the Dionex Chromatography Management System. Later, the data acquired during the network failure can be written back to the network datasource.

Wait until the network is available again. Stop the running ➢*Batch* (or wait until it is completed) and select **NFP Recovery** in the **Batch** menu. The server will write all data that were temporarily stored to the local disc during the network failure back to their proper locations on the network datasource. This procedure is logged in the **Audit Trail** as is the network failure.

In some cases, the network recovery can fail due to problems of the ➢*ODBC* or the network driver. If so, restart the server of the Dionex Chromatography Management System upon completion of the batch. In order to ensure that Windows and all other applications work properly we recommend rebooting the PC before.

Note: The ➢*Network Failure Protection* is available **for Windows NT** and **Windows 2000, only**! It is disabled on Windows 98 because these systems are unstable under network failure conditions.

During Backup / Non-Availability of the Network Database

In many companies/organizations, the ➢*Datasource / Database* is not available during the daily backup. In this case, however, it is known when the network will not be available so that the Dionex Chromatography Management System can be disconnected before.

Click the desired datasource or select the **Properties** command in the **File** or context menu. On the **Availability** tab, enter the time for which the datasource is not available. The time interval should start a few minutes before the backup starts.

Creating Backup Files

The Dionex Chromatography Management System offers its own backup program that allows creating backup files including all linked objects.

Before starting the ➢*Backup*, the objects to archive must be selected in the ➢*Browser*. All selection options of the Browser are supported. The backup dialog is then opened via **Export/Backup** from the **File** menu. Backup copies of the following objects can be created:

When selecting...	... a backup copy is created of:
a directory	all subdirectories and the included files, sequences, etc.
sequences	all samples and the files included in the sequence (QNT file and ➢*Program File (PGM File)*).
individual samples	the sequence information (name, directory, title, etc.), the selected samples as well as the ➢*PGM File* and ➢*QNT* file used by these samples.
other files	the corresponding files.

When using the ➢*Query* function in the Browser, the following options are available:

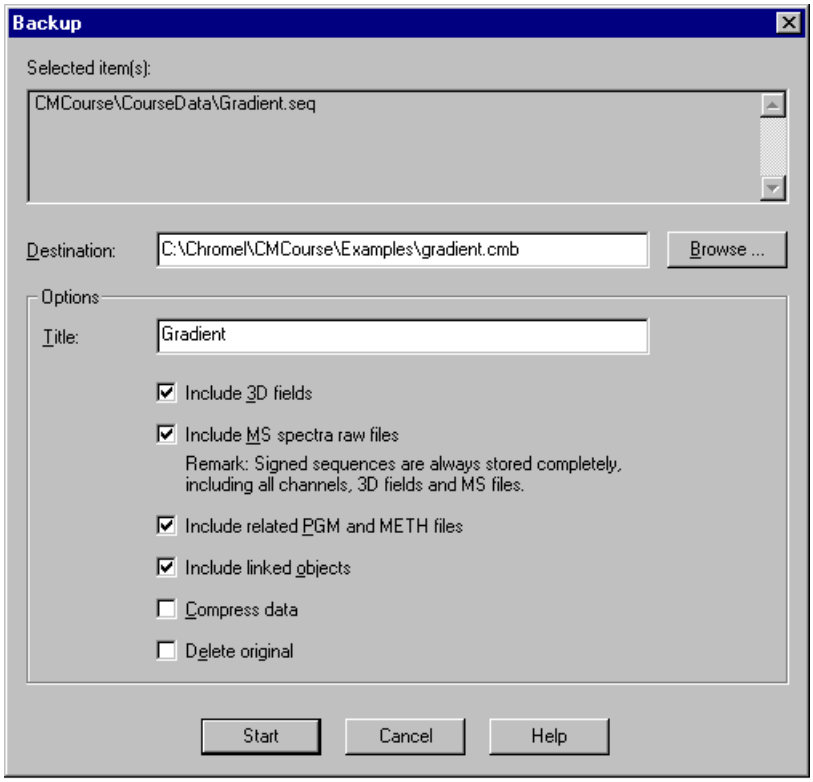
When selecting...	... a backup copy is created of:
individual samples	the sequence information (name, directory, title, etc.), the selected samples as well as the PGM and QNT files used by these samples.
sequences	all samples contained in the ➢*Query* of the corresponding sequence.

The following linked objects are copied when creating the backup:

Object	Link
sequence	Preferred ➢*Report Definition* file (RDF)
peak table	calibration list for the calibration mode "fixed"; blank run sample for blank run subtract mode "fixed sample"; spectra library for Spectra Library Screening.
Query	Preferred report definition file (RDF)
samples	QNT file PGM file

If a link refers to an object included in the list of selected objects, it is treated as a normal object.

Choose **Backup** to open the following dialog box:

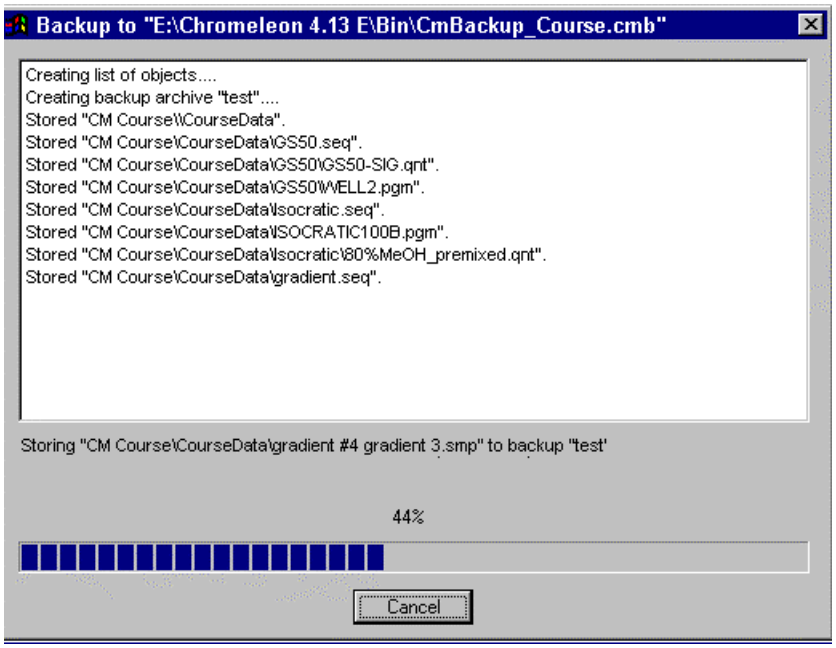


A description of the individual fields is available in the Online Help only (see *Backup*).

Before starting the backup, the required storage space is determined. In the case of hard disks and network drives, the Dionex Chromatography Management System checks whether sufficient storage capacity is available. If there is not enough space, an error message appears allowing the user to cancel the backup procedure.

If using removable media, the expected number of media is displayed. The user is prompted to keep the media ready. If using data compression, the number of actually required media may differ from the displayed number.

After that, the selected objects are stored. A dialog appears allowing to monitor the procedure. A progress bar indicates the status. The bar corresponds to the percentage of stored data already copied to the medium:



If the destination is a removable medium, the user is prompted to change the medium, as necessary.

To perform a backup, you must have the privilege **PRIV_Backup** (also refer to ➢*Privilege* groups) for all selected objects. The backup is indicated in the ➢*History*. The backup can be interrupted at any time by pressing the **Cancel** button. In this case, the backup contains all objects stored up to this point.

If the original objects should be deleted after the backup, a dialog appears where the user confirms the action. If the history mode is active, another dialog for entering a history comment will be opened.

Backup files have the extension **.cmb**. For information on how to open and restore backup files see **How to ...: Actions in the Browser Restoring Backup Files**.

Restoring Backup Files

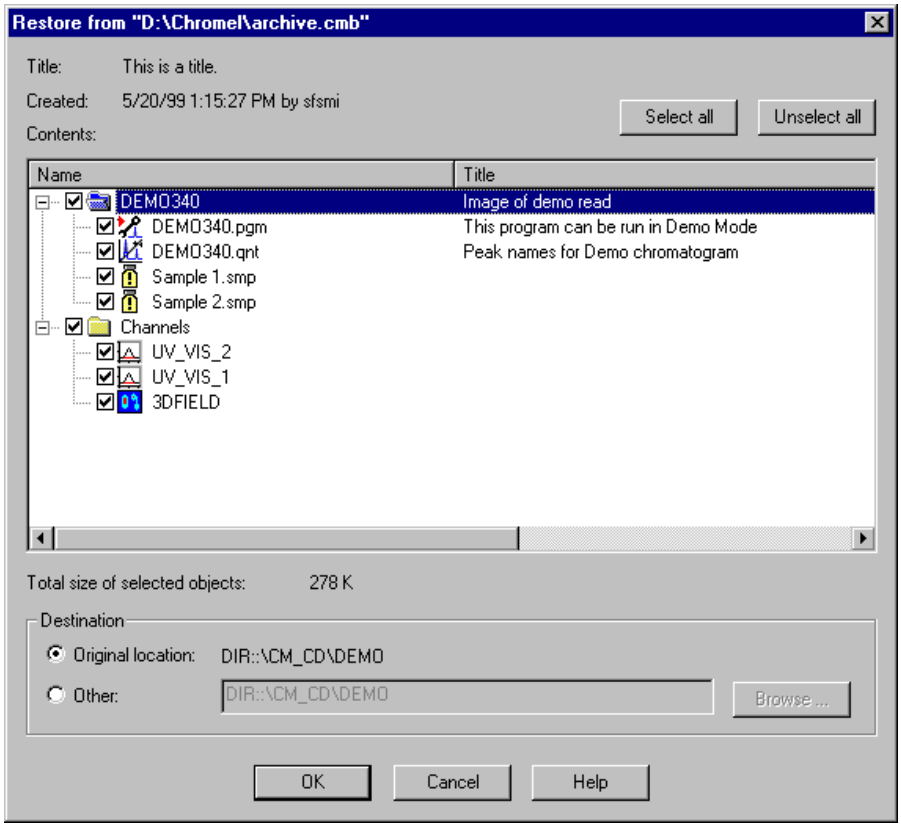
Backup files that were created via the ➢*Backup* function can be opened via the **Import** / ➢*Restore* command from the **File** menu of the Browser (also, see **Actions in the Browser** **Creating Backup Files**).

Tip: Besides, backup files can also be opened in the Windows Explorer by double-clicking the file name. Backup files are identified by their extension *.cmb.

After opening the Restore dialog, select the backup file to be restored. The Dionex Chromatography Management System recognizes whether the file is stored on a removable medium, a hard disk, or a network.

If the backup file is stored on removable media, insert the first medium, as it includes the contents list. Otherwise, an error message will be displayed.

The Dionex Chromatography Management System displays the contents list of the backup file:



A description of the individual fields is available in the Online Help only (see *Restore*).

In addition to the objects, the stored ➢*Channels* and linked objects are listed in separate groups.

Select the channels and the links to restore from the items in these groups. By default, all channels but no links will be restored.

Following this dialog, the selected objects are restored together with the raw data files of the selected channels, the audit trails, and the history. A dialog box appears similar to the Backup dialog. If the backup is located on several removable media, the user is prompted to insert the next medium, as necessary.

If the directory of an object to restore does not exist, it will be created. Links are always restored at the original location. The corresponding sequence and datasource must exist. Missing directories will be created, as necessary.

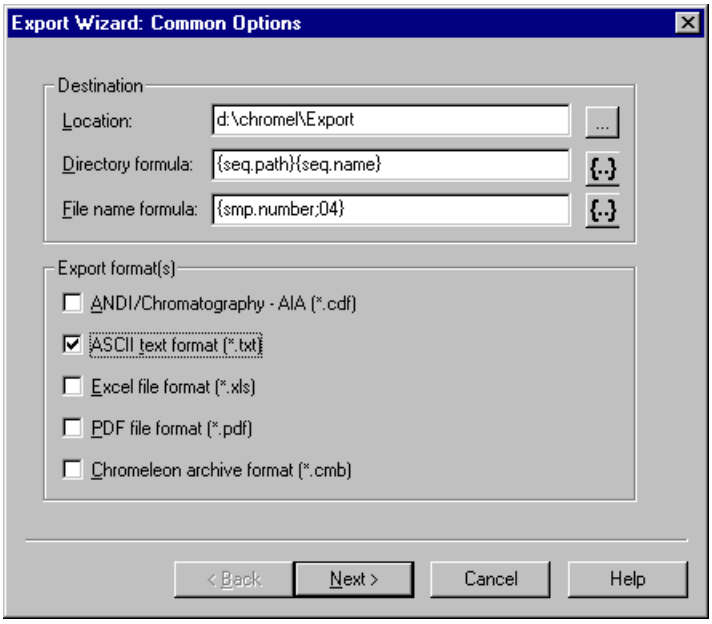
If the destination object already exists, the user is prompted whether to overwrite it. The following options are available: **Yes**, **Yes to all**, **No**, **No to all**, and **Cancel**. Each restored object will receive a corresponding history entry.

To perform the action **Restore**, the user must have the privilege **PRIV_Restore** for the destination directory. To overwrite an existing object, the privilege **PRIV_Copy** is required in addition. The restoration can be interrupted at any time by pressing the **Cancel** button.

Exporting Files

The Dionex Chromatography Management System offers various alternatives for exporting data (see **Data Export**). To export data in the Browser proceed as follows:

- Select **Batch Report** in the **File** menu to open the respective dialog box.
- Selecting the **Export** option opens the Export Wizard.



- Under **Location,** use the "..." button to define the position where to store the data.
- Use the **Directory** formula field to automatically create additional folders below the existing location folders in the Windows Explorer. In order to facilitate finding your files we recommend you to use the same structure as in the **Browser**. Use the {seq.path}\{seq.name}.seq formula to create the same structure.

  Use the **{...}** button to enter the formula if you do not know the syntax. For the above example, use the **Directory** variable of the **Sequence** category. Then enter a backslash (\) and select the **Name** variable of the same category.
- You can enter a formula for the file name in the **File name formula** field. As the individual files are normally created for the respective samples, the entry **{smp.name}**, i.e. the sample name, will be appropriate provided every sample has a specific name

  Use the **{...}** button to enter the formula if you do not know the syntax. For the above example, use the **Sample Name** variable of the **Sample** category.

  The default **{smp.number;04}** uses the number of the respective sample for the file name. 04 indicates a four-digit number, i.e. file names such as **0001.txt** or **0053.txt** will be created.
- Define the export format in the bottom part of the dialog box.
- Press **Next** to proceed to the following page(s) of the Export Wizard where you can define the options for the selected export format. For example, define for the ASCII format the pages you want to export and select the channel(s) if you want to export raw data together with your report.

  ☞ ***Tip***: Before you export a Summary page, ensure in the Printer Layout that a peak is selected in the individual columns. If the setting is **Selected Peak**, no data will be exported as no peak has been selected in the Browser.
- Press **Finish** to terminate the Export Wizard and start exporting by pressing **OK**.

Exporting Sequence Data in one Single File

Use the Summary page for exporting the data of a sequence in one single file. First, define the columns of interest in the Printer Layout as follows:

- Open the **Properties** column by double-clicking the headers of the individual columns. Select the desired peak and save the report.

  Tip: If the setting is **Selected Peak**, no data will be exported as this is done from the Browser where no peak can be selected.

- Go to the Browser and proceed as described in the previous chapter (**Exporting Files**). Make the following settings:
  - Use the export formats **ASCII**, **Excel**, and/or **PDF**.
  - Enter **{seq.name},** i.e. the sequence name, in the **File name formula** field, thus generating one single file for the sequence.
  - On the next page, just select **Summary** as the report page to be exported.
  - Press **Finish** to terminate the Export Wizard and start exporting by pressing **OK**.

Signing Sequences Electronically

The **Electronic Signature** is important for securing your data within the scope of quality assurance and ➢*GLP*. In order to sign sequences electronically, the ➢*CmUser* mode needs to be activated. In addition, the logged-on user must have the signature ➢*Privileges* (e.g. **SignResults)** assigned. For further details, see the CmUser Online Help.

Note: ➢*Electronic Signature* is available only for user databases that were created with a CmUser program version 6.10 or higher. Update your database if an error message notifies you that electronic signature will not be possible.

If these conditions are met, ➢*Sequences* can be signed in three steps:

- Submit
- Review
- Approve

Depending on the sequence's signature status, the corresponding menu item will be available in the context menu:

- **Submit Results...** (for unsigned samples)

- **Review Results...** (for submitted samples) or
- **Approve Results...** (for reviewed samples)

Access to the respective commands is via the **Sign Sequence** option in the **File** menu as well. Alternatively, the respective button on the standard ➢*Toolbar* can be used:

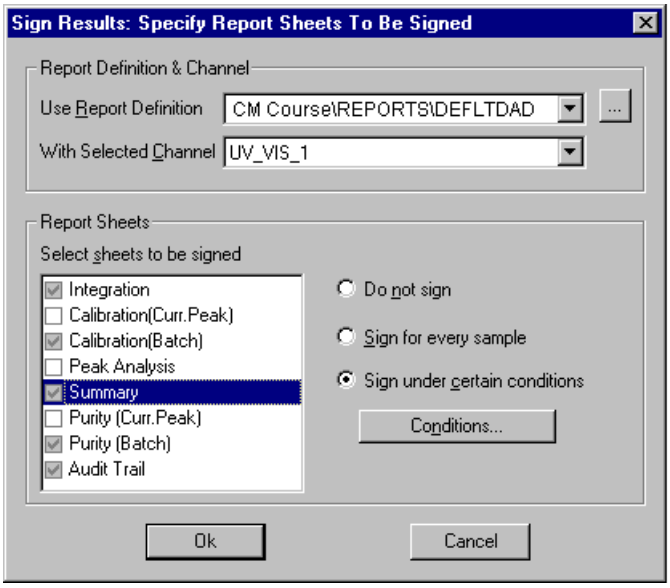
Depending on the sequence's signature status, the button has the corresponding meaning. For further information see

Individual Steps of the Electronic Signature

Checking the Signature Status and Undo Signature

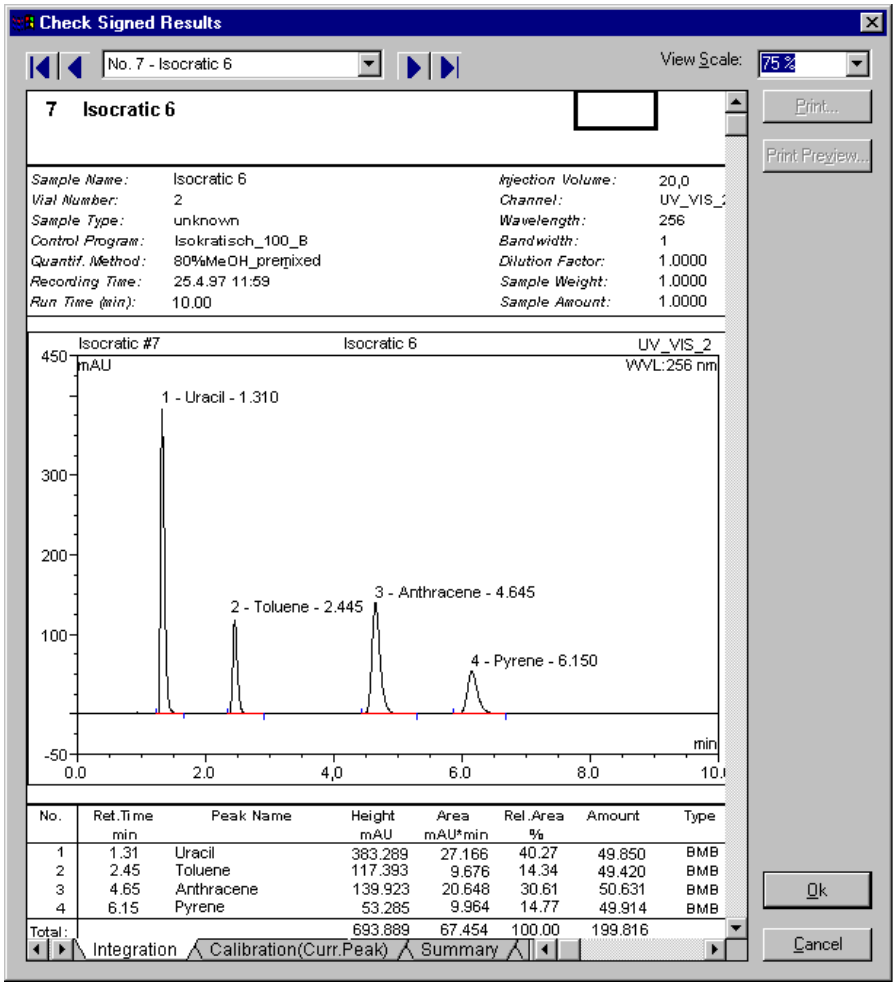
Individual Steps of the Electronic Signature

The first step of an **Electronic Signature** is the **Submit** process. Click a ➢*Sequence* that has not yet been signed and select the **Submit Results** command as described in the previous topic (for general information on electronic signature support in the Dionex Chromatography Management System, see **Signing Sequences Electronically**).

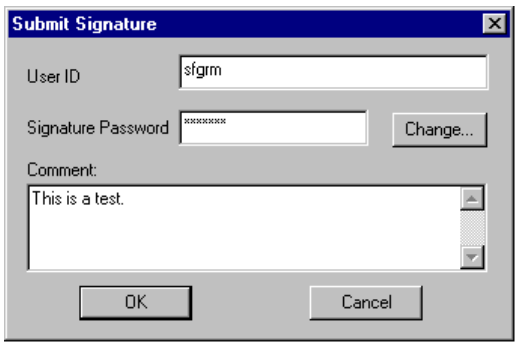


Select the ➢*Report Definition* file (RDF) to be used for displaying the sequence as well as the channel for which to show the results. In the lower window part, you can define the pages of the RDF file to be signed.

Selecting the RDF creates an SOR file (**S**igned **O**ff **R**esults file). Via the selected report definition file, the results are written to the SOR file. Meanwhile, the progress bar in the opening dialog box indicates the progress while the different pages of the report are frozen for the individual samples. Then, the **Check Signed Results** dialog box opens:

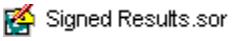


This allows you to check the report to be signed. Use the arrow keys to toggle between the different sequence samples. For each sample, the tabs for the selected report pages are displayed. Pressing OK when you have terminated your checks opens the **Submit Signature** dialog box opens in which the SOR file is signed by entering the User ID and the signature password:

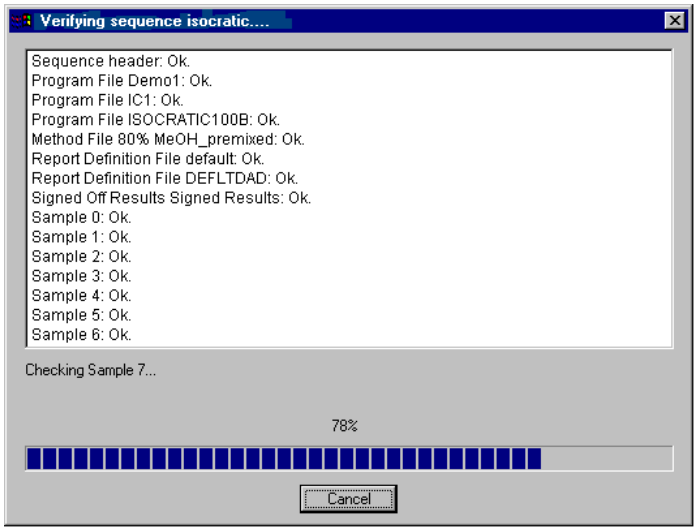


In the comment field, you can note e.g., critical or doubtful points noticed during the report creation.

With an open sequence, the SOR file is given below the other sequence files in the upper right Browser section and can be opened by double-clicking



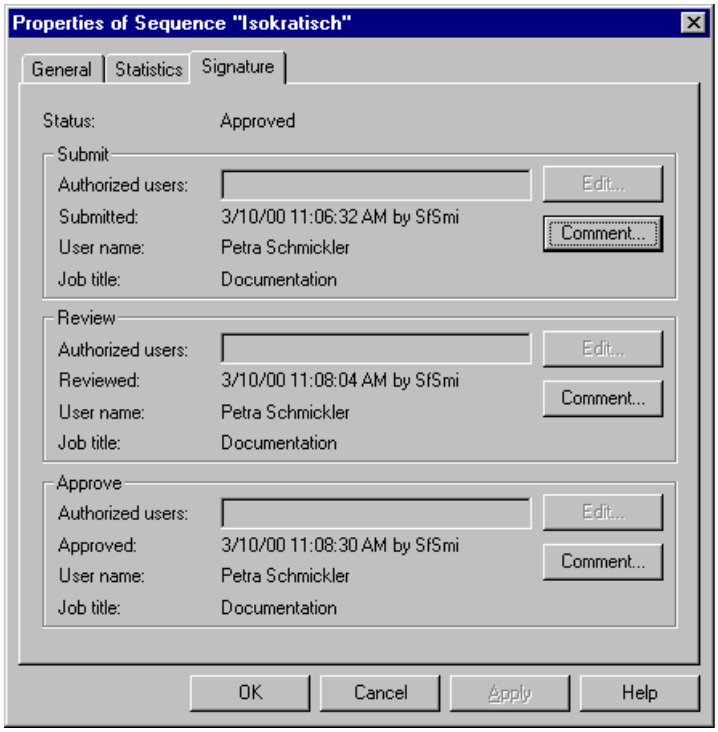
Having been signed and submitted the sequence can be reviewed via the **Review Results** command. Again, the progress is indicated by a progress bar in a dialog box. All files that are assigned to the sequence are reviewed followed by a review of the individual samples:



(This process is completed much faster than with **Submit** so that the above dialog box will be visible for a few seconds only, especially with short sequences.) To **approve** a sequence proceed in the same way.

Checking the Signature Status and Undo Signature

The current signature status of a ➢*Sequence* is given on the **Signature** tab on the sequence's **Properties** dialog. Here, you can also indicate which users are allowed to electronically sign this sequence (**Electronic Signature**).



To check the sequence signature, use the **Verify** command in the **File** menu under **Sign Sequence** or the respective button on the standard ➢*Toolbar*.

Hence, possibly tried manipulations of the signed sequence or errors in the signature are identified in any case. To check the reports once again in such a case, the signature must be removed by the **Undo Signature** command in the **File** menu under **Sign Sequence** or via the button:

However, to do so, the user must have the **UndoSignResults**➢ *Privilege* assigned. The corresponding SOR file will be deleted as well.

Performing a Query

The term ➢*Query* refers to the search for data based on specific search criteria. In the Dionex Chromatography Management System, you can search for samples and the corresponding sequences based on freely selectable parameters. Either you can use very detailed criteria to search for one specific sample, or you can use criteria that are more general to search for a specific series of samples with the same properties.

Proceed as follows to start a query:

- Change to the ➢*Browser* and select the **Query** command in the context menu or select **New / Query (using the Wizard)** in the **File** menu. Either way, a ➢*Wizard* opens and facilitates entering the required conditions.
- On the first Wizard page, define the ➢*Datasource* in which to perform the query. In addition, define whether to find certain ➢*Sequence* properties (**Sequences**) and/or sample properties (**Samples**), and/or other conditions (**Results**).
- Define the individual conditions on the following pages. Only those pages will open which refer to the properties selected on the first page.

Pressing **Finish** opens another dialog box, which offers another four tabs:

- Choose **General** to specify the datasource where to perform the search.
- Choose **Native SQL** to enter the SQL statement directly in the SQL syntax of the corresponding ➢*ODBC* driver (contains translated Dionex Chromatography Management System statements).

- Choose **SQL** to define the search statement in an entry dialog box.
- Choose **Result Restrictions** to limit the resulting sample list via further result queries.

For details, also see

Entering the Sample Query Using a Wizard

Selecting Search Criteria

Examples (Wizard)

Specifying the Sample Query Using the Dialog Box

Editing SQL Statements

Examples (Dialog Box)

Saving a Query

Entering the Sample Query Using the Wizard

On the first Wizard page, define whether to perform the ➢*Query* in the currently open ➢*Datasource* (**Selected Datasource**) or in a different one. If so, click the respective option to open the combo box and select the desired datasource from the list.

In addition, you can define the criteria types for the query:

- ➢*Sequences*
- Samples
- Results (variables from the different report categories)

On the following pages, use **Data Field** to choose the variable whose property you want to find. Enter an operator and define the value (also, see **Selecting Search Criteria**)

The combo box to the right of the respective line allows you to enter a logic connective with another search property. Only after having entered **AND** or **OR**, a second search property can be entered.

Press **Finish** to complete the Wizard and to open the **New Query Properties** dialog box. This dialog box allows you to specify your query further (also, see **Specifying the Sample Query Using the Dialog Box**).

Selecting Search Criteria

The ➢*Query* allows searching for samples and sequences using a variety of sample or sequence properties. Enter the search criteria (see table) on the pages **Query Wizard: Sequences** or **Samples**, respectively. To further restrict the query, double-click the **SQL** dialog and enter the respective criteria in the **Field** of the **Edit Conditions** sheet.

Designation	Search Criterion
Sample Name	⇒*Name*
Sample Number	⇒*No.*
Sample Type	⇒*Type*
Sample Status	⇒*Status*
Sample Comment	⇒*Comment*
Sample Inject Position	⇒*Pos.*
Sample Replicate ID	⇒*Replicate ID*
Sample Inject Volume	⇒*Inj. Vol.*
Sample Inject Time	⇒*Inj. Date/Time*
Sample Dilution Factor	⇒*Dil. Factor*
Sample Weight	⇒*Weight*
Sample Amount	⇒*ISTD Amount*
Sample Raw ID	Internal data system sample ID.
Sample User ID	Sample ID assigned by the user
Sample Program Name	⇒*Program* used for sample processing
Sample Method Name	⇒*Method* used for sample evaluation
Sequence Name	
Sequence Description	⇒*Sequence*
Sequence Preferred Channel	
Sequence Preferred Report	
Sequence Directory	
Sequence Timebase	➢*Timebase*
Sequence Creation Date	
Sequence Creation Operator	
Sequence Last Update	
Sequence Last Update Operator	

These criteria can be divided in four different groups (1 - 4, see table below for available groups):

- Text variables (e.g. **Sample** or **Sequence Name**, **Sample ID**, ...) (1),
- Numerical variables (e.g. **Sample Number**, **Sample Position**, ...) (2),
- Variables with specific values (**Sample Type** or **Sample Status**) (3), and
- Time variables (**Sample Inject Time**, **Sequence Creation Date**, ...) (4).

These search parameters must be further specified. Depending on the type, the search criterion can be linked with a value via various operators. The following operators are available:

Operator:	Searches all samples...	Group no.
=	that are equal to the specified character string.	1, 2, 3, 4
< >	that are not equal to the specified character string.	1, 2, 3, 4
>	that are larger than the specified character string.	1, 2, 4
<	that are smaller than the specified character string.	1, 2, 4
>=	that are larger than or equal to the specified character string	1, 2, 4
<=	that are smaller than or equal to the specified character string	1, 2, 4
contains:	that contain the specified character string.	1
contains not:	that do not contain the specified character string.	1
starts with:	that start with the specified character string.	1
does not start with:	that do not start with the specified character string.	1
ends with:	that end with the specified character string.	1
does not end with:	that do not end with the specified character string.	1
is like:	that fulfill the specified wildcard condition.	1
is not like:	that do not fulfill the specified wildcard condition.	1
is between:	that are between two values.	1, 2, 4
is not between:	that are not between two values.	1, 2, 4
during the previous:	that were created during a selectable time before the query.	4
is null	in which the variable does not exists	1, 2, 3, 4
is not null	in which the variable exists	1, 2, 3, 4

If the operators >, <, >=, or <= are used for text variables, the alphabetical order is considered (e.g.: A<B).

Note: All SQL-time queries containing a relative reference (operator **during the previous** in the **Edit Condition** window) are recalculated for each query.

Wildcards ("placeholders") represent character strings. The following wildcards are valid for text variables with the operator "is (not) like":

Wildcard	Significance
%	Any character string with 0 or more characters
_(underscore)	Any single character
[ ]	A single character within a specified range (e.g. [a-f]).
[^]	Any character with the exception of the specified range.

As soon as the search conditions have been completed, pressing the **Apply** button can start the query.

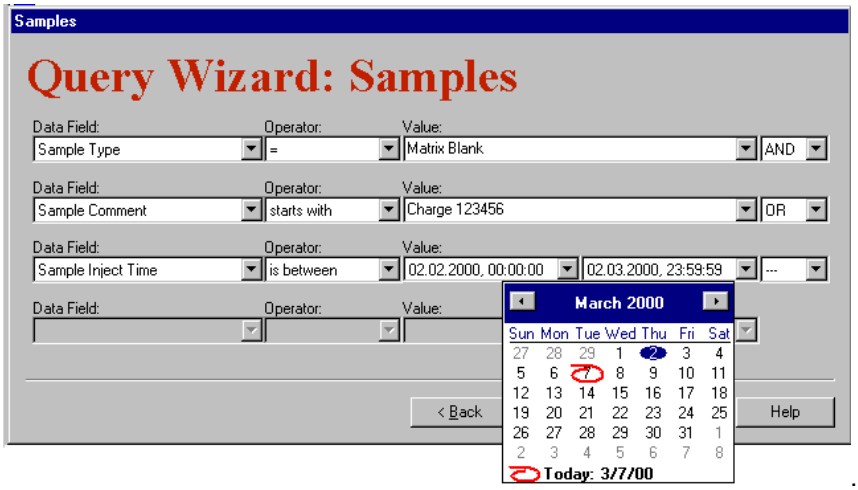
Further conditions can be entered in the Wizard on the **Result Restrictions** page or in the **Properties** dialog box via the **Edit Conditions** page of the **Result Restrictions**. Select a report variable (also, see ⇒*Report Categories*) by pressing the "**...**" button. Logical operations can be used according to the sample and sequence properties.

Note: Depending on the number of samples resulting from the SQL query, the execution of the result restriction may take some time. After approx. 3 seconds, a window will indicate the status of the result restriction (in % of the samples to test). The user can cancel the query. As the result of the query, only the samples of the SQL query that have "successfully passed" the result restrictions so far will be listed.

Examples (Wizard)

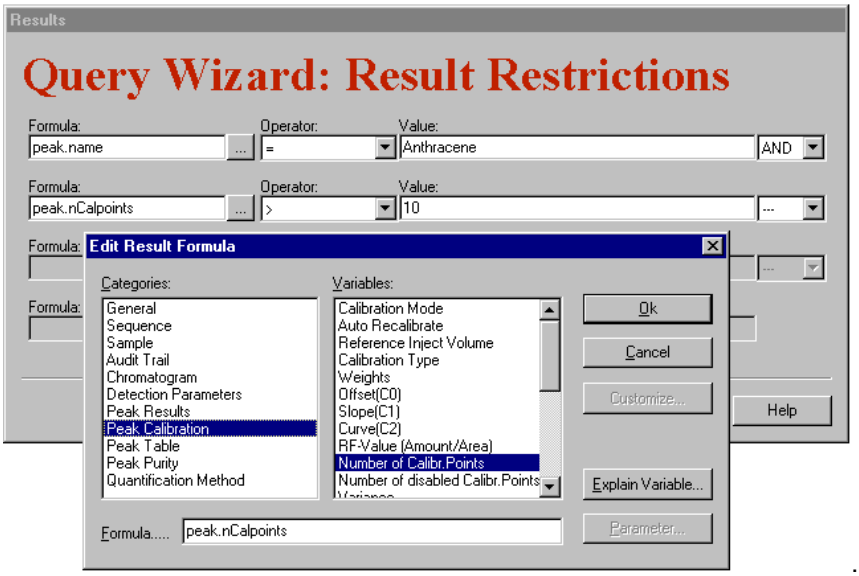
The following SQL query searches for all samples:

- With the sample type **Matrix Blank** and
- Whose comment starts with **Charge 123456** or
- An injection date between 2/2/2000 and 3/2/2000:



Use the following settings to restrict the ➢*Query* to samples

- Containing an Anthracene peak or
- Containing more than 10 calibration points:



For further examples on restricting the query via the dialog box, see **Examples (Dialog Box).**

Specifying the Sample Query Using the Dialog Box

Having entered the ➢*Query* properties using the ➢*Wizard*, the query can be specified further via the **New Query Properties** dialog box. In addition, this dialog box allows editing a performed query later. In this case, the dialog box is named **Properties of Query** "**xyz**". To access this dialog box, click the query and select **Properties** in the context or **File** menu.

The dialog box offers the following four tabs:

- **General** tab: In addition to entering a query title, it is possible to specify the datasource where the query is performed. If this field remains empty (default), the datasource is used where the query itself is saved. The settings **Preferred RDF-File** and **Preferred Channel** are used for opening a sample or for starting a batch report.
- **SQL** tab: This tab allows you to edit the SQL condition(s) the samples must fulfill. You can open an **Edit Condition** dialog box via the **Edit/Insert** button, by double-clicking the left mouse button, or via the context menu. This box allows you to add (Restrict/Expand Condition) or change SQL conditions (Change Condition).

  Via **Field**, you can select a search criterion. To restrict the criterion, SQL operators are available (see **How to ...: Actions in the Browser** **Selecting Search Criteria**). The corresponding comparison value can be defined in the edit field **Value**. For editing a search criterion, all ⇒*Sequence* and sample variables can be used.
- **Native SQL** tab: This tab dialog box translates the SQL statement into the SQL syntax of the corresponding ODBC driver. As the default, this sheet is "read only". It informs you about the SQL statement sent to the ODBC driver. By selecting the **Always use native SQL** option, it is possible to edit the SQL statement manually.

Caution: If SQL conditions were edited, this "translated" SQL statement will be used to perform the query.

- **Result Restrictions** tab: The list of samples found via the SQL query can be further limited by result restrictions. Similar to entering the SQL query, you can open the **Edit Conditions** dialog box by double-clicking the left mouse button or via the context menu. Here, result conditions can be edited. **Result Restrictions** generally limits the query to samples that contain raw data.

In the **Formula** field, you can select a report variable (also, see ⇒*Report Categories*) via the "**...**" button. Again, SQL operators (see **How to ...: Actions in the Browser Selecting Search Criteria**) are supported. Enter the reference value in the **Value** field.

- As soon as the search conditions have been completed, you can start the search by pressing the **Apply** button.

Editing SQL Statements

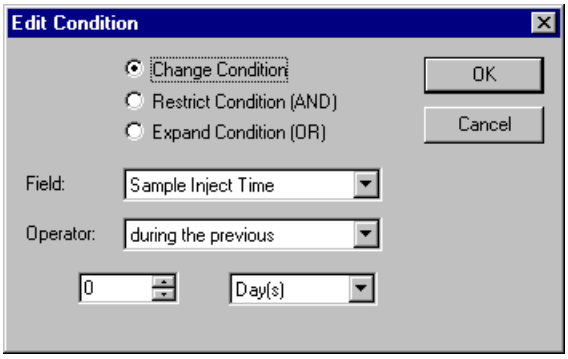
The **Native SQL** tab dialog box shows the SQL statement the Dionex Chromatography Management System created from the database query specified via the **SQL** tab dialog box.

Users with a good knowledge of the SQL database language can specify further conditions for their ➢*Query*. For this purpose, **Always use native SQL** must be selected. The statement can then be modified or extended via the keyboard.

Caution: If you edited the SQL statement via the **Native SQL** tab, this "translated" SQL statement will be executed whenever the query is performed as long as this box is checked.

Examples (Dialog Box)

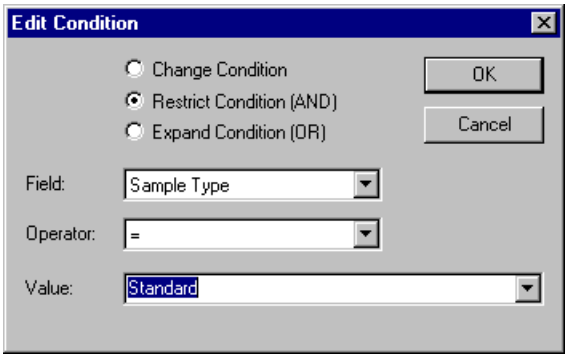
The following SQL query searches for all samples of the current day:



The SQL sheet will show the following:

Samples.smp_inject_time >= CURRENT_INTERVAL '0' DAY.

To restrict the search to the current day's standard samples instead of all sample types, the SQL query must also include the following input:

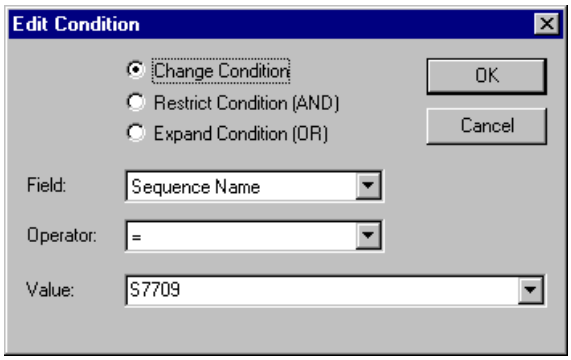


The SQL sheet now shows the following:

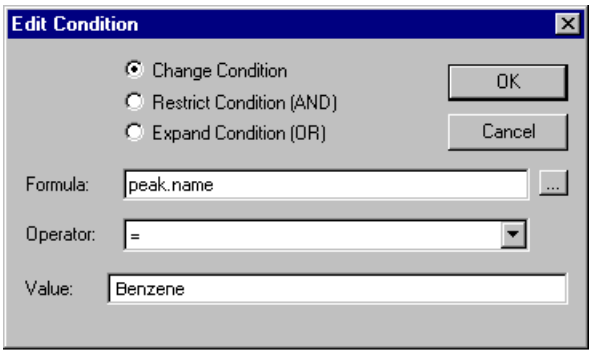
Samples.smp_type = 'S'

AND Samples.smp_inject_time >= CURRENT_INTERVAL '0' DAY

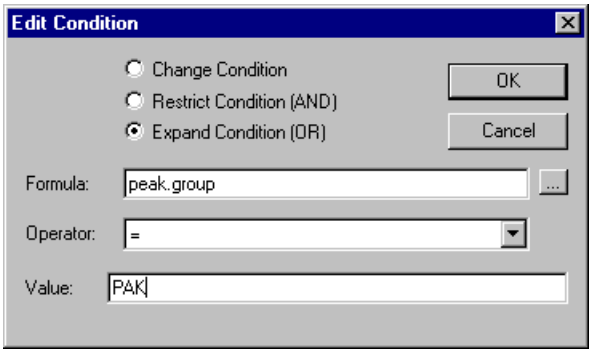
To search for all samples in a ⇒*Sequence* named **S7709**, in which the peak **Benzene** or a peak of the **PAK** (PAH) peak group was identified, first enter the following:



In addition, specify the following conditions in the **Result Restrictions** box:



Finally, enter the condition **or PAK** (PAH) in the **Result Restrictions** box:



The **SQL** sheet now shows:

Sequences.seq_name = 'S7709'

The **Result Restrictions** sheet indicates:

peak.name = 'Benzene'

OR peak.group = 'PAK'.

For examples on entering the query using the Wizard, see **Examples (Wizard).**

Saving a Query

Queries can be saved as a file in the datasource, similar to ⇒*Sequences*. For this purpose, open the ➢*Query* Wizard via the **File** menu or in the context menu. After entering the conditions, press the **OK** button to save these conditions as a query object under any file name.

In the Browser, the ➢*Query* is indicated by the symbol: .

If the cursor is positioned on a query, the Dionex Chromatography Management System acts as if displaying a sequence: If the query is located in the left window section of the ➢*Browser*, the sample query is immediately executed. The result will be displayed in the right window section. If the query is located in the right window section of the Browser, pressing **Return** or double-clicking the file will execute the query.

A previously saved query can be edited via the **Properties** command from the **File** menu (or via the context menu).

Performing the Chromeleon/PeakNet OQ

If the respective **Preconditions for the Chromeleon/PeakNet Operational Qualification** are met, the **Data System OQ** can be performed manually or automatically using the ➢*Wizard*. For further information on the individual steps, see the following pages:

Performing the Chromeleon/PeakNet OQ Automatically

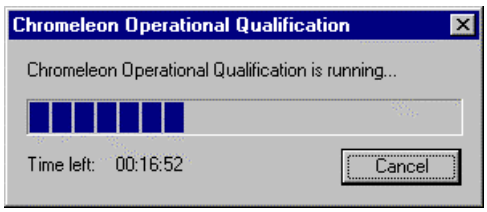
Performing the Chromeleon/PeakNet OQ Manually

Performing the Chromeleon/PeakNet OQ Automatically

For performing the **Operational Qualification of the Dionex Chromatography Management System** automatically using the ➢*Wizard*, the following steps must be taken:

1. Establish a connection to the ➢*Datasource* on the Dionex Chromatography Management System CD or to a copy thereof.
2. In the Client, select the menu item **Chromeleon OQ** or **PeakNet OQ** in the **Qualification** menu. The **Wizard** opens and guides you through the OQ. Press **Next** to proceed to the next step.

3. Select the source directory of the sample sequence that holds the ➢*Sequence* CM_OQ.
4. Specify a data path and a sequence name for saving the results. Specify whether the report shall be printed automatically upon termination of the OQ.
5. Select **Finish** to start the OQ automatically. The following dialog box allows you to monitor the progress:



6. While the OQ is running, the Dionex Chromatography Management System is locked. This lock can be removed only by pressing **Cancel** in the active window **Chromeleon (or PeakNet) Operational Qualification**.
7. If specified in step 5, the report will be printed automatically when the OQ is finished.
8. The server is stopped and the configuration used before starting the OQ is reloaded. Then the server starts again.

For information on how to perform the Data System OQ manually, see **How to ...: Actions in the Browser Performing the Chromeleon/PeakNet OQ Manually**.

Performing the Chromeleon/PeakNet OQ Manually

For performing the **Operational Qualification of the Dionex Chromatography Management System** manually, the following steps must be taken:

1. Ensure that the ➢*Server* of the Dionex Chromatography Management System is running and no process is active.
2. Start the program module ➢*Server Configuration*.
3. Save the actual configuration under a unique name.

4. Load the CM_OQ.CFG configuration from the **Bin** subdirectory of the Dionex Chromatography Management System directory.
5. Start the ➢*Client* of the Dionex Chromatography Management System if it is not yet running.
6. Close all windows except the ➢*Browser*.
7. Establish a connection to the ➢*Datasource* that holds the sequence template.
8. Copy the sequence template.
9. Open the ➢*Control Panel* of the copied ➢*Sequence* and connect it to the ➢*Timebase* CM_OQ.
10. Open the batch list. If necessary, delete any sequences stored in the batch list and add the copied sequence.
11. Start the ➢*Batch*.
12. Ensure that no modifications are made in the Dionex Chromatography Management System while the sequence is processed (duration: 25 minutes).
13. Upon termination of the sequence, print the report by selecting the menu item **Batch Report** in the **File** menu of the Browser.
14. Start the program module **Server Configuration**.
15. Reload the configuration used before starting the OQ.

For information on how to perform the Data System OQ automatically, see **How to ...: Actions in the Browser Performing the Chromeleon/PeakNet OQ Automatically**.

System Wellness

System Wellness provides built-in diagnostic and calibration features that help prevent unscheduled system shutdowns and assure reliable operation of system devices. System Wellness support is provided for devices that are connected via the Dionex ➢*DX-LAN*.

For an overview of System Wellness features and a list of supported devices, see **System Wellness Overview**.

System Wellness tasks are performed from the Browser. For details, see the System Wellness section under **How to ...: Actions in the Browser**:

Opening a Wellness Control Panel

Viewing and Restoring Calibration Data

Performing Device Calibrations

Performing Device Diagnostics

Entering Device Parameters

Also, see **How to ...: Actions in the Server Configuration**
Enabling/Disabling System Wellness Functions

Opening a Wellness Control Panel

➢*Control Panels* for performing System Wellness functions are provided for various system configurations.

1. In the ➢*Browser* under the local ➢*Datasource*, open the **Panels** folder and then open the **Wellness** sub-folder.
2. Double-click the panel name that corresponds to your ➢*Timebase* configuration.
3. The control panel opens and then the Dionex Chromatography Management System attempts to connect to the timebase assigned to the panel.
4. If an error message appears stating that the timebase was not found, close the message and then select **Connect to Timebase** from the **Control** menu. Select the timebase to be connected to the panel.
5. After communication is established with the timebase, the various calibration and diagnostic controls on the panel are enabled.

Viewing and Restoring Calibration Data

Calibration data for a System Wellness supported device is displayed on the Wellness ➢*Control Panel* (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).

The Dionex Chromatography Management System stores three sets of calibration data for each System Wellness supported device.

- Current is the data most recently sent (uploaded) from the device. It is the data currently stored in the device memory.
- Previous is the data from the previous time calibration data was uploaded from the device.
- Factory is the data obtained (uploaded) from the device when it was initially configured in the System Configuration program (see **How to ...: Actions in the Server Configuration Enabling and Disabling System Wellness Functions**).

The Wellness control panel displays the current data and the date the current calibration function was performed. If the factory value is the current data, the date field displays "---."

- To view previous or factory data or download calibration data from the Dionex Chromatography Management System to the device, click the **Detail** button.

  A Calibration Detail dialog box appears that displays the three sets of calibration data values and their corresponding dates. The dates indicate when the values were uploaded from the device to the Dionex Chromatography Management System.
- To download calibration data to the device, select **Current**, **Previous**, or **Factory** from the list to the right of the **Download** button. Then, select **Download**.

Performing Device Calibrations

Wellness ➢*Control Panels*, which are supplied with the Dionex Chromatography Management System, display calibration data and provide command buttons for performing device calibrations. After a calibration is performed, the device uploads the new calibration data to the Dionex Chromatography Management System.

Tip: Many calibrations require setup steps before the actual calibration command is given. Before selecting a calibration command button on a control panel, see the topics below for details about the particular calibration task you are performing.

Devices	Calibration Procedures
Pumps, Detectors, Autosamplers	**Leak Detector**
Pumps	**Flow Rate**
	Pressure Transducer Offset
	Degas
Detectors	**Wavelength (AD25/PDA-100)**
	Conductivity Cell (CD20/25/25A, ED40/50/50A, IC20/25/25A)
	pH Reference Electrode (ED40/50/50A Amperometry Mode)
AS50 Autosampler	**Inject Port Volume**

Calibrating the Leak Detector

When to Calibrate: After installing a new leak detector
If the leak detector diagnostic test fails
Every 6 months

Many System Wellness supported devices are equipped with leak detectors. The calibration procedure for all of the sensors is the same.

1. Thoroughly dry the sensor.
2. Open the System Wellness ➢*Control Panel* for the device (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).

3. Under **Calibration**, **leak detector**, press the **internal** command button to calibrate the sensor installed in the device itself. Press the **external** command button to calibrate the sensor on a controlled device. For example, for a pump, internal refers to the sensor in the pump and external refers to the sensor in a chromatography oven controlled by the pump.
4. The device calibrates the sensor and uploads the new value to the Dionex Chromatography Management System. The Dionex Chromatography Management System stores this new calibration value as the current value.

Calibrating the Pump Flow Rate

When to Calibrate:	Every 6 months
Items Needed:	Backpressure tubing to create 14 MPa ± 2 MPa (2000 psi ± 300 psi). Use 0.076 mm (0.003 in) ID yellow PEEK tubing (P/N 049715)
	Deionized water
	Tared beaker

1. Verify that there is about 14 MPa (2000 psi) of backpressure.
2 Pump deionized water at 1.0 mL/min.
3. Allow the pump to stabilize for at least 5 minutes.
4. Collect water into a tared beaker for ***exactly*** 5 minutes.
5. Open the System Wellness ➢*Control Panel* for the pump (see **How to ...: Actions in the Browser** **Opening a Wellness Control Panel**).
6. Enter the weight of the water into the **weight** entry field under **flow rate** and press the **Enter** key. The Dionex Chromatography Management System downloads the value to the pump and stores this calibration value as the current value.

Calibrating the Pressure Transducer Offset

When to Calibrate: Every 6 months

1. Turn off the pump flow.
2. Open the waste valve.
   - For GP40/50, IP20/25 pumps: The waste valve is on the pressure transducer. To open the valve, turn the knob about two turns counterclockwise.
   - For GS50/IS25 pumps: The waste valve is on the secondary pump head. To open the valve, turn the knob one-quarter to one-half turn counterclockwise.
3. Open the System Wellness ➢*Control Panel* for the pump (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).
4. Press the **offset** command button under **pressure transducer**. The pump calibrates the offset and uploads the new value to the Dionex Chromatography Management System. The Dionex Chromatography Management System stores this new offset as the current value.
5. Close the waste valve.

Degas Calibration

When to Calibrate: Every 6 months

1. Open the System Wellness ➢*Control Panel* for the pump (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).

2 Select the **degas** command button. The pump performs the degas calibration and uploads the new calibration value to the Dionex Chromatography Management System. The Dionex Chromatography Management System stores this new value as the current degas value.

Wavelength Calibration

Use this calibration procedure for the Dionex AD25 and PDA-100 detectors. Wavelength calibration occurs automatically whenever the detector power is turned on. In addition, manually run wavelength calibration at the following times:

When to Calibrate:	After a failed wavelength verification test

1. Verify that there is solvent flowing through the cell, the background absorbance is low, and there are no bubbles in the light path.
2. Open the System Wellness ➢*Control Panel* for the detector (see **How to ...: Actions in the Browser** **Opening a Wellness Control Panel**).
3. Press the **wavelength** command button under **Calibration**. The detector performs the wavelength calibration routine and uploads the results (Pass or Fail) to the Dionex Chromatography Management System.

If wavelength calibration fails, see the troubleshooting section of the detector operator's manual.

Calibrating the Conductivity Cell

When to Calibrate:	After installing a new cell (use Method A) Every 6 months (use Method B)
Items Needed (Method B Only):	1.0 mM KCl solution: Prepare by dissolving 0.07456 g of reagent grade KCl in one liter of 18 megohm deionized water Backpressure tubing to provide at least 7 MPa (1000 psi). Use 0.076 mm (0.003 in) ID yellow PEEK tubing (P/N 049715)

Method A: For Calibrating New or Replacement Cells

1. Open the System Wellness ➢*Control Panel* for the detector (see **How to ...: Actions in the Browser** **Opening a Wellness Control Panel**).
2. In the **conductivity cell calibration** entry field, type the cell calibration constant (written on a tag on the conductivity cell's cable) and press the **Enter** key. The Dionex Chromatography Management System downloads the value to the detector and stores the value as the current cell calibration constant.

Method B: For Calibrating After Every 6 Months of Use

1. Disconnect the pump output line from the injection valve.
2. Connect the pump output line directly to the inlet of the DS3 or cell.
3. Verify that there is a minimum of 7 MPa (1000 psi) of backpressure.
4. Pump 1.0 mM KCl through the cell at 1.0 mL/min.
5. If using a DS3, set the DS3 temperature to the intended operating point and allow it to reach this temperature.
6. Allow the conductivity to stabilize for about 5 minutes.
7. Open the System Wellness control panel for the detector (see **How to ...: Actions in the Browser**  **Opening a Wellness Control Panel**).
8. Press the **calibrate** command button under **conductivity cell**. The detector calibrates the cell and uploads a new cell calibration constant to the Dionex Chromatography Management System. The Dionex Chromatography Management System stores this value as the current cell calibration constant.

   After calibration, the conductivity reading should be 147.00 ± 2 µS/cm and the cell calibration constant should be between 130 and 190. If this is not the case, refer to the troubleshooting section of your detector operator's manual.
9. Flush the KCl solution from the system by pumping deionized water through the cell. When the conductivity drops to near zero, stop the pump.
10. Reconnect the pump to the injection valve and reconnect the line from the suppressor to the cell inlet.

Calibrating the pH Reference Electrode

When to Calibrate:	Every 6 months
Items Needed:	pH 7 buffer A second buffer of known pH (usually a calibration buffer that most closely matches the pH of the eluent used in your application)

1. Carefully remove the combination pH/Ag-Ag/Cl reference electrode from the amperometry cell, making sure to leave the electrode leads connected to the cell.
2. Place the electrode into a pH 7 buffer.
3. Wait for the pH reading to stabilize (about 1 minute).

4. Open the System Wellness ➢*Control Panel* for the detector (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).
5. Press the **pH 7** command button under **pH electrode**.
6. Remove the electrode from the pH buffer, rinse, and then dry it.
7. Place the electrode in the second buffer.
8. Wait for the pH reading to stabilize.
9. Enter the pH of the second buffer into the edit field above the **2nd buffer** command button.
10. Press the **2nd buffer** command button.

Entering the AS50 Inject Port Volume

The inject port volume is the volume of tubing between the AS50 inject port and the injection valve. The AS50 uses this information to determine how much fluid to push through the line in order to position the sample correctly in the loop for precision injections.

When to enter a new inject port volume:	Only after installing a new needle seal assembly or after recalibrating the inject port volume on an existing needle seal assembly.

For detailed instructions on replacing a needle seal assembly or calibrating the inject port, refer to the AS50 operator's manual.

1. Open the System Wellness ➢*Control Panel* for the autosampler (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).
2. In the **Inject Port Volume** field, enter the volume written on the tag on the new needle seal assembly, or enter the volume determined during recalibration of the inject port volume on an existing needle seal assembly.
3. Press the **Enter** key. The Dionex Chromatography Management System downloads the value to the autosampler and stores this calibration value as the current value.

Performing Device Diagnostics

Wellness control panels, which are supplied with the Dionex Chromatography Management System, display diagnostic test results and provide command buttons for performing the tests.

The following tests are available - see **How to ...: Actions in the Browser**:

Leak Detector (for any device equipped with a leak detector)

Wavelength Verification (for AD25 and PDA-100 detectors)

Testing the Leak Detector

Many System Wellness supported devices are equipped with leak detectors. The test procedure for all of the sensors is the same.

1. Thoroughly dry the sensor.
2. Open the System Wellness ➢*Control Panel* for the device (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).
3. Under **Diagnostic Tests**, **leak detector**, select the **internal** command button to test the sensor installed in the device itself. Select **external** to test the sensor on a controlled device. For example, for a pump, internal refers to the sensor in the pump and external refers to the sensor in a chromatography oven controlled by the pump.
4. The device tests the sensor and reports the results to the Dionex Chromatography Management System. Possible test results are:
   - Passed (Dry)
   - Failed (Wet)
   - Failed (Open circuit): The sensor may be disconnected. Check the connection.
   - Failed (Short circuit): The sensor may need replacing. Contact Dionex for assistance.
   - Failed (Out-of-calibration): Calibrate the sensor (see **How to ...: Actions in the Browser Calibrating the Leak Detector**) and retest. If the test still fails, the sensor may need replacing. Contact Dionex for assistance.

Wavelength Verification

Use this procedure for the Dionex AD25 and PDA-100 detectors. The **Wavelength Verification** test verifies the wavelength accuracy of the AD25 or PDA-100 detectors. When this test is run, a holmium oxide filter is placed in the

light path and measured wavelengths are compared to theoretical wavelengths for holmium oxide.

1. Verify that there is solvent flowing through the cell, the background absorbance is low, and there are no bubbles in the light path.
2. Open the System Wellness ➢*Control Panel* for the detector (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).
3. Under **Diagnostic Tests**, **wavelength verification**, press the **verify** command button. The detector runs the test and then reports the results to the Dionex Chromatography Management System. The overall results (**Passed** or **Failed**) are reported and the theoretical and measured values for three peaks in the holmium oxide spectrum.

If the test fails, run the wavelength calibration (see **How to ...: Actions in the Browser Wavelength Calibration**) and then rerun the verification test.

Entering Device Parameters

For some devices, System Wellness ➢*Control Panel* include fields that let you enter various device parameters.

Applying a Sodium Correction (for ED40/ED50/ED50A Amperometry detectors)

Applying a Sodium Correction

If you are using a NaCl reference electrode with an ED40, ED50, or ED50A detector in amperometry mode, turn on the sodium correction parameter. This adjusts the detector's signal response for the NaCl electrode, instead of for the default AgCl reference electrode.

1. Open the System Wellness ➢*Control Panel* for the detector (see **How to ...: Actions in the Browser Opening a Wellness Control Panel**).
2. Under **Device Parameters**, **sodium correction**, select **On**.

Importing PeakNet (Release 4.5 Through 5.2) Method Files

Overview

In order to use Method files from PeakNet 5 (PeakNet release 4.5 through 5.2) with the Dionex Chromatography Management System, they must first be imported into the Dionex Chromatography Management System.

When imported, the PeakNet 5 Method file is converted into a ➢*PGM File* and/or ➢*Quantification Method (QNT Method)* of the Dionex Chromatography Management System. Converted PGM files contain timed events and setup parameters for all modules included in the original PeakNet 5 Method. Converted QNT files contain component names, retention times, reference peaks, tolerance, calibration options, groups, and level amounts for each detector in the PeakNet 5 Method.

PeakNet 5 Methods from the following modules can be imported: AS50, GP40/GP50, IP20/IP25, AD20, AD25, CD20, ED40, IC20, UI20, DX-120. For Methods that were created with AI450 software, only the QNT portion of the Method is converted.

Because of differences in the way that PeakNet 5 and the Dionex Chromatography Management System function, some features available in a PeakNet 5 Method file are not imported into the Dionex Chromatography Management System. These include:

- Replicate calibration information
- CE Method parameters
- High/low limit values
- Outlier rejection
- Linear weighting options

In addition, the Dionex Chromatography Management System allows only a single component table per injection, whereas PeakNet 5 allows one table per detector. When the PeakNet 5 Method contains multiple detectors, the first detector is converted entirely, that is, information about every component and unknown peak is added to the peak table. Then, for the other detector(s), only unique components and unique unknown groups, which were not in the first detector's data, are added to the table. This means that any reference component information for detectors other than the first may be lost.

How To

1 In the ➢*Browser*, select a ➢*Datasource* folder (not a sequence name).

2 Select the **Import/Restore** command from the **File** menu and then select **PeakNet 5** and **Method Files**.

3 In the Import PeakNet 5 Method Files dialog box, navigate to the folder that contains the PeakNet 5 Method file(s) to be imported. These files are named with a .MET extension.

4 Select one or more of the Method files and click the **Open** button. The files appear in the Selected files list.

5 To convert the PeakNet 5 Method into a PGM file for the Dionex Chromatography Management System, select the **Program** box. The PGM file is created in the folder shown next to the **Program** box. The default is the datasource folder currently selected in the Browser. To choose a different location, click the **Browse** button and select the desired location.

6 To convert the PeakNet 5 Method component table and calibration parameters into a QNT method for the Dionex Chromatography Management System, select the **QNT** box. The QNT file is created in the folder shown next to the **QNT** box. The default is the datasource folder currently selected in the Browser. To choose a different location, click the **Browse** button and select the desired location.

7 Click the **Import** button. The selected PGM and/or QNT files are created.

The new files have the same name as the PeakNet 5 Method file, but with PN5 appended and with PGM and QNT extensions. Once a Method file is converted, the file name is removed from the Selected files list.

☞ ***Tip***: If the QNT option is selected, but the PeakNet 5 Method does not contain a detector module, an empty QNT method file is created.

Also, see: **Importing PeakNet (Release 4.5 Through 5.2) Data Files**

Importing PeakNet (Release 4.5 Through 5.2) Data Files

Overview

In order to use data files from PeakNet 5 (PeakNet release 4.5 through 5.2) with the Dionex Chromatography Management System, they must first be imported into the Dionex Chromatography Management System (Dionex CMS).

When the PeakNet 5 data file is imported, a ➢*Sequence* for the Dionex Chromatography Management System is created. The sequence includes the raw data from the data file, the embedded PeakNet 5 Method (converted into ➢*PGM File* and ➢*Quantification Method (QNT Method)* of the Dionex Chromatography Management System), and additional information required to complete the sequence. If multiple data files are selected for import, they are grouped into one sequence.

If the PeakNet 5 data file contains multiple detectors, a separate sample line in the sequence is created for each detector (up to four).

How To

1 In the ➢*Browser*, select a ➢*Datasource* folder (not a sequence name).

2 Select the **Import/Restore** command from the **File** menu and then select **PeakNet 5** and **Data Files**.

3 In the Import PeakNet 5 Data Files dialog box, navigate to the folder that contains the PeakNet 5 data file(s) to be imported. These files are named with a .DXD or .Dxx extension (where xx is 01 - 99).

4 Select one or more data files and click the **Open** button. The files appear in the **Selected files** list.

5 The selected data files will be imported into the folder shown in the **PeakNet Folder** box. The default is the datasource folder currently selected in the Browser. To import the data file(s) into a different location, click the **Browse** button and select the desired location.

6 In the **Sequence Name** box, enter a name for the sequence to be created from the imported data files.

7 Click the **Import** button. The selected PeakNet 5 data files are imported into the Dionex Chromatography Management System.

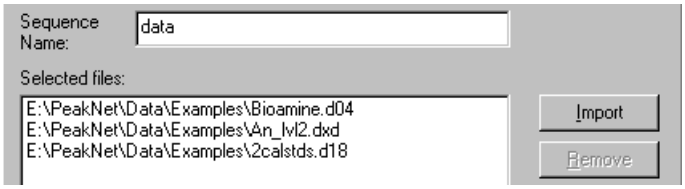
The following files are created:

- One sequence, which contains a sample line for each PeakNet 5 data file selected for import. If any of the data files contained data from multiple detectors, separate sample lines are created for each detector's data.
- One PGM file and one QNT file for each sample in the sequence. The PGM and QNT files are created from the PeakNet 5 Method embedded in the PeakNet 5 data file.

The PGM and QNT files are named as follows: the Method file name from the PeakNet 5 data file is used, followed by a three digit identifier, which corresponds to the detector's position in the sequence, and then a pgm or qnt extension.

Example

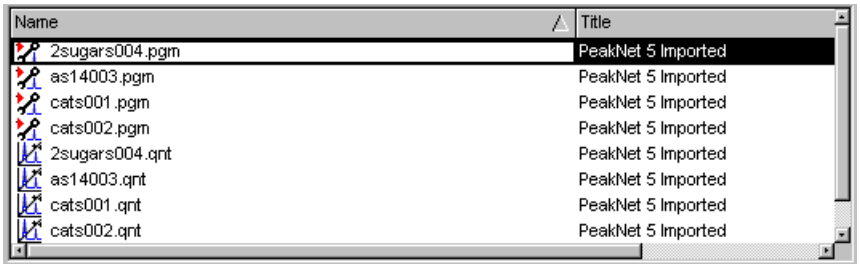
In the Import PeakNet 5 Data Files dialog box, three data files are selected for import.



After importing, the following sequence is created. Notice that because the Bioamine.d04 data file contained data from two detectors, two sample lines were created in the sequence:

No.	Name	Type	Pos.	Inj. Vol.	Program	Method
1	biogenic amines/31.2ppm/TBAO	Unknown	0	10.0	cats001	cats001
2	biogenic amines/31.2ppm/TBAO	Unknown	0	10.0	cats002	cats002
3	Level 2 Standard	Unknown	0	10.0	as14003	as14003
4	Diabetic Candy Sample	Unknown	0	10.0	2sugars004	2sugars004

The following PGM and QNT files were also created. These correspond to the programs and methods listed in the sequence:



Also, see **Importing PeakNet (Release 4.5 Through 5.2) Method Files**

PeakNet (Release 4.5 Through 5.2) Translation Tables

See the following topics for how PeakNet (releases 4.5 through 5.2) setup and timed event Method parameters are translated to PGM file commands of the Dionex Chromatography Management System.

AS50 Autosampler

Pump Modules and Eluent Generator

AD20 Detector

AD25 Detector

CD20 Detectors

ED40 Detectors

IC20 Systems

DX-120 System

UI20 Module

See the following topic for how PeakNet (release 4.5 through 5.2) component table parameters are translated to QNT method parameters of the Dionex Chromatography Management System.

Detector Component Table Translation

AS50 Autosampler Setup and Timed Event Parameter

Translation

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
TTL 1 (checked/unchecked)	Sampler_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2 (checked/unchecked)	Sampler_TTL_2.State (=0v/5v)	Setup & timed portions
Relay 1 (checked/unchecked)	Sampler_Relay_1.State (=Closed/Open)	Setup & timed portions
Relay 2 (checked/unchecked)	Sampler_Relay_2.State (=Closed/Open)	Setup & timed portions
CSV (A/B)	ColumnValve.State(=Col_A/Col_B)	Setup & timed portions
Sample NeedleHeight	NeedleHeight	Setup portion
ColumnTemperature	ColumnTemperature	Setup portion
TrayTemperature	TrayTemperature	Setup portion
Cycle Time	Cycle	Setup portion
Valve (Load/Inject)	Load/Inject If Inject, command "Wait InjectState" is added	Setup & timed portions
Pipet function (Source/Volume/Destination)	Pipet (SourceVial/Volume/ DestinationVial)	Setup portion
Mix function (Vial/Volume/Cycles)	Mix (SourceVial/Volume/NumberOfTimes)	Setup portion
Flush function (Volume)	FlushSP (Volume)	Setup portion
Delay function (Delay Time)	DelaySP (Time)	Setup portion
Needle function (Height)	SetNeedleHeight (Height)	Setup portion
Dilute function (Concentrate Source/ Concentrate Volume/ Diluent Source/ Diluent Volume/ Destination)	Dilute (SourceVial/ ConcentrateVolume SourceReservoir/ DiluentVolume/ DestinationVial)	Setup portion
Dispense function (Source/Volume/Destination)	Dispense (SourceReservoir/Volume/ DestinationVial)	Setup portion
Wait function	Wait (SamplePrep)	Setup portion
PeakNet (Release 4.5 Through 5.2) Method Parameter	**PGM Command of the Dionex Chromatography Management System**	**Comments**
Wait for stable temperature (checked/unchecked)	WaitForTemperature (=True/False)	Setup portion

	In any case 2 commands are added: 1."Flush Volume=100" 2."Wait FlushState"	Setup portion
	Syringe Speed always set to default value = 3	Setup portion
	CutSegmentVolume always set to default value = 0	Setup portion
Output Labels	Not converted	
Comments	Comments	
Description	Comments	

Pump and Eluent Generator Setup and Timed Event Parameter Translation

Pump Modules Translation Table

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Oven Temperature	Temperature	Setup portion
High Pressure Limit	Pressure.UpperLimit	Setup portion
Low Pressure Limit	Pressure.LowerLimit	Setup portion
Eluent Label(A/B/C/D)	(%A/%B/%C/%D).Equate	Setup portion
Eluent percentage (B/C/D)	%B/%C/%D	Timed portion
Inject (checked/unchecked)	InjectValve.State (=InjectPosition/LoadPosition)	Setup & timed portions
Column (checked/unchecked)	ColumnValve.State (=Col_B/Col_A)	Setup & timed portions
TTL 1 (checked/unchecked)	Pump_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2 (checked/unchecked)	Pump_TTL_2.State (=0v/5v)	Setup & timed portions
Relay 1 (checked/unchecked)	Pump_Relay_1.State (=Closed/Open)	Setup & timed portions
Relay 2 (checked/unchecked)	Pump_Relay_2.State (=Closed/Open)	Setup & timed portions
Flow	Flow	Setup & timed portions
PeakNet (Release 4.5 Through 5.2) Method Parameter	**PGM Command of the Dionex Chromatography Management System**	**Comments**
Eluent percentage (%A)	Not converted	Calculated from %B, %C, and %D
Pump (On/Off)	Not converted	
Curve	Curve	

Comment	Comments	
Piston Size	Not converted	Set in Server Configuration instead
Pressure Units	Not converted	Set in Server Configuration instead
Description	Comments	

Eluent Generator Translation Table

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Eluent Concentration	Concentration	Timed portion
TTL 1(checked/unchecked)	EluentGenerator_TTL_1.State (=0v/5v)	Timed portion
Offset Volume	Not converted	Set in Server Configuration instead
Curve	Curve	
Eluent Label	Not converted	
TTL 1 Output	Not converted	

AD20 Setup and Timed Event Parameter Translation

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Rate	Data_Collection_Rate	Setup portion
Time	UV_VIS_1.AcqOff (at time=time of AcqOn + Time)	Timed portion
TTL 1(checked/unchecked)	UV_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2(checked/unchecked)	UV_TTL_2.State (=0v/5v)	Setup & timed portions
Relay 1 (checked/unchecked)	UV_Relay_1.State (=Closed/Open)	Setup & timed portions
PeakNet (Release 4.5 Through 5.2) Method Parameter	**PGM Command of the Dionex Chromatography Management System**	**Comments**
Relay 2 (checked/unchecked)	UV_Relay_2.State (=Closed/Open)	Setup & timed portions
Offset (checked)	Autozero	Setup & timed portions
Mark (checked)	UV_Analog_out.Mark	Setup & timed portions
Range	UV_Analog_out.Recorder_Range	Setup & timed portions
Wavelength	Wavelength	Setup & timed portions

Collection Begin (checked)	UV_VIS_1.AcqOn	Setup or timed portion
UV Lamp (Off/Low/High)	UV_Lamp (=Off/Low/High) If =Low/High, command "Wait UV_Lamp_Ready" is added	Setup portion
Visible Lamp (Off/Low/High)	Visible_Lamp (=Off/Low/High)	Setup portion
Plot Scales (Minimum/Maximum)	Not converted	
Detector Units	Not converted	
X-Y Data	Not converted	

AD25 Setup and Timed Event Parameter Translation

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Rate	Data_Collection_Rate	Setup portion
Time	UV_VIS_1.AcqOff (at time=time of AcqOn + Time)	Timed portion
TTL 1(checked/unchecked)	UV_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2(checked/unchecked)	UV_TTL_2.State (=0v/5v)	Setup & timed portions
Relay 1 (checked/unchecked)	UV_Relay_1.State (=Closed/Open)	Setup & timed portions
Relay 2 (checked/unchecked)	UV_Relay_2.State (=Closed/Open)	Setup & timed portions
Offset (checked)	Autozero	Setup & timed portions
Mark (checked)	UV_Analog_out.Mark	Setup & timed portions
Range	UV_Analog_out.Recorder_Range	Setup & timed portions
Wavelength	Wavelength	Setup & timed portions
Collection Begin (checked)	UV_VIS_1.AcqOn	Setup or timed portion

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
UV Lamp (On/Off)	UV_Lamp (=On/Off) If =On, command "Wait UV_Lamp_Ready" is added	Setup portion
Visible Lamp (On/Off)	Visible_Lamp (=On/Off)	Setup portion
Offset Level	UV_Analog_out.Offset_Level	Setup portion
Calibration (Off/Zero/Full Scale)	Recorder_Calibration (AU/Zero/Full_Scale)	Setup portion

Polarity (Negative/Positive)	UV_Analog_Out.Polarity (=Negative/Positive)	Setup portion
Rise Time	Rise_Time	Setup portion
Comment	Comments	
Description	Comments	
Labels	Not converted	
Plot Scales (Minimum/Maximum)	Not converted	
Detector Units	Not converted	
X-Y Data	Not converted	

CD20 Setup and Timed Event Parameter Translation

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Rate	Data_Collection_Rate	Setup portion
Time	AcqOff (at time=time of AcqOn + Time)	Timed portion
Range (µS)	ECD_Analog_Out.Recorder_Range	Setup & timed portions
TTL 1(checked/unchecked)	ECD_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2(checked/unchecked)	ECD_TTL_2.State (=0v/5v)	Setup & timed portions
Relay 1 (checked/unchecked)	ECD_Relay_1.State (=Closed/Open)	Setup & timed portions
Relay 2 (checked/unchecked)	ECD_Relay_2.State (=Closed/Open)	Setup & timed portions
Offset (checked)	Autozero	Setup & timed portions
Mark (checked)	ECD_Analog_Out.Mark	Setup & timed portions
PeakNet (Release 4.5 Through 5.2) Method Parameter	**PGM Command of the Dionex Chromatography Management System**	**Comments**
Temp. Comp.	Temperature_Compensation	Setup portion
Cell Temp.	DS3_Temperature	Setup portion
SRS Current (Off/50/100/300/500 Ma)	SRS_Current (=Off/50/100/300/500)	Setup portion
Collection Begin (checked)	AcqOn	Setup or timed portion
Plot Scales (Minimum/Maximum)	Not converted	
Detector Units	Not converted	
X-Y Data	Not converted	

ED40 Setup and Timed Event Parameter Translation

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Rate	Data_Collection_Rate	Setup portion
Time	AcqOff (at time=time of AcqOn + Time)	Timed portion
Range (µS)	ECD_Analog_Out.Recorder_Range	Setup & timed portions
TTL 1(checked/unchecked)	ECD_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2(checked/unchecked)	ECD_TTL_2.State (=0v/5v)	Setup & timed portions
Relay 1 (checked/unchecked)	ECD_Relay_1.State (=Closed/Open)	Setup & timed portions
Relay 2 (checked/unchecked)	ECD_Relay_2.State (=Closed/Open)	Setup & timed portions
Offset (checked)	Autozero	Setup & timed portions
Mark (checked)	ECD_Analog_Out.Mark	Setup & timed portions
Temp. Comp.	Temperature_Compensation	Setup portion. Only for ED40/ED50c (conductivity)
Cell Temp.	DS3_Temperature	Setup portion. Only for ED40/ED50c

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
SRS Current (Off/50/100/300/500 mA)	SRS_Current (=Off/50/100/300/500)	Setup portion. Only for ED40/ED50c
Amperometry Cell (On/Off)	Cell (=On/Off)	Setup portion. Only for ED40/ED50d (DC amperometry) & ED40/ED50i (integrated amperometry)
Oven Temperature (enabled)	Oven_Temperature	Setup portion. Only for

		ED40/ED50d & ED40/ED50i
Voltage	DC_Voltage	Setup portion. Only for ED40/ED50d
Collection Begin (checked)	AcqOn	Setup or timed portion
Plot Scales (Minimum/Maximum)	Not converted	
Detector Units	Not converted	
X-Y Data	Not converted	

IC20 Setup and Timed Event Parameter Translation

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Rate	Data_Collection_Rate	Setup portion
Time	ECD_1.AcqOff (at time=time of AcqOn + Time)	Timed portion
High Pressure Limit	Pressure.UpperLimit	Setup portion
Low Pressure Limit	Pressure.LowerLimit	Setup portion
SRS Current (Off/50/100/300/500 Ma)	SRS_Current (=Off/50/100/300/500)	Setup portion
Oven Temp.	DS3_Temperature	Setup portion
Temp. Comp.	Temperature_Compensation	Setup portion
PeakNet (Release 4.5 Through 5.2) Method Parameter	**PGM Command of the Dionex Chromatography Management System**	**Comments**
Inject(checked/unchecked)	Pump_InjectValve.State (InjectPosition/LoadPosition)	Setup & timed portions
TTL 1(checked/unchecked)	Pump_ECD_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2(checked/unchecked)	Pump_ECD_TTL_2.State (=0v/5v)	Setup & timed portions
Relay 1 (checked/unchecked)	Pump_ECD_Relay_1.State (=Closed/Open)	Setup & timed portions
Relay 2 (checked/unchecked)	Pump_ECD_Relay_2.State (=Closed/Open)	Setup & timed portions
Offset (checked)	Autozero	Setup & timed portions
Mark (checked)	Mark	Setup & timed portions
Flow	Pump_ECD.Flow	Timed portion
Range	Recorder_Range	Setup & timed portions

Eluent (A/B)	Pump_ColumnValve.State (=Col_A/Col_B)	Setup & timed portions
Collection Begin (checked)	ECD_1.AcqOn	Setup or timed portion
Pressure Units	Not converted	Set in Server Configuration instead
Piston Size	Not converted	Set in Server Configuration instead
Pump (On/Off)	Not converted	
Comment	Comments	
Description	Comments	
Labels	Not converted	
Plot Scales (Minimum/Maximum)	Not converted	
Detector Units	Not converted	
X-Y Data	Not converted	

DX-120 Setup and Timed Event Parameter Translation

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Rate	Data_Collection_Rate	Setup portion
Time	ECD_1.AcqOff (at time=time of AcqOn + Time)	Timed portion
Pump (On/Off)	Pump (=On/Off)	Setup portion
Column (A/B)	Column (=A/B)	Setup portion
	Wait RinseComplete command added	Only if System Mode is Column
Pressure (psi/MPa)	PressureUnit (=psi/MPa)	Setup portion
SRS/Cell (On/Off)	SRS (=On/Off)	Setup portion
Eluent Pressure (On/Off)	EluentPressure (=On/Off)	Setup portion
Offset (checked)	Autozero	Setup & timed portions
Inject(checked/unchecked)	Pump_InjectValve.State (InjectPosition/LoadPosition)	Setup & timed portions
TTL 1(checked/unchecked)	ECD_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2(checked/unchecked)	ECD_TTL_2.State (=0v/5v)	Setup & timed portions
Controlled AC (checked/unchecked)	ControlledAC (=On/Off)	Setup & timed portions
Eluent (A/B)	Eluent (=A/B)	Setup & timed portions Only if System Mode is Eluent
Collection Begin (checked)	ECD_1.AcqOn	Setup or timed portion
System Mode	Not converted	
Comment	Comments	
TTL Output Labels	Not converted	
Plot Scales (Minimum/Maximum)	Not converted	
Detector Units	Not converted	
X-Y Data	Not converted	

UI20 Setup and Timed Event Parameter Translation

PeakNet (Release 4.5 Through 5.2) Method Parameter	PGM Command of the Dionex Chromatography Management System	Comments
Rate (A&B)	Data_Collection_Rate	Setup portion
Time (A&B)	Channel_A.AcqOff for Channel A Channel_B.AcqOff for Channel B (at time=time of AcqOn + Time)	Timed portion
TTL 1(checked/unchecked)	Interface_TTL_1.State (=0v/5v)	Setup & timed portions
TTL 2(checked/unchecked)	Interface_TTL_2.State (=0v/5v)	Setup & timed portions
TTL 3(checked/unchecked)	Interface_TTL_3.State (=0v/5v)	Setup & timed portions
TTL 4(checked/unchecked)	Interface_TTL_4.State (=0v/5v)	Setup & timed portions
Relay 1 (checked/unchecked)	Interface_Relay_1.State (=Closed/Open)	Setup & timed portions
Relay 2 (checked/unchecked)	Interface_Relay_2.State (=Closed/Open)	Setup & timed portions
Full Scale Voltage (mV)	Full_Scale_Voltage	Setup portion
(10/100/1000/10000)	(0.011/ 0.110/ 1.100/ 11.000)	
Collection Begin (checked)	Channel_A.AcqOn for Channel A Channel_B.AcqOn for Channel B	Setup or timed portion
Comment	Comments	
Labels	Not converted	
Plot Scales (Minimum/Maximum)	Not converted	
Units	Not converted	
X-Y Data	Not converted	
TTL Inputs	Not converted	
Trigger	Not converted	

Detector Component Table Parameter Translation

PeakNet Release 4.5 Through 5.2 (PN5) Component Table Parameter	QNT Method Parameter of the Dionex Chromatography Management System	Comments
Component Name	Peak Name	
Retention Time	Retention Time	If peak Reference Component column = None then Retention Time options are set to Absolute. If peak Reference Component = <Component> then Retention Time options are set to Time Distance to Reference Peak and Reference Peak = <Component> is assigned
Tolerance	Window	If Tolerance = time then Window options are set to Absolute and Greatest. If Tolerance = % then Window options are set to Relative and Greatest.
Reference Component	Retention Time Options	See Retention Time comments for rules.
Internal Standard Component	Standard	If global PN5 calibration options = External then all DDS Standard = External If global PN5 calibration options = Internal then - If Internal Standard Component = Internal Standard then "Use this peak as Internal Standard" option is set. - If Internal Standard Component = <Component> then Internal Standard is set and Associated ISTD Peak is assigned.
Calibration Standards Level [1...32] Amounts	Amount column for each level	An amount column for each level labeled Std1, Std2, … Stdn is inserted where n = total levels. The amounts for each peak in the table are filled in.
Check Standards Level [1...32] Amounts	Amount column for each level	An amount column for each level labeled CStd1, CStd2, … CStdn is inserted where n = total levels. The amounts for each peak in the table are filled in.

PeakNet Release 4.5 Through 5.2 (PN5) Component Table Parameter	QNT Method Parameter of the Dionex Chromatography Management System	Comments
Curve Fit Type	Calibration Type	If Cubic in PN5 then set to quadratic. - PN5 Fit Linear/quadratic with Origin = Force is Linear/quadratic in the DDS. - PN5 Fit Linear/quadratic with Origin = Ignore is Linear/quadratic with Offset in the DDS. - PN5 Fit Linear/quadratic with Origin = Include is Linear/quadratic with Offset and Include point (0,0) options in the DDS. - All DDS are set to No Weights. - No Average Response Factor in the DDS so set to Linear.
Origin	Calibration Type	See Curve Fit Type for rules.
Calibrate By	Calibrate By	- Area or Height - If Relative then set to Relative Area for Identified Peaks Only.
Relative Response Component	Response Factor	Relative to Peak is set and correct peak is assigned.
Relative Factor	Response Factor	Value for factor is assigned.
Groups	Groups	- For each peak in a group the DDS group item is set to that name. - For each time range in a group, the range is added to Unidentified Peaks list.
Standardization	External/Internal	See handling in Quantification section above.
Calibration Standard Volume	Reference Inject Volume	
Amount Units	Dimension of Amounts	
Replace Retention Time	Use recently detected retention times checkbox is checked	Last Standard Options = Last Value
Low Limit Amount	Not Available (N.A.)	
High Limit Amount	N.A.	
Total Levels for Calibration Standards	N.A.	

PeakNet Release 4.5 Through 5.2 (PN5) Component Table Parameter	QNT Method Parameter of the Dionex Chromatography Management System	Comments
Total Levels for Check Standards	N.A.	
Replicates Table	N.A.	No replicate information will be converted from PN5.
Replicates	N.A.	
Rejection of Outlier	N.A.	
Linear Weighting	N.A.	
Replace/Average Response	N.A.	
Sample Volume Default	N.A.	
Sample Weight	N.A.	
Dilution Factor	N.A.	
Internal Standard Amount	N.A.	
Unknown Response Factor	N.A.	
Response for Unknowns	N.A.	
CE Information	N.A.	If CE information is contained it will not be converted to the DDS.

Actions in the Control Panel

See the following topics for details on how to load a **Control Panel** and how to modify controls and the timebase assignment.

Loading a Control Panel

Connecting a Control Panel with a Timebase

Modifying a Control Panel

Modifying a Control

Linking a Control to a Device

Creating a Command Button

Creating Hidden Windows

In addition, data acquisition can be simulated in a control panel and sample and sequence information can be displayed:

Using/Recording Demo Data

Displaying Sample and Sequence Information

Loading a Control Panel

Before processing a new unknown samples or operating a controllable instrument, a ➢*Control Panel* must be loaded, either manually or automatically:

Manually

- Choose the **Open** command from the **File** menu and search for files with the extension ***.pan**. In the **Open** dialog box, choose the object type **Control Panel**.
- Alternatively, you can search for the file directly in the ➢*Browser*.

The Dionex Chromatography Management System includes various default control panels that offer all standard functions required for operation. Normally, you will find these in the **Panels** directory of the local ➢*Datasource*.

- Select a control panel and open it by double-clicking its name.

Each window must be connected with a ➢*Timebase*. When opening the window, the Dionex Chromatography Management System automatically establishes a connection to the most recently used timebase. Usually, this timebase was assigned during installation by the Dionex Service. Naturally, each window can be connected with any other timebase (see **How to ...: Actions in the Control Panel Connecting a Control Panel with a Timebase**).

Automatically

When starting the Dionex Chromatography Management System, the most recent ➢*Workspace* is loaded. If this view contains a control panel, it will also be loaded.

If it is not possible to load a workspace, e.g. because no such view was arranged by the user, the control panel must be opened manually.

Connecting a Control Panel to a Timebase

When loading a ➢*Control Panel*, it is automatically connected with the previously stored ➢*Timebase*. You can modify the timebase assignment any time.

- Open a control panel and choose the **Connect to Timebase** command from the **Control** menu.

On the left, the input dialog box shows the name of the current timebase, the computer name of the corresponding ➢*Server* and the communications protocol. On the right, there is the icon for the local computer (**My Computer**). If the computer is connected to a network, you will also find an icon for the network neighborhood.

- Open the directory tree by clicking on the **+** character.
- If the server is started, all timebases of the local server are listed below **My Computer**. If the server is not active, or if no server is installed, the message **The server is not running** will be displayed.
- Below **Network Neighborhood**, you see all PCs currently connected to the network. Open the directory tree below a computer name to see whether a Dionex Chromatography Management System server is installed on this computer. If the server is active, the names of the corresponding timebases are visible. Otherwise, you will receive the message **The server is not running**.
- Select the name of a timebase and complete the input by pressing **OK**.

The Dionex Chromatography Management System now connects your control panel to the corresponding timebase. If the action is successfully completed, the connected instruments can be controlled via the controls in various colors.

Problems in Establishing a Connection

It depends on the selected network protocol whether a non-local server is visible or can be accessed. The system requires several seconds to check whether the selected protocol can be used or not! If no connection is established to a specific timebase, this can be due to several reasons.

- First, check whether the corresponding server is running.
- If this is ensured, try another network protocol. The Dionex Chromatography Management System can communicate via various network protocols, e.g. IPX, TCP/IP, or NetBEUI.

⚠ ***Caution***: Communication between two stations is possible only if the same (!) network protocol is installed and selected. Generally, it is sufficient to install the corresponding Microsoft (**IPX/SPX compatible protocol**; **NetBEUI**; **TCP/IP**) or Novell (**Novell IPX ODI Protocol**) network protocols via **Settings/Control Panel/Network/Configuration**. Which protocol is actually used depends on the current network installation. Please contact your network administrator. If a connection is to be established to a Windows NT/Windows 2000 computer, this is usually possible via the protocol **Named Pipes**.

- Sometimes it may happen that the required timebase exists (Server is running) but that it is not displayed. If so, open the **Connect to Timebase** dialog box again. This may also happen when linking two computers via an ISDN connection. Usually, the reason is a slightly incorrect network installation.
- If the **IPX/SPX compatible protocol** is used, the **Activate NetBIOS with IPX/SPX** option should be used under **Settings/Control Panel/Network/Configuration/Properties/NetBIOS**.

If it is still not possible to establish a connection, please contact Dionex Service.

Problems with Controlling Instruments

In addition to the control mode, the Dionex Chromatography Management System offers the **Monitor Only** mode. If a user establishes a connection to a timebase via a network, the user receives the monitor only status on this timebase.

The monitor only status is also assigned, when a user attempts to access a local timebase that us currently used by an external user.

- Deactivate the **Monitor Only** command in the **Control** menu to enable complete control of the timebase.

Modifying a Control Panel

Select the ➢*Control Panel* you intend to modify (see **How to ...: Actions in the Control Panel** **Loading a Control Panel**).

Activating the Layout Mode

- Change to the ➢*Layout Mode* by selecting it in the context menu.

Adding a Control

- Move the mouse cursor over the ➢*Layout Toolbar*:

  The **quick info** gives information on the ➢*Control* where the mouse cursor is situated.
- Select the desired control via a mouse click. The mouse cursor is now "loaded" with the corresponding control.
- Position the mouse cursor to where you want to add the new control and press the left mouse button.

Removing a Control

- Click the left mouse button on the control to be removed. The selected control is marked by the control frame.
- Press the **Delete** key to remove the control.

Modifying the Size and Position of Controls

- Select a control with the left mouse button and assign the desired size by drawing the ➢*Control Frame*.
- Select a control, position the mouse cursor on the control, and move it while pressing the left mouse button. Select several controls by simultaneously pressing the **Shift** key.
- Select the function ➢*Align* (in the Edit menu) to align several controls. The control frame of the control first selected is used as reference point and reference size for the other controls.

For information on how to change control properties, see **How to ...: Actions in the Control Panel Modifying a Control**

Modifying a Control

Online Mode

- Position the mouse cursor over the corresponding ➢*Control* (= object) and open the context menu (right mouse button).
- Open the edit box via the **Properties** option.

Layout Mode

- Click the object with the left mouse button.
- Press the right mouse button within the control frame and open the edit box via **Properties**.

Dialog Box "Properties"

Depending on the selected control, the **Properties** dialog box contains different tab dialog boxes with the following functions:

	Name	Function
1.	General	Determines the size and the text of the control
2.	Link	Establishes the connection to the device the properties of which shall be displayed
3.	Autosize	Determines how the size of the control will change when the complete panel is increased or decreased in size
4.	Color	Selects the color for the individual components of the control

	Name	Function
5.	Style	Selects the shape of the control
6.	Button	Defines if additional ➢*Control Panel* windows shall be opened via the respective **Command Button** and if so which ones (also, see: **How to ...: Actions in the Control Panel** **Creating Hidden Windows**)
7.	Command	Enters the command/program to be executed when the **Command Button** is pressed.
8.	Axis/Decoration	Determines the scaling of the axes and the display of the online signals and the 3D plot
9.	Signals	Determines which signals shall be displayed using which offset
10.	Chrom.	Selects overlapping chromatograms in the signal plot
11.	Device	Selects the pump(s) for which the course of the gradient shall be displayed
12.	Timebase	Connects to the selected ➢*Timebase*

The individual tab dialog boxes are available for the following controls (links to the respective topics in the Online Help only):

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
Form	X			X	X							X
Check Box	X	X	X									
Color Box	X	X	X	X								
String Display	X	X	X									
Gauge Indicator	X	X	X	X	X							
Command Button	X		X			X	X					
Online Signal Plot	X		X	X				X	X	X		
Group Box	X		X		X							
Gauge/Slider	X	X	X	X	X							
Lamp	X	X	X	X	X							
Switch	X	X	X		X							
Edit Field	X	X	X	X	X							
Audit Trail	X		X									

	1	2	3	4	5	6	7	8	9	10	11	12
Gradient Display	X		X	X							X	X
3D-Plot	X		X	X				X				
Rack Display	X	X	X									
Online Mass Spectrum Plot	X		X	X								

For information on how to specify the property of a control, see **How to ...: Actions in the Control Panel Linking a Control to a Device.**

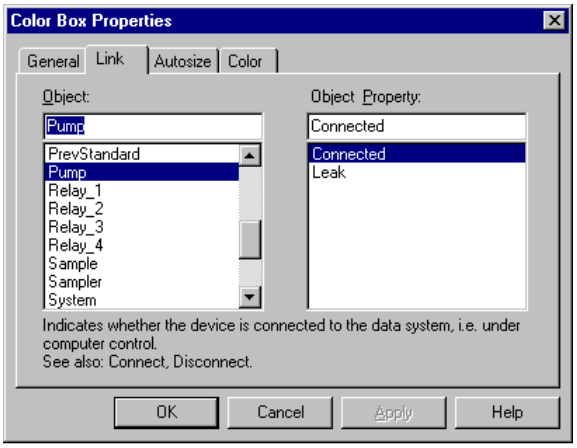
Linking a Control to a Device

Controls that should display the status or parameters of an instrument must be "linked" with this instrument.

- Place the mouse cursor over the ➢*Control* and open the context menu (right mouse button). Click the **Properties** and select the **Link** tab.
- In the field **Object**, select the destination of the link (e.g. an instrument, a function (relay), a ➢*Channel* or a system). In the field **Object Properties** select the property or the quantity to be measured which is available for this destination. Confirm your entry with **OK** to link the control to the destination and the property.

Example

If you wish to use e.g. a color box to see whether your pump is connected to the Dionex Chromatography Management System, select the following setting:



☞ ***Tip***: Not every control is ideal for representing certain functions or

parameters. Depending on the selected control, the corresponding device functions are listed in the field **Object Properties**.

Note: The signal plot, the gradient profile, and the 3D-plot are not linked via the **Link** dialog box. The parameters are selected either via the **Signals** (signal plot) tab or via the **Device** (gradient profile) tab or they cannot be modified (3D-plot).

Creating a Command Button

A command button can be assigned a command or a sequence of commands. The command or the program is then executed upon a key click. To create command buttons, users must have the corresponding authorization.

- Place the mouse cursor over the corresponding button, open the context menu, select **Properties**, and open the **Command** tab dialog box.
- In the list box, all commands to be executed are entered successively. The syntax corresponds to the ➢*Program*. Analogous to there, the syntax can be checked by pressing the **Check...** button and the operation can be tested via **Try it now** before programming is completed.
- You can also start a complete program, which was written previously, via a **Command** Button. To do so, copy the full program text and insert it in the **Command** tab dialog box. Another possibility is via the command ⇒*Branch*. Enter the program (+ location) that shall be started after the command **Branch**:

  ```
  Branch „CM_Seminar\\Programs\\Equilibration"
  ```

  Using this button you could start e.g. program for the equilibration of the column which is stored on the datasource **CM_Seminar** under the directory **Programs**.

For further details, see **Control** **Program Syntax**.

For practical tips, see **How to …:**

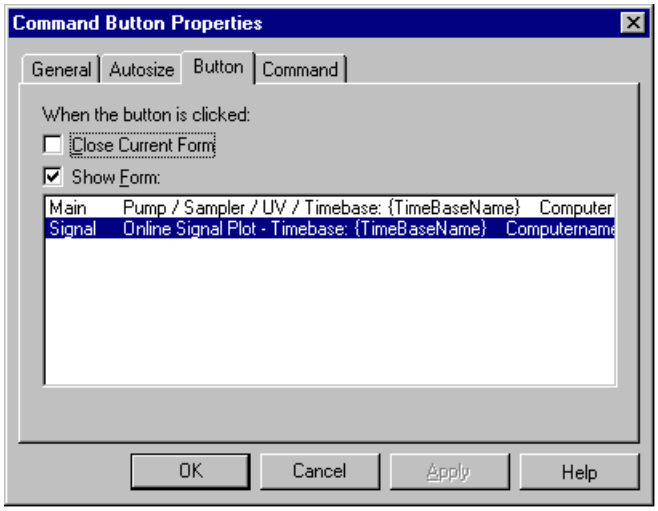
Actions in the PGM Editor **Creating a Program**

Device Control **Extending a Program**

Creating Hidden Windows

In some cases, a ➢*Control Panel* has to fulfill so many different functions that they cannot all fit in one window. In this case, a **Command Button** can be created to open an additional window, which may then contain the remaining controls. For example, the additional window can contain a large signal plot. Please proceed as follows:

- First, create an additional window: Activate the **Layout Mode** and select the command **New Window** from the menu **Window**.
- Add a signal plot to the new window, determine its size, and select the desired properties via the corresponding dialog box (**Properties**).
- Click on the background of this window (i.e., beside the signal plot) and from there, open the accompanying dialog box **Properties**.
- On the tab dialog box **General**, enter a name (e.g. **Signal**) and on the tab dialog box **Style** deactivate the **Initially Visible** option.
- Now add a **Command Button** to the original window and open its **Properties**.
- The tab dialog box **Button** indicates the names and headings for all windows that belong to this button. Select the new window and activate **Show Form**.



Using this control, you may now open the **Signal** plot.

Using/Recording Demo Data

Simulating Data Acquisition

➢*Demo Mode* lets you simulate data acquisition by loading a pre-recorded demo file and then displaying the data from the demo file in the ➢*Control Panel's* signal plot. The demo file is "read back" as though the data were being acquired in real time.

1. To select Demo Mode for a device, start the **Server Configuration** and select the device under the ➢*Timebase*.
2. Select **Properties** from the **Edit** or context menu.
3. For detectors, select **Read** under **Demo Mode** on the **General** tab page and select an existing demo file from the **Demo File Name** drop-down list.
4. In addition, activate the Demo Mode for all other devices of the timebase on the corresponding **General** tab pages.
5. To run the demo file, open the control panel for the device, connect to the timebase, and then turn on data acquisition. The **Data Acquisition** dialog box appears.
6. If the demo file contains more than one channel, select the desired channel(s) and click **OK**. The demo file begins running. It runs continuously (repeats) until data acquisition is turned off.

Recording Demo Data

1. To create a demo file for an installed detector, open the **Properties** dialog box in the **Server Configuration** and select **Write** under **Demo Mode** on the General tab page.
2. Enter a name for the demo file. If the device is connected via the Dionex DX-LAN, select the **Device ID** under **Communication**.
3. To write the demo file, open the control panel for the device and turn on data acquisition. The data acquired from the detector is recorded in the demo file.
4. To stop recording data, turn off data acquisition. The demo file is then complete. Alternatively, instead of starting and stopping data acquisition manually, you can run a ➢*PGM File* that turns acquisition on and off.

Displaying Sample and Sequence Information

In a ➢*Control Panel*, information that is specific to sequences and samples can be displayed in addition to the current analysis and status values. The

information can include the processed sample, the ➢*Sequence*, the ➢*Datasource*, the sample status etc.

To display this type of information, a ➢*Control* (alphanumeric display) is linked to one of the following functions (**Object Properties**):

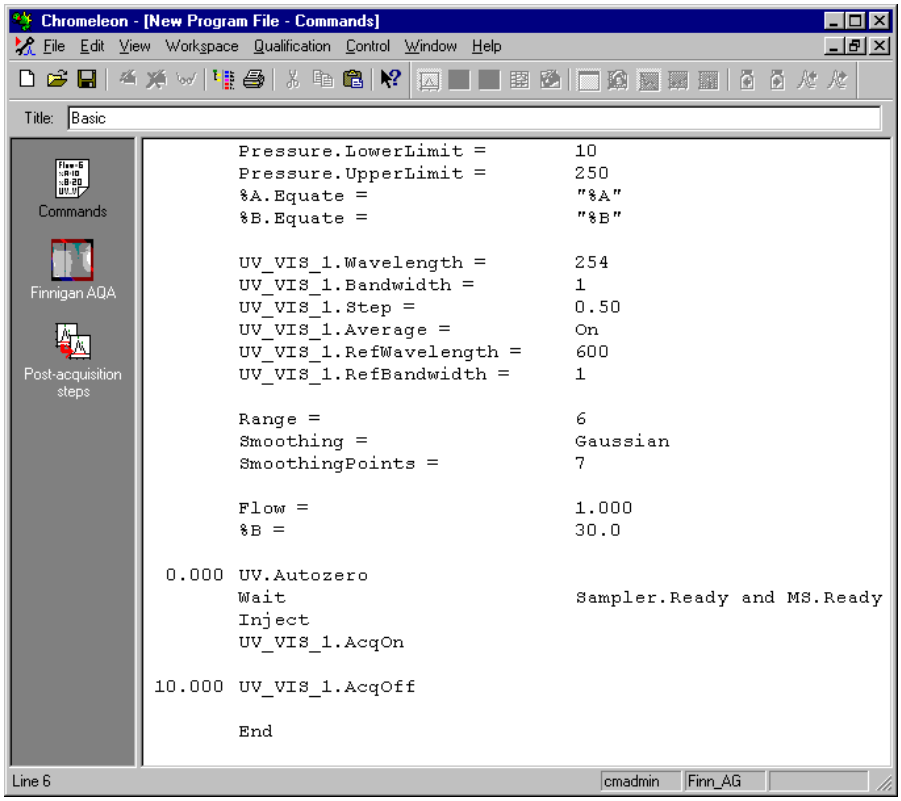
Comment	**Datasource**	**Program**
Name	**Sequence**	**ProgramMoniker**
Number	**SequencePath**	**Moniker**
Type	**SequenceMoniker**	**ID**

For details on how to change controls, see:

How to ...: Actions in the Control Panel.

Actions in the PGM Editor

The PGM editor is used for editing PGM files. It includes three views that can be accessed via the corresponding icons in the left pane (the so-called shortcut bar):



- **Commands** (for creating the program). For details, see **How to …: Actions in the PGM Editor** **Creating a Program** below.

- **Finnigan AQA** (creating the MS method). For details on the MS instrument method, see **How to …: Actions Related to the aQa-MS Creating a Method for the aQa-MS**.
- **Post-acquisition steps** (extraction and data smoothing steps after the data acquisition). For information, see **How to …: Actions in the PGM Editor Adding Post-Acquisition Steps**.

For further details on the PGM Editor, see **Basic Operation PGM Editor**.

Creating a Program

To create a ➢*Program*, various start conditions and ⇒*Control Commands* must be recorded precisely. Usually, program creation is via the Program Wizard while editing is via the **PGM-Editor** (Basic Operation topic). However, creating the program directly in the PGM Editor is possible as well. . The following minimum entries are required to receive a functioning program:

- Determination of recording signals and their parameters
- Determination of ⇒*Flow* rate and solvent composition (⇒*%A, %B, %C, %D* - for controlled pumps, only)
- ⇒*Inject* command
- Start of data acquisition (⇒*AcqOn/Off*)
- End of data acquisition
- End of program (⇒*End*)

Ensure that all relevant parameters are defined in the program. For parameters that are not explicitly defined, the Dionex Chromatography Management System uses the settings of the last sequence.

We recommend creating programs using the **Program Wizard**:

First, create the program automatically (see **Automatically Creating a Program** on the next page), and then edit the file manually (see **Manually Creating a Program** on the following page).

With respect to GLP/GMP we also recommend to add comments to the program on all chromatographic settings, e.g. column, detector, pumps, and, if necessary, the sample components plus explanatory notes. However, this is possible only when editing the file manually.

To see the structure of a simple program, see **How to …: Actions in the PGM Editor Program Example**

Experienced users of the data system GynkoSoft will find useful information under **How to :..: Actions in the PGM Editor**:

Differences from GynkoSoft

GynkoSoft Translation Table

Automatically Creating a Program

The basic structure of a ➢*Program* can be created with the **Program Wizard**.

- Choose **File / New** and select **Program File**.
- Enter the required information in the corresponding edit field.
- Press F1 if you need further help.

At the end of the input procedure, the system creates a functioning program based on your entries, without any requiring a special syntax or programming.

This program is a basic structure that can be modified or extended, as described under **How to ...: Actions in the PGM Editor Manually Creating a PGM File**

For a simple example, see **How to ...: Actions in the PGM Editor**

Program Example

For examples for the corresponding special programs, see **How to ...: Actions in the PGM Editor**

Creating an Emergency Program

Creating a Power-Failure Program

For an overview of the numerous programming capabilities, see **How to …: Device Control Extending a Program**

Manually Creating a Program

The following steps describe how to manually modify and save a ➢*Program*. (Note: For information on how to create a new program, see **Actions in the PGM Editor** **Automatically Creating a Program**).

General

- Choose the **File Open** command and select an existing PGM file.
- Ensure that the server has been started via the ➢*Monitor Program*.
- Connect the PGM file to a timebase by choosing the **Connect to Timebase** command from the Control menu. Select the timebase that will use the completed PGM file.
- Position the cursor on the place you wish to modify, or press Enter to create a new program line.

Entering commands/status variables

- Press the F8 key to open the edit box facilitating input.
- Choose the instrument (in the following called **Device**) for which you want to edit an instruction. A device can be any instrument of a timebase, but also an installed channel, a relay, a remote input, or the system itself. A device is represented by the symbol. Click the preceding **+** character to see details.
- Each device has its own **commands** ( ) and/or **properties** (, , ,).
- As soon as you select a command or a property, further edit fields and a short help text (**Help**) will appear in addition to the retention time field.
- Enter the retention time at which to execute the command.
- Assign the required value (e.g. a number) or a status (e.g. **On**) to the command / property.
- Press **OK** to complete the input, press **OK & Prev** or **OK & Next** to change the previous or the next program line.
- Repeat the input procedure until all commands are changed.

Checks during command input

- During the entry, the Dionex Chromatography Management System checks the commands from different angles (also, see ➢*Check Command*):

  Syntax check: Does the entry correspond to the formal rules of the PGM language?

  Semantics check: Does the PGM file make sense with regard to chromatography?

- If an error is detected, the corresponding line is written in red. Check and correct the entry. If necessary, repeat this procedure using the F8 input box.

Adding comments

- Use a semicolon to start the comment. The complete line following the semicolon is written in green to indicate that the Dionex Chromatography Management System treats the text as comment.
- Save the result as a new PGM file (**Save as**).

Note: Experienced users can enter these commands directly, i.e. without opening the F8 edit box. However, this requires profound knowledge of the **Program Syntax**.

For a simple example of a PGM file and an overview of the available programming possibilities, see **How to ...: Actions in the PGM Editor**

Program Example

For examples for the corresponding special programs, see **How to ...: Actions in the PGM Editor**

Creating an Emergency Program

Creating a Power-Failure Program

For an overview of the numerous programming capabilities, see **How to ...: Device Control**

Extending a Program

Program Example

A ➢*Program* for a 20 minute chromatogram, at a flow rate of 1 ml/min, with the components A (60%) and B (40%), the signals UV_VIS_1 (256nm), UV_VIS_2 (300nm) and a 3D-field that is recorded in the 200 to 360 nm range at a step of 0.5 seconds, could thus have the following appearance:

```
Pressure.LowerLimit =          5
Pressure.UpperLimit =          250
%A.Equate =                    "%A"
%B.Equate =                    "%B"
%C.Equate =                    "%C"

3DFIELD.MaxWavelength =        360.0
3DFIELD.MinWavelength =        200.0
3DFIELD.BunchWidth =           1.9
3DFIELD.Step =                 0.5
3DFIELD.RefWavelength =        600.0
3DFIELD.RefBandwidth =         1.9

UV_VIS_1.Wavelength =          256
UV_VIS_1.Bandwidth =           1
UV_VIS_1.Step =                2
UV_VIS_1.Average =             On
UV_VIS_1.RefWavelength =       600
UV_VIS_1.RefBandwidth =        1

UV_VIS_2.Wavelength =          300
UV_VIS_2.Bandwidth =           1
UV_VIS_2.Step =                2
UV_VIS_2.Average =             On
UV_VIS_2.RefWavelength =       600
UV_VIS_2.RefBandwidth =        1

Flow =                         1.000
%B =                           60
```

```
0.000   UV.Autozero
        Inject
        3DFIELD.AcqOn
        UV_VIS_1.AcqOn
        UV_VIS_2.AcqOn

20.000  3DFIELD.AcqOff
        UV_VIS_1.AcqOff
        UV_VIS_2.AcqOff

        End
```

Notes:

- A program for processing a sample batch must contain the ⇒*Inject*, ⇒*AcqOn/Off*, and ⇒*End* commands.
- It is possible but not necessary to include the commands for controlling the pump and the detector. Instead of entering the ⇒*Flow* rate, eluent composition (⇒*%A, %B, %C, %D*), and signal parameters directly on the instruments, these values can be set via the program, as shown in the example. This is possible only for controllable chromatography instruments connected to the data system via a RS232 interface.
- By definition, the injection time is t = 0.000. All commands that are to be executed before the injection time, have the time entry of t < =0.000 (e.g. detector lamp on command, here -10.000 min).
- The ⇒*LampOn/Off* command can be omitted if it is ensured that the lamp was given enough time to reach operating temperature.
- Commands that are not listed but are automatically considered (e.g. ⇒*Step* parameters of the UV_VIS_1 channel) are used with their default values or the values that were last used (e.g. Step = 0.25). The decision that value is considered depends on the respective device driver.
- In your programs, bear in mind that the instruments need a certain time to execute the different processes. If you use an HP autosampler, for example, the program files must be at least 2 min long to allow the ➢*Autosampler* sufficient time until the next injection.

For special PGM file examples, see **How to ...: Actions in the PGM Editor**

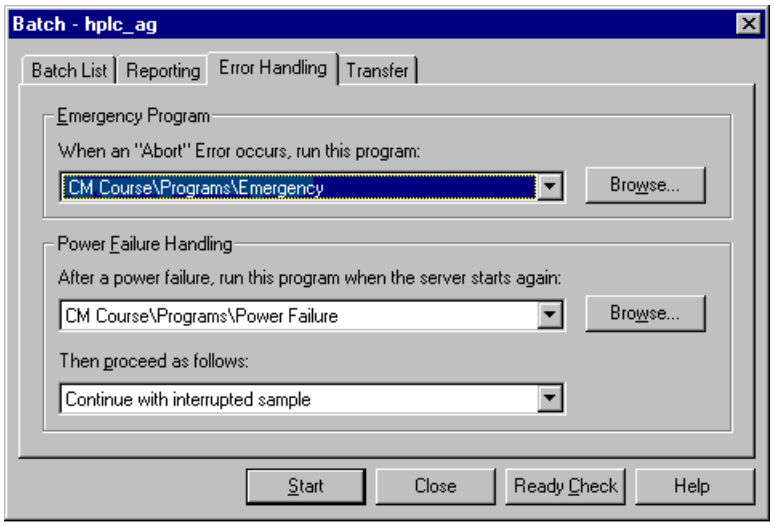
Creating an Emergency Program

Creating a Power-Failure Program

Creating an Emergency Program

If a ➢*Batch* was aborted automatically due to a severe error, an ➢*Emergency Program* can be started. This action can be defined as a rule. This ➢*Program* can be executed automatically.

Open the **Batch - <Timebase>** dialog box via the **Error Handling** command of the **Batch** menu. On the **Error Handling** tab, select the desired emergency program in the **Emergency Program** section via the **Browse** button.



Example 1:

A failure of the detector lamp represents a serious error, as no data can be recorded. However, this error should not immediately stop the flow. Instead, the column should be reconditioned after the abortion of the batch. The following emergency program can be used for this:

```
;       Program: Emergency.PGM
        Recondition column after abort.
0.000   Flow                    = 1
        %A.Value                = 0
        %B.Value                = 100
        %C.Value                = 0
10.000  Flow                    = 1
10.500  End
```

Example 2:

A serious error occurs, e.g. when the ➢*Autosampler* has a power failure. In this case, the entire system should be stopped immediately to prevent further damage. The emergency program **Abort.PGM** stops the pump flow and switches off the detector lamp.

```
;       Program: Abort.PGM
        The detector lamp and the pump flow are switched off.
0.000   Flow          = 0
        Lamp          = Off
0.500   End
```

Also, see:

How to ...: Actions in the PGM Editor Creating a Power-Failure Program

Creating a Power-Failure Program

You can define how the Dionex Chromatography Management System shall react after a power failure (see ➢*Power-Failure Protection*). After booting the server, run a power-failure program first.

Open the Batch <Timebase> dialog box via the **Error Handling** command in the **Batch** menu. On the Error Handling tab, select the desired power-failure program in the **Power Failure Handling** section via the **Browse** button.

If you do not have a power-failure program yet, create one for your respective timebase. Please ensure that all instruments are reconnected to the Dionex Chromatography Management System first. As very often self-tests have to be performed, the ⇒*Connect* commands should be given 1-2 minutes before the first ⇒*Control Commands* are sent to the instruments.

Example:

The following program example can be used e.g. for a ➢*Timebase* which contains an ASI-100 ➢*Autosampler*, a UVD 340S ➢*Photodiode Array Detector*, and a P580 pump:

```
-2.000   UV.Connect
   Sampler.Connect
   Pump.Connect
-1.500 Lamp =                On

; After being switched on, the UVD 340S needs some time for spectra
; calibration. That is why this command as well needs to be given some
; minutes before starting the data acquisition.

 0.000 Flow =                0.300

 1.000 Flow =                1.000

       End
```

Also, see:

How to ...: Actions in the PGM Editor Creating an Emergency Program

Differences from GynkoSoft

The following description is intended for experienced **GynkoSoft** users who are interested in the modifications in the new ➢*Program*.

General Information

If a command is intended for a specific instrument, this is no longer specified as a parameter *(Device, Signal,...)*, but the instrument is stated before the command. Between the device name and the command, a period is inserted. In GynkoSoft the syntax was:

```
0.000 Autozero     Detector=UVD320S
```

The new syntax in the Dionex Chromatography Management System is:

```
0.000 UVD320S.Autozero
```

As before, the instrument can be omitted if no confusion is possible. If there are several instruments for which the command could be valid, the instrument MUST be explicitly specified.

The retention time can be omitted if it does not change. It must be specified for the first command in a group of combined commands.

Wherever numerical input is expected, a mathematical expression can be entered, if required. This can include variables (parameters and values such as signal value, pressure etc.) and the usual operators (+ - * /, brackets).

Wherever a logical value is expected, a logical expression can be entered with the operators = <>, <, >, <=, >=, AND, OR, NOT. All relays, inputs, and further status parameters can be used as logical variables.

Text, Names

Text parameters (for ⇒*Protocol*, ⇒*Message*, Equate) must be in quotation marks. This does not apply to the names of devices, triggers, commands, etc.

Names can include the letters A-Z, numbers, percent characters, and underscores. Some names had to be changed, as they contained invalid characters (e.g. blanks, hyphens or minus signs).

Names can start with a number if no confusion with other numbers is possible (valid name: **3DFIELD**; invalid name: **1E2** as this could be interpreted as exponential function).

Currently, commands and names cannot be abbreviated.

Variables

Whenever possible commands are replaced or completed by variables (or, as in Online, **Object Properties**). Instead of the **Lamp On** and **Lamp Off** commands, there is now the ⇒*LampOn/Off* variable that can assume the values **On** and **Off**. The value of a variable is changed via **Variable = Value** (e.g. Lamp = Off). The character **="** can be omitted, i.e. **Lamp Off** is also valid.

Variables considerably improve the readability of a program, as several variables are defined instead of entering a long command with numerous parameters. The GynkoSoft command

```
...    Signal Parameter, Signal=UV_Vis_1, Step=0.25, Average=On,
       Wavelength=250, Bandwidth=0
```

reads in the Dionex Chromatography Management System:

```
...    UV_Vis_1.Step          0.25
...    UV_Vis_1.Average       On
...    UV_Vis_1.Wavelength    250
...    UV_Vis_1.Bandwidth     0
```

The ➢*Sample Data* (**Name**, **ID**, **Comment**, **Program**, and others) includes variables that can be used in the program. There are four **sets** of sample

variables (Sample, PrevSample, NextSample, PrevStandard) referring to the current, the previous, the next, and the last standard sample. The entry is similar to devices, e.g. **Sample.Name**.

In this sense, ⇒*Position* and ⇒*Volume* are not sample variables, but are assigned to a sampler or a driver for manual injectors. The program can read and change these variables. The modifications are re-entered in the sample data record.

All data points recorded by the Dionex Chromatography Management System (signal values, inputs, pressure, temperature...) are also available as variables, but cannot be modified.

Some variables include several values (e.g. nominal and actual temperature). Generally, the Dionex Chromatography Management System recognizes the **correct** value. For the oven, the actual value is shown, but the nominal value is changed. Changing this is theoretically possible by explicitly specifying the value (separated by a period). The nominal temperature is thus **Temperature.Nominal**, and the actual temperature is **Temperature.Actual**.

The following sub-variables are possible:

Actual	Actual value
Nominal	Nominal value (e.g. temperature)
UpperLimit	Upper limit (e.g. pressure)
LowerLimit	Lower limit (e.g. pressure)
Equate	Name (e.g. %A)

Trigger

A ⇒*Trigger* can now actuate an entire list of commands. It is no longer necessary to define several triggers with the same condition. EndTrigger must mark the end of the list. The commands in the trigger list need *not* have a time definition.

Triggers must always have a name that may not coincide with the name of a device or a command.

GynkoSoft has a fixed hysteresis of 5%. In the Dionex Chromatography Management System, the hysteresis can be set for the trigger command with the parameter hysteresis=*x*.

DELTA is no longer a trigger variable but can be assigned to any signal as a property.

 ***Note:*** All commands, variables, and their spelling can be viewed via the

Control menu and the **Command** command. Use this possibility to see the syntax of a specific command.

GynkoSoft Translation Table

The following table shows the translation of each GynkoSoft command in the Dionex Chromatography Management System (Dionex CMS):

GynkoSoft	Dionex CMS	Comment
%B, Percent=*x*	%B = *x (see ⇒%A, %B, %C, %D)*	%C, %D etc.
Abort Batch		Not yet supported
Acquisition On	*Channelname*.AcqOn (see ⇒*AcqOn/Off*)	For each channel separately
Acquisition Off	Acquisition Off	To switch off all channels, *or:*
	Channelname.AcqOff	For an individual channel
Autozero, Detector = *Name*	*Name*.Autozero	
Branch		
Column Temperature, Temperature = *x*	⇒*Temperature* = *x*	
Connect	⇒*Connect*	*Or with variables:* Connected=Connected
Continue	⇒*Continue*	*Or with variables:* HoldMode = Off
DELTA Signal name	Signalname.Delta	
Disconnect	Disconnect	*Or with variables:* Connected=Disconnected
Dispense Position=*x*, Volume=*y*, Duration=*z*	⇒*Dispense* ⇒*Position*=*x*, ⇒*Volume*=*y*, Duration=*z*	
Equate %A = *text*	%A.Equate = "*text*"	
End Program	⇒*End*	
Execute Device=*Name*, Function=*Func*, ...	*Name.Func* ...	
Flow Total, Flow = *x*	⇒*Flow* = *x*	
Hold	⇒*Hold*	*(Or with variables:* HoldMode = On)

GynkoSoft	Dionex CMS	Comment
Inject	⇒*Inject*	
Lamp On	Lamp = On (see ⇒*Lamp on/off*)	"=" can be omitted...
Lamp Off	Lamp = Off	
Message *text*	⇒*Message* "*text*"	
Pressure Limits, Lower Limit = *x*, Upper Limit = *y*	Pressure.LowerLimit = *x* Pressure.UpperLimit = *y* (See ⇒Pressure Limits)	Two separate commands required
Protocol *text*	⇒*Protocol* "*text*"	
Relay On, Relay = *r*, Duration = *x*	*r*.On Duration = *x*	*Or with variables:* *r*.Duration = x *r* On
Relay Off, Relay = *r*, Duration = *x*	*r*.Off Duration = *x*	*Or with variables:* *r*.Duration = x *r* Off
Reset	⇒*Reset*	
Segment, Volume = *x*	Suck Position=100, Volume=*x*	Position=100 *means that the air volume is drawn* (Command available for GINA 50 only)
Signal Parameter, Signal = *Name, Parameter=x*	*Name.Parameter=x*	For each parameter a separate line is required
Sound, Frequency=*x*, Duration=*y*	⇒*Sound*, Frequency=*x*, Duration=*y*	
Stop Flow	⇒*StopFlow*	*Or with variables:* StopMode = On
Suck Position=*x*, Volume=*y*, Duration=*z*	⇒*Draw* Position=*x*, Volume=*y*, Duration=*z*	
Trigger Name=*n*, Cond=*y*, ... *Command*	⇒*Trigger n* Condition=*y*, ... *Command* *Further Commands optional...* EndTrigger	See below
Trigger Off	Trigger *n,* Condition = 0 EndTrigger	Must be entered separately for each trigger
Wait, Input=*Name*	Wait *Name*	Apart from an input, the data system can wait for any condition (as trigger)

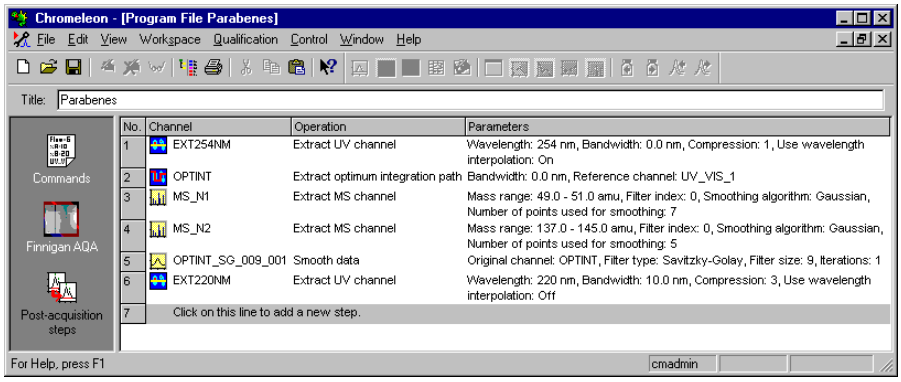
Adding Post-Acquisition Steps

The **Post-acquisition steps** view of the PGM editor allows defining extraction and data smoothing steps to be performed after data acquisition. These steps can be performed either online after the data acquisition or offline outside of chromatograms, UV spectra, and mass spectra.

Click the gray line to add a new post-acquisition step. In the opening dialog box, select the desired step. The following options are available:

- **Extract MS channel** (➢*Mass Trace* extraction - possible only after MS data were acquired.)
- **Extract optimum integration path** (extraction of the optimum integration path - possible only after a 3D-field was acquired)
- **Extract UV channel** (UV channel extraction - possible only after a 3D-field was acquired)
- **Smooth data** (chromatogram ➢*Smoothing*).

For example, the following steps can be added:



In step 1 and step 6, two UV channels are extracted at 254 and 220 nm, respectively. The EXT254NM channel does not use compression; data that were acquired at 254 nm are used only. For the EXT220NM, a range von 10 nm was selected, i.e., the wavelengths from 215 to 225 nm were used. In addition, compression is used during channel extraction. Compression = 3 means that every third datapoint is saved only.

In step 3 and step 4, two MS channels (MS_1 and MS_2) are extracted. The first of these mass traces covers the mass range 49.0 to 51.0 amu while the second once covers masses from 137.0 to 145.0 amu. For both channels, the Gaussian algorithm is used for data smoothing. Seven points are used for data smoothing when extracting the MS_N1 channel, while five points are used when extracting the MS_N2 channel.

In step 2, the ➢*Optimum Integration Path* is saved as OPTINT channel. In step 5, data smoothing is performed for this new channel using the Savitzky-Golay ➢*Filter*. Then, it is saved again as OPTINT_SG_009_001 channel. **Filter size: 9** indicates that 9 input datapoints each were used for creating one output datapoint.

Adding additional steps is via the bottom line or the Insert and Append Line commands of the context menu.

The post-acquisition steps are performed by the server when data acquisition of the last channel is terminated and before the ➢*System Suitability Test (SST)* is started. In case of network failure (see ➢*Network Failure Protection*), execution of the post-acquisition steps is delayed until the network source is available again.

Actions in the Chromatogram

The window shows the integrated chromatogram of a sample. Determining and integrating the peak areas was performed automatically based on the ⇒*Detection Parameters*. If you want to change the detection parameters for example because peaks are integrated that are too small or unimportant or because the baseline does not meet your requirements, you can perform the change graphically in the chromatogram:

Defining Detection Parameters Graphically

This function allows defining the detection parameters according to your requirements. In addition, the detection parameters are available on the Detection tab of the ⇒*QNT Editor* (see: **How to ...: Actions in the QNT Editor** **Defining Detection Parameters**).

If, even then, the representation and/or evaluation of single samples do not correspond to the expected result, the peak delimiters and the baseline can be modified manually. It is also possible to display further chromatograms for comparison. In addition, peaks can be assigned manually and a baseline for the entire chromatogram (averaged baseline) can be defined. A data filter can be applied, which smoothes the chromatogram and improves the reproducibility of peak baselines. For details, see the topics below:

Manual Re-Integration

Manual Peak Assignment

Performing a Chromatogram Comparison

Performing Data Smoothing

Due to the heavy noise, we recommend performing background subtraction for mass spectra. This can be defined in the chromatogram as well (see **Subtracting MS Background Spectra**).

For details on displaying a ➢*Report* or a Spectra Plot, see **How to ...:**

Actions in the UV Spectra and Mass Spectra

Actions in the Report

Defining Detection Parameters Graphically

Their graphical input considerably facilitates defining the ⇒*Detection Parameters*. Proceed as follows:

- If no parameter is indicated in the chromatogram, click the **Detection Parameter Tool** that is available via the context menu or the respective symbol on the integration ➢*Toolbar*.

- In the chromatogram, move exactly to the location where to enter a parameter.
- In the context menu, select the **Detection Parameter** option.
- Here you can directly

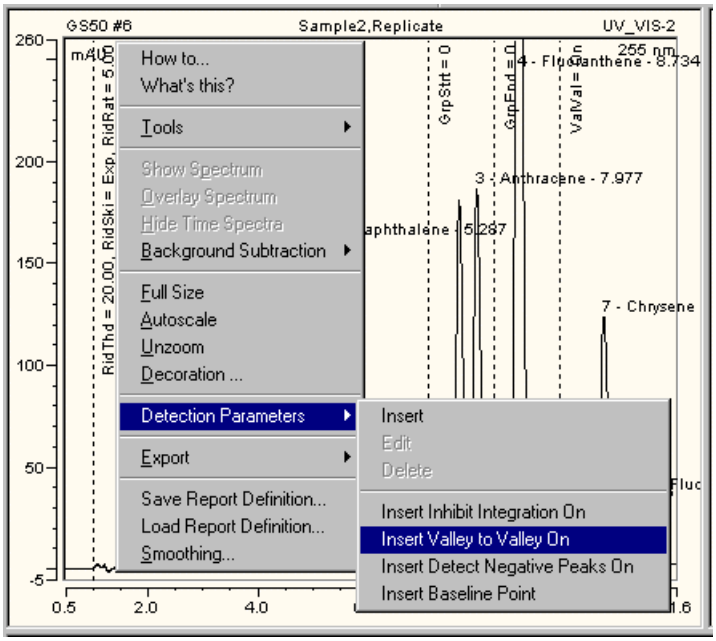
  Enable/disable to inhibit the integration (**Insert Inhibit Integration On** - see **How to ...: Actions in the QNT Editor** **Inhibiting Peak Integration**),

  Enable/disable the integration from valley to valley (**Insert Valley to Valley On**),

  Enable/disable negative peak integration (**Insert Detect Negative Peaks On**), or

  Insert a new baseline point (**Insert Baseline Point**) (for the latter, see **How to ...: Actions in the QNT Editor** **Modifying the Baseline**.
- Select **Insert** to insert another parameter.
- The **Detection Parameter Tool** allows moving the entered parameters to the desired location in the chromatogram.

The following example corresponds to the table input under **How to ...: Actions in the QNT Editor** **Defining Detection Parameters**.



In the chromatogram, a dotted vertical line at which the abbreviation for the parameter and its respective value are given indicates the parameters. In the illustration, see e.g. the values for the Rider Threshold (in short: RidThd), Rider Skimming (RidSki) and Maximum Rider Ratio (RidRat) parameters at 1.000 min.

For another way to enter detection parameters graphically, select a chromatogram area via the right mouse button. The opening context menu offers the following possibilities:

- Set an averaged baseline (**Set Averaged Baseline Start/End**), - see **How to ...: Actions in the Chromatogram Defining an Averaged Baseline**
- Define the minimum peak area (**Set Minimum Area**)
- Define the minimum peak height (**Set Minimum Height**)
- Define the minimum peak width (**Set Minimum Width**) (for all **Set Minimum ...** commands see **How to ...: Actions in the QNT Editor Reducing the Number of Evaluated Peaks**)

- Define the peak recognition algorithm (**Set Peak Slice & Sensitivity**, see **How to ...: Actions in the QNT Editor Modifying the Peak Recognition Algorithm**) or
- Select a range for the peak inhibition (**Set Inhibit Integration Range**)

Note: You can undo the graphical input of detection parameters. Click into one of the tables of the QNT editor and select the **Undo** command of the **Edit** menu. (In the chromatogram itself, you can only undo the modifications of the currently open chromatogram.)

Their graphical input enters the newly defined detection parameters to the **Detection** tab of the ⇒*QNT Editor*. They will be used for all samples that are evaluated using the QNT file of the current sample. Input of the detection parameters is also possible directly on the **Detection** tab (see **How to ...: Actions in the QNT Editor Defining Detection Parameters**).

Manual Re-Integration

Manual Re-Integration includes all actions performed directly in the chromatogram via mouse-click and the different tools on the integration ➢*Toolbar*. Thus, changes will always be performed in the current chromatogram only. This includes the following topics:

Moving Peak Delimiters
Modifying the Baseline
Inserting / Deleting a Peak
Changing the Peak Type
Defining an Averaged Baseline

Prerequisite

An integrated chromatogram can be recognized by the red baseline below the peaks and by the peak delimiters on the left and right of the baseline (= integration limit).

Caution: These elements must be displayed in the chromatogram (see Decoration / Peak Decoration in the context menu).

For all manual re-integration actions, it is recommended to zoom the area in which you want to perform modifications. Choose **Automatic** in the context menu to mark each place in the chromatogram that you can modify manually. The shape of the mouse cursor indicates which action is currently possible.

All modifications in the chromatogram can be undone as long as they are not stored.

In the **Edit** menu, select the **Delete Manipulations** command.

Moving Peak Delimiters

Near the blue peak delimiters, the mouse cursor changes its appearance (if the **Automatic Tool** or the **Delimiter Tool** are selected). It symbolizes peak start (⇂) and peak end (↾).

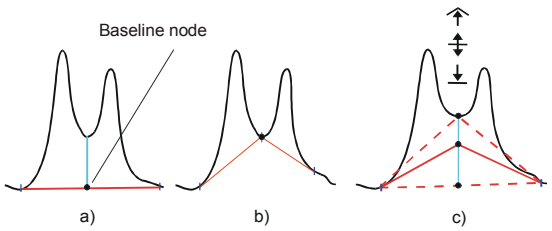
Press the left mouse button and move the mouse cursor to the new peak start or peak end.

It is not possible to "run over" a peak delimiter. The peak delimiter would be moved in the same direction. After positioning, the Dionex Chromatography Management System draws a new baseline. The modified peak properties Area, Width, Amount etc. are immediately updated and displayed in the integration report.

Peak delimiters of negative peaks can also be moved. In this case, the presentation of the mouse cursor is mirrored.

Modifying the Baseline

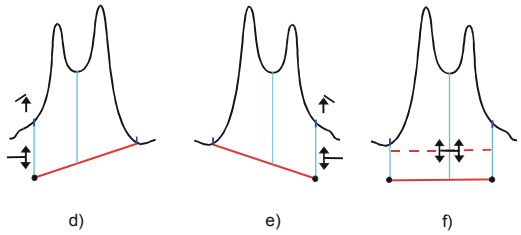
If two peaks that are not completely separated in the chromatogram are to be integrated individually, this is performed by dropping a perpendicular line from the minimum between the two peaks to the baseline. The intersection with the baseline is referred to as "baseline node" (a).



If the baseline should be drawn from peak end to peak end, activate the ⇒*Valley to Valley* detection parameter. The baseline node is automatically moved towards the signal curve until it rests on the curve in the minimum between two peaks (b).

Each baseline node can be moved along the perpendicular line and can be freely positioned ("freely floating baseline node" (c)). If either state (a) or (b) is approached, the mouse cursor automatically clicks into place. The shape of the mouse cursor (,) indicates the currently performed action. Use the **Automatic Tool** or the **Delimiter Tool**.

At the end of a baseline, freely floating baseline nodes can be generated (d, e).



The system automatically makes a distinction between moving a peak delimiter horizontally and a baseline node vertically depending on the direction in which the mouse cursor is drawn.

Between two baseline nodes, the entire baseline can be moved in vertical direction (f). The shape of the mouse cursor ( ) indicates whether the action is possible.

***Note**:* Inserting freely floating baseline nodes was not possible with the data system "GynkoSoft."

Inserting / Deleting Peaks

Inserting a Peak

In each free position of the chromatogram, and on the ascending and descending flanks of a peak, a new peak (i.e. a baseline and two peak delimiters) can be inserted later.

A small peak (⅄) on the right side of the mouse cursor indicates the places where this is possible. A warning sign (⃠) indicates the places where this is not possible.

- Open the context menu and select the **Insert Peak Tool** command. The mouse cursor now indicates the places where a peak can or cannot be inserted. Other actions (edit modes) are not possible at this point.

Deleting a Peak

If the mouse cursor is positioned over a peak, the peak can be deleted.

- Open the context menu and select the **Delete** command.

The peak delimiters and the baseline of the peak are removed.

Changing the Peak Type

If the mouse cursor is positioned over a peak, the peak type can be changed.

- Open the context menu and select the **Change to Main Peak** or **Change to Rider** command.

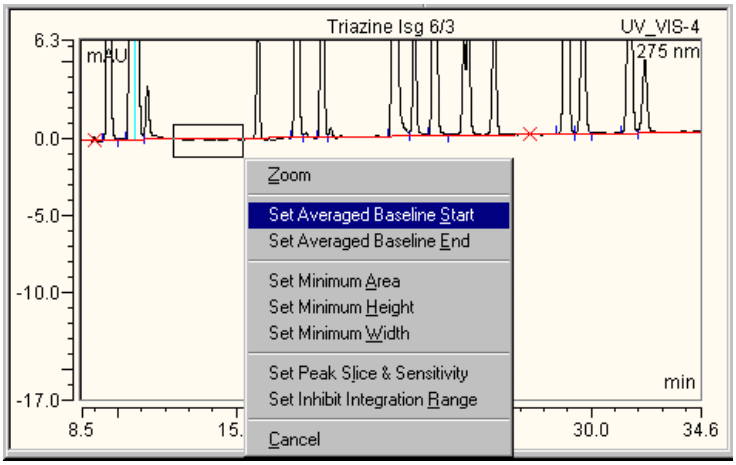
Use this function to change a main peak into a rider and vice versa. Single peaks are always interpreted as main peaks and, therefore, cannot be converted into rider peaks. The context menu indicates: **Can't Change Peak Type**.

Whether a peak is classified as a main peak or a ➢*Rider* depends in the automatic classification exclusively on the ⇒*Rider Threshold* and ⇒*Maximum Rider Ratio* parameters.

Defining an Averaged Baseline

By means of two points, which can be entered in the chromatogram, you can define a baseline for the entire chromatogram (= averaged baseline) as follows:

- In the chromatogram, use the right mouse key to select an area at the beginning of the chromatogram. The first ⇒*Baseline Point* shall be in the middle of this area.
- In the context menu, select the **Set Averaged Baseline Start** command.



This sets the first baseline point. The x-value is the middle of the selected area while the y-value is the averaged value of the signal values weighted by the data rate. This first value will not be marked, as it is not sufficient for setting the baseline. A second point is required as well.

***Note**:* If you exit the Dionex Chromatography Management System without having entered the second point, the first point will be deleted.

To enter the second point proceed as follows:

- In the chromatogram, use the right mouse key to select an area somewhere at the end of the chromatogram. The second baseline point shall be in the middle of this area.
- In the context menu, select the **Set Averaged Baseline End** command.

This action sets the second baseline point. The new baseline is drawn through both points, which are marked by a red cross.

You can modify the averaged baseline later in two ways:

1. by selecting a new baseline point, which then replaces one of the former ones.

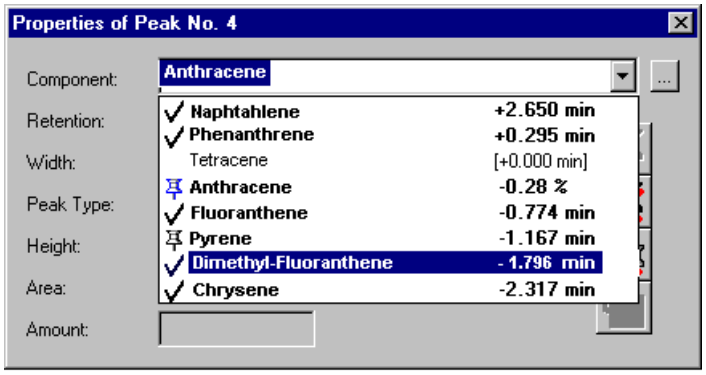
2. by means of the baseline tool on the Integration ➢*Toolbar*. (See **How to ...: Actions in the Chromatogram** **Modifying the Baseline**)

Manual Peak Assignment

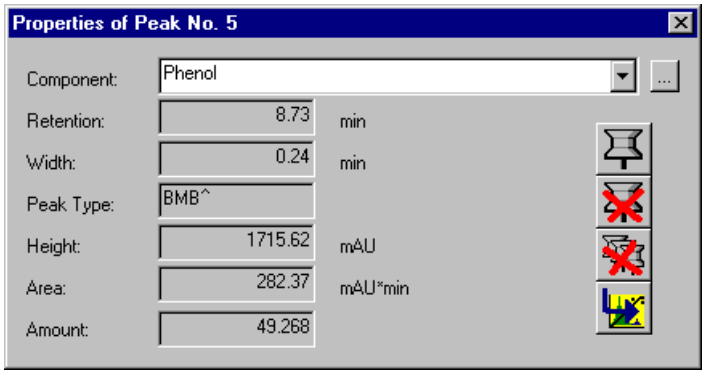
(Dialog box "Properties of Peak No. x")

If you have inserted a new peak, or wish to name existing or unidentified peaks, or rename incorrectly identified peaks, you can do this in the chromatogram either via the **QNT Editor** or in a report.

- Click the respective peak and use the **Peak Properties** command in the context menu to open the dialog box **Properties of Peak No. x** or double click the peak.
- Enter the corresponding name under **Component** or select one of the names listed in the combo box. Pressing <Return> or the lowest symbol bottom inserts the peak into the peak table of the QNT method using the retention time of the current chromatogram and the settings of the previous peak (as far as sensible).



- It is also possible to rename an identified peak by manually assigning it a different name. Enter the new name or select one of the names listed in the combo box and confirm your entry by pressing the first symbol button. Via the additional symbol buttons, you can cancel this action or delete all manual peak assignments (see quick info for the buttons). Manual peak assignments of identified peaks are not transferred to the QNT method but apply to the currently open chromatogram only.



You do not have to close the dialog box to continue working in the chromatogram. <Return> accepts a new entry in the peak table of the QNT editor (provided that the peak has not yet been assigned there). The dialog box then indicates the values of the next peak to be assigned. The dialog box remains open until explicitly closed or until the chromatogram is closed.

***Note**:* The manual peak assignments are saved in the ➢*Quantification Method*. However, manual peak assignments for identified peaks are not included in the QNT method but are valid for the currently open chromatogram only.

Performing a Chromatogram Comparison

The Dionex Chromatography Management System allows comparing several chromatograms. Different options are available for displaying different samples or several ➢*Channels* of the same sample. Comparing different channels of different samples is possible as well. The samples / channels must be selected and related to each other.

For details, see the following topics:

Selecting the Samples and Channels

Displaying Several Chromatograms

Normalizing Chromatograms

Selecting the Samples and Channels

Different alternatives are available to select samples and channels that are to be displayed as ➢*Overlays*:

- Display the chromatogram of a sample in an integration window by opening the sample, e.g., by double-clicking its name in the ➢*Browser*.

  Select one or several samples of one ⇒*Sequence* in the Browser and drag the sample(s) into an open integration window while pressing the left mouse button. The action is indicated by a **+** sign on the mouse cursor. After letting go the mouse button, the chromatogram of the sample(s) is displayed. The same channel is used as for the reference sample.

  Instead of selecting a sample in the Browser and dragging it into an open integration window, you may also select the sample in the integration view using the **Add Overlay** command of the **File** menu. The chromatogram of the first sample will then be overlaid by the chromatogram of the selected one.

Or:

- Select several samples in the Browser, open the context menu, and select **Compare**. The submenu of this command offers a list of all recorded channel types. After selecting a channel, the chromatograms of all samples with raw data for this channel are compared.

Or:

- Select a sample in the Browser, open the context menu, and select **All Channels** to compare all channels of a sample in a separate window. Pressing F4 key or the key combination Shift+F4 displays the channels of all samples in a sequence successively.

  If several samples are selected, all channels of the first selected sample are displayed. By pressing the F4 key or the key combination Shift+F4, you can browse through the selected samples.

Or:

- Click the **Next/Previous Chromatogram** icons ( / ) while pressing the Ctrl key to insert the chromatogram of the next or previous sample.

Or:

- Perform a ➢*Query* over several sequences or ➢*Datasources*. Open the context menu and select the **Compare** command. The submenu of this command offers a list of all recorded channel types. After selecting a channel, the chromatograms of all samples with raw data for this channel are compared.

Or:

- Click the **Next Channel** icon () while holding down the Ctrl key to insert the next channel of the same sample.
- Click the **Previous Channel** icon () while holding down the Ctrl key to insert the previous channel of the same sample.

Displaying Several Chromatograms

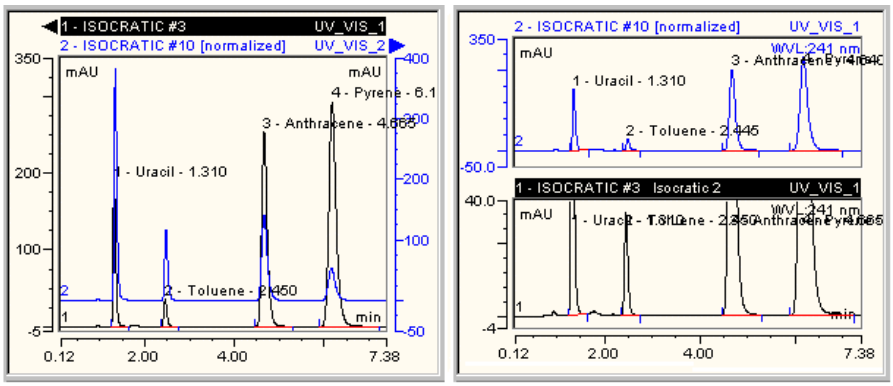
After adding an ➢*Overlay* (= an additional chromatogram), you can define the display arrangement for the two chromatograms. Proceed as follows:

- Select the **Decoration...** command in the context menu of the chromatogram plot.
- In the **Chromatogram Decoration** dialog box, choose the **Comparison** tab and define the chromatogram **Arrangement**:

  The **Overlay** option allows displaying the overlay of the single chromatograms in one single plot (see the left section of the screenshot below).

Use the **Stack** option to display the chromatograms one below the other in different plots (see the right section of the screenshot below).

The **Mixed** option combines the **Overlay** and the **Stack** option. Chromatograms of different detectors are displayed as single plots.



The **Overlay** view allows adding an additional signal axis (on the right) for the overlaid chromatogram that was added last via the **Overlay with right signal axis** command. This command, too, is available on the **Comparison** tab of the **Chromatogram Decoration** dialog box. Thus, you can select a different signal range for the chromatogram that was added last. The **Stack** view allows individual scaling of the signal axis for each single chromatogram.

To offset the chromatograms in x- and/or y-direction in the **Overlay** view, use the signal or time offset that can be set on the **Comparison** tab.

- Activate the **Time** checkbox to move the current chromatogram in the x-direction.
- Activate the **Signal** checkbox to move the current chromatogram in the y-direction.

The offset is specified in percent of the signal or time axis. A signal offset of 5% shifts each of the following chromatograms upwards by 5%. Accordingly, a time offset causes a percentage alteration in the x-direction. This results in a "pseudo-3D" presentation.

Normalizing Chromatograms

For a sensible comparison of different chromatograms, often a common reference point is chosen for the overlaid chromatograms (see ➢*Overlay*). The

chromatograms are normalized. As the default, the ⇒*Retention Time* is used for the normalization, i.e., all chromatograms are arranged so that their start points match (t = 0).

Alternatively, chromatograms can use a common peak as their reference point.

- Choose the **Decoration** command of the context menu and open the **Comparison** tab dialog box.
- Select the reference peak from the **At Peak** list box.
- Choose **Shift** if this is to be performed independently from the length of the chromatogram.
- Choose **Stretch** if the chromatograms are to be stretched or compressed in x-direction, so that there is a time scaling in all chromatograms. The stretch 0 to 1min (or n min) has the same length for all chromatograms.
- Activate the **Normalize Signal** check box if the height of the desired chromatogram peak should match in addition. Depending on how much the reference peak must be stretched or compressed, all other peaks in the chromatogram are also stretched or compressed. This enables amount estimation for the same peaks from different chromatograms. This option is not available in the **Stack** view.

Performing Data Smoothing

Data ➢*Smoothing* can help improve the appearance of chromatograms and the reproducibility of peak baselines by reducing noise through digital filtering. Smoothing affects both, the display and the integration of the chromatogram. When smoothing is completed, the new chromatogram is displayed overlaid on the original chromatogram. The original data file is **not** altered and the smoothed data is saved separately.

For chromatogram smoothing, proceed as follows:

1. Display the sample's chromatogram by double-clicking its name in the ➢*Browser*.
2. Right-click on a blank section of the chromatogram window and select **Smoothing** from the menu. The **Smoothing** dialog box appears.
3. Select the **Filter Type, Filter Size, and Iterations**. See **Data Smoothing** for details.
4. To smooth all the samples in the sequence or ➢*Query*, select the **Apply to all samples in the current sequence or query** check box.
5. In the **Smoothed Channel** box, enter the name of the smoothed sample

data that will be created. The suggested name is the current channel name, followed by the type of filter (MA for Moving Average, OL for Olympic, and SG for Savitzky-Golay), the filter size, and the number of iterations.

6. Click **OK** to start the smoothing.

For information on how to smooth MS chromatograms during mass trace extraction, see **How to ...: Actions Related to the aQa-MS Extracting Mass Traces Afterwards**).

Subtracting MS Background Spectra

As ➢*Mass Spectra* usually show heavier noise than UV spectra, we recommend subtracting the background spectra:

Peak-Depending Background Subtraction

Select the **Background Subtraction** command in the context menu of the chromatogram. Enable background subtraction via the **Enable Background Subtraction** option and select **Peak Dependent Range**. Depending on the peaks, the Dionex Chromatography Management system will automatically determine two ranges for calculating the background and then subtract the entire mass spectrum of these ranges. The **MS** tab of the ⇒*QNT Editor* allows defining the number of mass spectra to be used for the two ranges (see **How to …: Actions in the QNT Editor Processing Mass Spectra**).

Fixed Background Subtraction for the Entire Chromatogram

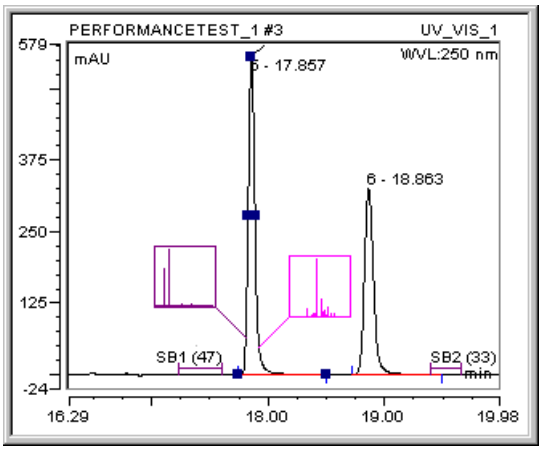
At the beginning of the chromatogram, press the right mouse button and select a baseline range for which to subtract the mass spectra. The corresponding context menu opens. Select **Set Background Subtraction Range 1** to use the defined range as the first range for which to subtract the mass spectra from the mass spectra of the single peaks and/or from the retention time spectrum.

Note: Selecting **Set Background Subtraction to Range 1** automatically activates the **Fixed Background Ranges** option of the **Background Subtraction** command in the context menu.

In the same way, select a baseline range at the end of the chromatogram. Select **Set Background Subtraction Range 2** to define this range as the second range for which to subtract mass spectra from the mass spectra of the single peaks.

Note: Defining the second range is useful but not imperative, as background subtraction can also be performed using the mass spectra of the first range only.

The two defined ranges are marked by a horizontal line (in the same color as the respective spectrum or blue if no spectrum is available) and labeled with SB1 or SB2 (SB = subtracted background). The number of single mass spectra that are averaged is given in parenthesis if the background subtraction range was used:



Note: Setting the two ranges for background subtraction of mass spectra is possible in a UV channel as well. However, we recommend setting the two ranges in the corresponding MS channel, as only there the respective peaks will be visible.

The **Clear Background Subtraction Ranges** option allows removing the previously defined ranges.

Effects

The settings made in the chromatogram are saved in the QNT file of the current sample. They overwrite the settings on the **MS** tab of the QNT editor. It makes no difference whether background subtraction is defined in the **Integration** view or in the QNT Editor. Thus, your input affects all samples that are evaluated using this QNT file.

Tip: Ensure that no peak of another sample is within the retention time used as **Background Subtraction Range** in **Fixed** mode.

If you have defined two ranges, these ranges are averaged and the result is subtracted from the mass spectrum that has been recorded between the two ranges. The mass spectra of the two ranges are weighted based on the time distance from where the respective mass spectrum was recorded, i.e., the range that is nearer to the respective mass spectrum is considered more.

If a mass spectrum is not located between the two ranges, only the averaged mass spectrum of the range next to the spectrum is subtracted.

Actions in the UV Spectra and Mass Spectra

The **Spectra** window is activated via the **Show Spectra** command in the **View** menu or via the

button and allows representing UV spectra as well as their identification via a spectra library.

The **Mass Spectra** window, which is very similar to the **Spectra Plot** window, is activated correspondingly via the **Show Mass Spectra** command or the

button.

For details, see the following topics:

Displaying a Peak Spectrum (UV or MS)

Displaying and Overlaying Single (UV or MS) Spectra

Match Factor, Difference Spectra, 1st /2nd Derivatives of UV Spectra

Starting a UV Spectra Search

as well as

How to ...: Actions Related to the aQa-MS Extracting Mass Traces Afterwards

☞ ***Tip***: The prerequisite for the spectra representation is the availability of the corresponding raw data. It is obtained by recording a 3D-field with a ➢*Photodiode Array Detector*.

Displaying a Peak Spectrum (UV or MS)

- In the neighboring chromatogram window, select the peak of which you want to view the UV / ➢*Mass Spectrum*.

The spectrum of the peak is visible (note: if the corresponding raw data is not available, an error message is displayed).

- Choose the **Decorations..** command from the context menu of the (Mass) Spectra window and determine the peak height at which to extract and display spectra via **Peak Spectra**.

Depending on the settings, up to five spectra of the same peak are displayed in different colors. Normally, the spectra are extracted at 10 and 50% peak height from the ascending and the descending peak flanks and at the run time of the peak. The representation of the spectrum is normalized. If the spectra largely match, this can be a criterion for peak purity.

Displaying and Overlaying Single (UV or MS) Spectra

In addition to peak spectra (= UV or ➢*Mass Spectrum* in the peak maximum or spectrum at a defined peak height), the Dionex Chromatography Management System is capable of displaying any other spectrum of a chromatogram at the time t.

Perform the following steps to extract any spectra of a chromatogram via a mouse click.

- Activate the **Spectra Tool** command in the context menu or press the corresponding icon on the *Integration Toolbar* (for details, see *Integration Toolbar* in the Online Help).

- The changed mode is indicated by a spectra symbol that is added to the mouse cursor.
- Click anywhere in the chromatogram to view the corresponding spectrum.
- Repeat the action while pressing the Shift key to overlay several spectra.

Displaying Spectra of Different Samples

To objectively compare spectra of different samples, it is necessary to perform a chromatogram comparison.

- Compare two chromatograms by displaying an additional chromatogram in the Integration window (see **Chromatogram Comparison** in the chapter **Integration**).
- Activate the **Spectra Tool** command and select single spectra by clicking various places in the chromatogram while pressing the Shift key.

***Note**:* UV spectra are overlaid in one window. MS spectra are displayed one below the other to enhance the clearness of representation. For a large enough representation, enlarge the upper section of the entire window, if necessary.

Match Factor, Difference Spectra, 1st/2nd Derivatives of UV Spectra

As soon as two or more spectra are represented via the Spectra Plot, the similarity of the UV spectra becomes an issue.

The Match Factor can express the similarity, by forming difference spectra or by representing the first or second derivative of a UV spectrum.

- Choose the **Decorations** command of the **View** or context menu and activate the **Show match** checkbox on the **Label** tab. The Dionex Chromatography Management System issues a value for each represented spectrum, expressing the match degree relative to the main spectrum (0 = no match; 1000 = perfect match).
- On the **Analysis** tab choose whether the difference spectrum or the first or second derivative of a spectrum are displayed in a second window in addition to the actual spectra.

In the case of the match factor and the difference spectrum, the question of which UV spectrum is considered a main spectrum is especially important, as this is the basis of comparison or the basis for all calculations.

Usually, this is the peak spectrum extracted at the retention time. If there is no peak spectrum, a distinction is made between two situations: If the UV spectra were extracted individually from the chromatogram via spectra tool, the spectrum that is first extracted is the main spectrum. If spectra are automatically extracted at different peak heights, the spectrum with the "oldest" retention time is considered the main spectrum. When representing difference spectra, the **Difference to ...** entry indicates the basis of calculation.

Starting a UV Spectra Search

To facilitate substance identification, the peak spectrum, which is displayed in the **Spectra Plot** windows of the **Integration** or **PPA** method, can be compared to the UV spectra of a spectra library.

Based on the available library, the Dionex Chromatography Management System creates a spectra list sorted by the degree of similarity, the **Hit List**. The number of possible hits can be limited via comprehensive search criteria.

- If the cursor is positioned in a spectra window, choose the **Library Search ...** command from the context menu to start the spectra search.

In the edit box, specify the library that should be searched. The following are minimum entries required to receive a valid search result:

- In the field **Spectra Library to be searched in ...** choose a spectra library (LIB file). If no LIB file is offered, press the **Browse** button to search for a corresponding file.
- In the field ⇒*Match Criterion*, determine the mathematical method based on which the original spectrum and the library spectrum are compared with each other. The best search results are generally received with the setting **Least Squares**.
- Press the **OK** button to start a spectra search.

Note: To be able to compare UV spectra with each other, the spectrum and the reference spectrum should be recorded under identical conditions. For best results, compare spectra to your own spectra library.

Result

A list of possible candidates will be displayed. The top spectrum has the highest match value and the best similarity to the original spectrum.

Detailed Search

To accelerate the search and to receive very specific results, there are numerous options:

- Normally, the **Spectrum Derivative** option is deactivated, i.e. comparing spectra is based on the actual curve shape. If the **1´st Derivative** option is selected, the comparison of the two spectra is performed based on the first derivative. This has the consequence that the curve characteristics will be more significant (shoulders become real extremes), which allows a more precise comparison. The drawback of this option is the reduction of the signal to noise ratio, which causes sections with weaker signals to loose significance.
- Select **Hit Threshold** and enter a value between 0 and 1000, e.g. 950. Only the spectra with a match above 950 will be displayed. Spectra with a lower match value will not be displayed. Spectra with a match value below 900 are usually spectra of other substances (if derivatives are not used for the comparison). Exceptions to this are acceptable only if e.g. the signal to noise ratio is low.

To ensure a precise search result, use the following options:

- Enter the number of relative extremes the spectrum should have (**Number of Relative Extrema)**. This option is useful to exclude spectra that are similar but have an additional side maximum.
- Select **Check Greatest Relative Maximum** to use only spectra with the greatest relative maximum at the same position. Choose **Allowed Deviation** to define a tolerance range. The range should not be more than 10 nm. Otherwise, the criterion weakens.
- Via **Retention Time Window**, define a time window that includes the retention time of the peak. Use this option to exclude substances with very similar spectra, but which are eluted at very different retention times.

Additional criteria are only required in special cases. However, they are useful for searching large libraries containing numerous spectra of the same substance, but extracted under different conditions (e.g. different solvents and detectors, different users, different date etc.).

Note: When creating your own spectra library, please enter information in all fields, even in the fields that may seem unnecessary. In the course of time and with a growing library, this may become a major advantage.

Actions in the Report

The Dionex Chromatography Management System offers numerous options to work with reports. It is possible to use existing default reports or create special ➢*Reports* to meet individual requirements.

For details, see the following topics:

Displaying a Report
Defining the Contents of a Report
Defining the Appearance of a Report
Saving a Report
Linking Report Variables
Calculating the Peak Variable Amount
Adding/Renaming a Worksheet
Peak Summary
Audit Trail (Sample Protocol)
History
MS Reports
Other Special Reports

Displaying a Report

In each of the six method windows (Integration / PPA / QNT Editor / Spectra / Calibration Curve / Spectra Calibration), a numerical ➢*Report* can be included.

- Choose the **Report** command from the **View** menu.

If you have not generated a report before, a default report will be opened. It contains the worksheets **Integration**, **Calibration**, **Peak Analysis**, **Summary**, and **Audit**. If you are working with a ➢*Photodiode Array Detector*, it is recommended to select the default report **DEFLTDAD**. This report contains the additional worksheets **Peak Purity** and **Lib Search**.

- Via the tab in the lower left corner of the report, choose the worksheet to change from one report type to the next.

Each worksheet has a number of default variables that are an integral part of the respective report type. In an integration report, this includes the columns **Ret.Time**, **Area**, and ⇒*Amount*. A calibration report contains the columns **Offset (c0)**, **Slope (c1)**, and **Curve (c2)** etc.

Without requiring additional input, these predefined report sheets are available for various purposes.

Defining the Contents of a Report

Via the **Table** command of the context menu or double-clicking a table column, the *contents* of a ⇒*Report Definition File* can be changed.

- Choose **Add / Insert Column** to add a column with any content to the report at the right or left of the current cursor position.
- Choose **Fix Column** to move the selected columns to the far left. Columns of this type are permanently visible, even when scrolling.
- Choose **Delete Column** to delete one or several columns.
- Choose **Column Properties** to modify the column properties. Thus, the current column contents (e.g. number of theoretical plates) can be replaced by a different variable.

☞ ***Tip***: Each column usually shows one report variable. However, it is possible to link several report variables (see: **How to ...: Actions in the Report Linking Report Variables**). Mathematical and statistical functions such as SUM, AVERAGE, etc. are only available in the Report and the ➢*Printer Layout* together with the ➢*Report Publisher*!

- Choose **Table Properties** to modify the properties of the entire report. Use this command to sort the table in groups or remove peaks below a certain area value.

Defining the Appearance of a Report

The *appearance* of a report is modified via the **Table** menu. Choose **Format / ...**

- **Alignment** to position the text horizontally and vertically within a cell or a column.
- **Font** to determine the font type and size.
- **Border** to determine the location, the color, and the shape of the frame.
- **Pattern** to determine the color and the pattern of the cell background.
- **Number Format** to determine the format of the represented values.
- **Autoformat** to design the entire report by selecting a ready-made default template. The Preview window shows the various formats.

Saving a New Report Definition File

All modifications to a report can be saved in a ⇒*Report Definition File*.

- Choose **Save Report Definition ...** and enter the file name under which to save the modifications.
- Overwrite the **DEFAULT.RDF** file to change the default settings for reports. (Note: Overwriting the **DEFAULT.RDF** file is generally not necessary, as the report definition file (RDF) you saved last will be used when you open a report.)

Linking Report Variables

Linking two or more report variables via the four basic arithmetic operations or via powers allows you to generate user-defined report variables.

Use the formulas of the ⇒*Report Categories* to link individual variables.

Perform the following steps:

- Select a report column and choose the **Add Column** command from the **Table** menu.
- In the **Formula** field of the edit box (**Add Report Column**), enter the formulas you wish to link via mathematical operators.

- Note that the variable names are not identical with their "formulas" (e.g. **peak height** and **peak.height**). For the correct syntax, refer to ⇒*Report Categories*. You can copy the syntax there by selecting the required formula and pressing the key combination CTRL+C. Change to the edit box again and insert the formula by pressing CTRL+V.

  Example: If the peak height should be put in relation to the corresponding ⇒*Amount*, this can be expressed as follows:

  peak.height / peak.amount

- Alternatively, expressions can be linked via the operators **+**, **-**, **x**, and **^** (for powers)
- In the field **Header**, enter the desired column header.
- Press **Customize** to include newly defined variables in the report variables list.
- Complete your input by pressing **OK**.

☞ ***Tip***: Mathematical and statistical functions such as SUM, AVERAGE, etc. are only available in the Report and in the ➢*Printer Layout* together with the ➢*Report Publisher*!

Calculating the Peak Variable "Amount"

If you wish to check the indicated ⇒*Amount* values, have a look at the respective coefficients of the calibration function first. Then, add the columns offset (c0), slope (c1), and curve (c2), which are all part of the category **Peak Calibration**.

For the amount calculation of an unknown sample the inverse function f(y) of the calibration function F(x) must be calculated. Calibration functions are calculated as follows:

Linear: $$f(y) = \frac{1}{c_1} y$$

Linear with offset: $$f(y) = -\frac{c_0}{c_1} + \frac{1}{c_1} y$$

Quadratic: $$f(y) = \frac{1}{2 * c_2} * \left(- c_1 \pm \sqrt{{c_1}^2 + 4 * c_2 * y} \right)$$

Quadratic with offset: $$f(y) = \frac{1}{2 * c_2} * \left(-c_1 \pm \sqrt{{c_1}^2 - 4 * c_2 * (c_0 - y)} \right)$$

Exponential: $$f(y) = \left(\frac{1}{c_0} \right)^{\left(\frac{1}{c_1} \right)} * y^{\left(\frac{1}{c_1} \right)}$$

***Note**:* For ambiguous inverse functions (two possible values for quadratic with or without offset) always use the value which comes "closest" to the X values of the respective calibration.

If it is not possible to calculate the expression (c1=0 for linear with or without offset, the radiant < 0 for quadratic with or without offset, or c0=0, or c2=0 for exponential), "n.a." is given as amount.

Adding/Renaming a Worksheet

You may add new worksheets with any contents and appearances to the ⇒*Report Definition File*.

- Choose the **Insert Report** command of the **Table** menu and determine the type of report to be created.

Audit Trail	Shows the Audit Trail of the current sample.
Calibration History	Shows all variables documenting the course of the calibration.
Calibration Report	Shows all variables required for creating a calibration report.
Database Query	Inserts any kind of database queries into the report. Enter the search criteria in SQL code.
Detection Parameter Report	Shows all ➢Detection Parameters of the current sample.
History Report	Shows all variables required for creating a ➢History report.
Integration Report	Shows all variables required for creating an integration report.
MS Instrument Info Report	Shows information on the ➢Mass Spectrometer.
MS Instrument Method Report	Indicates the MS method.
MS Raw Report	Shows the raw data of the current ➢*Mass Spectrum*.

MS Status Log Report	Indicates the mass spectrometer settings.
MS Tune Data Report	Indicates the tune data of the ➢*Xcalibur* raw data file.
Peak Summary	Shows all variables required for creating a peak summary.
Program Report	Shows the ➢*Program* for the current sample.
SST Report	Lists all variables which are required for the representation of the ➢*System Suitability Test*.

- From the variables that are available on the right-hand side, click those you wish to include in the new report. Pressing **OK** creates the desired worksheet of the report.
- In the report, double-click the newly added tab to assign it a new name.

Saving

The contents and the appearance of a report are saved via the **Save Report Definition** command.

☞ ***Tip***: Please note that the appearance and the contents of this (screen) report needs not to be identical with the actually printed report, the **Report Templates**. The printout is defined exclusively in the Printer Layout and enables printing independently of the screen contents.

Peak Summary

Use the **Summary** worksheet in the **Report** (see **Peak Summary Report**) to show certain results from all samples.

The required steps are described under **How to ...: Actions in the Report**:

Displaying a Report and

Adding/Renaming a Worksheet.

In contrast to the **Integration** and **Calibration** worksheets of the ⇒*Report Definition File* that list the data of the peaks of *one* sample, the **Summary** represents data of a specific peak from *all* samples (generally a ⇒*Sequence*).

If you wish to show e.g. the amount of different peaks of all samples of a sequence in a table, select the **Amount** variable of the **Peak Result** category via the **Column Properties** command of the context menu and display the value for **Fixed Peak(s)**. The default setting shows the values for the currently **Selected Peak** so that you can determine the peak for which to display the data by clicking the peak in the above chromatogram.

The default Summary report contains several columns. In addition to the sample name and the retention time, it also offers the columns **Area**, **Height**, ⇒*Amount*, **Types**, and **Plates**. As soon as a user selects a peak in the chromatogram, the values of this peak are included in the Summary report. If the selected peak is not contained in a sample, this line remains empty (n.a. = not available).

Below the sample list, there are the lines **Average** and **Relative Standard Deviation**. The average value of a column is calculated and displayed. The relative standard deviation from this value is indicated in percent.

The user can modify the default Summary report at any time. However, it is recommended to keep this report sheet. If another report is required, create an additional Peak Summary report sheet with new column assignments.

Note: Instead of a single sequence, the Summary report can also be started based on a ➢*Query*. Then, the Summary may include different samples from different sequences.

Audit Trail (Sample Protocol)

The **Sample Protocol (Audit Trail)** can be included in a ⇒*Report Definition File* as a worksheet. The sheet always shows the Audit Trail for the currently selected sample.

- In the **Day Time** column, the time of a command or message is entered.
- The **Ret.Time** column indicates the corresponding retention time.
- The **/Message** column command shows the command itself, a message text or an event.

The contents of the worksheet can be included in other documents via **Cut & Paste**. Printing the entire **Audit Trail** via the ➢*Printer Layout* is possible as well.

Using Audit Trail Variables in other Worksheets

Certain events (as performing a ⇒*Trigger* or changing the wavelength at a specific time) can be included in any Report worksheet.

- Open the corresponding worksheet and choose the **Column Properties** command from the context menu.
- Choose **Audit Trail** from the **Categories** list.
- Choose one of the Audit Trail variables from the **Variables** field. The available selection depends on the events listed in the **Audit Trail** of the sample.
- If you would like to display events that are not listed here (e.g. the system pressure recorded via a Log command), this is possible via the **Formula** field. In this case, the event variable is appended to the name AUDIT, separated by a period (AUDIT.pressure). This output makes sense only if these values were actually recorded!
- Confirm your input with **OK**.

Your report now includes an additional column with an **Audit Trail** variable. Normally, the value for the corresponding peak at the retention time is entered in each line. If there is no value at this time, the last recorded value is entered. When forming a gradient, the data system calculates the corresponding values (%A, %B, %C ...).

If you want to display a specific **Audit Trail** event for all peaks in a report at a specific time, the Dionex Chromatography Management System offers the following option:

- Choose the **Column Properties** command and choose an **Audit Trail** variable.
- Press the **Parameter...** button.

You now have the possibility to specify a retention time. Confirming the action with **OK** generates a report column with a fixed retention time. The **Wavelength** audit trail variable displays the wavelength at the time t.

History

The ➢*History* report is not part of a default report. So, use the **Insert Report** command to add a history worksheet to a ⇒*Report Definition File* (see: **How to ...: Actions in the Report Adding/Renaming a Worksheet**).

By default, the sheet shows the history of the current sample. Use the **Table Properties** command of the context menu to open the **History Report Properties** dialog box where you can change the settings.

- On the **History Objects** tab, select the object for which to display history entries.
- On the **Time Restrictions** tab, specify the time when the history entries to be displayed must have been made.
- On the **Operations** tab, determine the changes to be displayed.
- On the **Users** tab, determine the user(s) whose changes shall be displayed.
- On the **Sorting** tab, define the sorting order for the history entries.
- The **Layout** tab allows enabling the special layout mode for the history report. This is possible only if detail columns are available. If detail columns exist, a shortened history report is displayed when **Design template mode** is enabled, thus, simplifying layout definition.

MS Reports

Similar to the ➢*History* report, the different MS reports are not part of the default ⇒*Report Definition Files*. Use the **Insert Report** command to add them as separate worksheets to a report definition file (see: **How to ...: Actions in the Report Adding/Renaming a Worksheet**):

- Select the **MS Instrument Info Report** to view information on the ➢*Mass Spectrometer*. If there is no MS data, the report just says: *"No MS Instrument Info found."*
- The **MS Instrument Method Report** indicates the MS method. If there is no MS data, the report just says: *"No MS Instrument Method found."*
- The **MS Raw Report** shows the raw data (mass, intensity, and relative intensity) of the current ➢*Mass Spectrum*. If there is no MS data, the report just says: *"No MS Raw Data found."*

- The **MS Status Log Report** shows the mass spectrometer settings. If there is no MS data, the report just says: *"No MS Status Log found."*
- Select the **MS Tune Data Report** to view the tune data of the ➢*Xcalibur* raw data file. If there is no MS data, the report just says: *"No Tune Data found."*

***Note**:* If you do not have the MS Control option enabled on your PC, the MS reports will not be displayed in the Insert Report dialog.

All MS reports comprise the default columns only; further columns cannot be added.

Other Special Reports

Similar to the ➢*History* report and the MS reports, the following reports are not part of the default ⇒*Report Definition Files* either. Use the **Insert Report** command to add them as separate worksheets to a report definition file (see: **How to ...: Actions in the Report Adding/Renaming a Worksheet**):

- Select the **Database Query** report to integrate any kind of database query in the report. Open the **Table Properties** in the context menu and specify the datasource in which the query shall be performed. Use ➢*SQL* statements to define the properties for which the query shall be performed.
- The **Detection Parameter Report** indicates the ⇒*Detection Parameters* used for the current sample.
- The **Program Report** indicates the ➢*Program* of the current sample.
- The **SST Report** indicates the results of the ➢*System Suitability Test*. The default SST report columns are part of the ⇒*System Suitability Test* category. They cannot be edited.

***Note**:* The Database Query report, the Detection Parameter Report, and the Program Report comprise the default columns only. Further columns cannot be added.

Actions in the QNT Editor

The settings performed in the quantification window determine which ⇒*Detection Parameters*, and calibration and peak table parameters (see ⇒*QNT Parameters*) are used for evaluating a peak or an entire chromatogram.

As the peak table offers more columns than can be displayed clearly on the screen, the columns are distributed to three tabs:

- **Peak Table** (general peak table)
- **Amount Table** (parameters to determine the amount)
- **Peak Tracking** (parameters for peak assignment via reference spectra)
- **MS Tracking** (parameters for peak assignment via ➢*Mass Spectra*)

Use the **Display Columns** command in the **View** menu to select the columns for the respective tab.

The QNT editor offers additional tabs to enter parameters:

- **General** (general settings)
- **Detection** (detection/detection parameters)
- **Calibration**
- **Spectra Library Screening** (spectra search parameters)
- **SST** (➢*System Suitability Test* parameters)
- **MS** (➢*Mass Spectrometry* parameters)

You can disable the display of any tab via the **Select Sheets** command from the **View** menu. To rename a tab, simply double-click the tab in the **QNT Editor** and enter a new name.

For further details, see the following topics:

Creating a Peak Table
Defining Detection Parameters
Combining Peaks
Subtracting a Blank Run Sample
Disabling Standard Samples
Calibration
Spectra Library Screening
Defining the System Suitability Test
Processing Mass Spectra

Creating a Peak Table

The peak table contains data for

- Peak identification
- Amount calculation

Specific peaks of a chromatogram are thus identified via a name (= identified). The determined peak areas are converted in amount values (= ➢*Formula for Amount Calculation*). The peak table serves as the basis for each calibration, as it contains the substance concentration of all standard samples. Input is usually before the analysis start.

Use the command **Display Column** from the context or **View** menu to determine which columns are displayed on the sheets. This option allows adjusting the **Peak Table**, **Amount Table**, and **Peak Tracking** sheets to individual requirements.

For further details, see the following topics:

Identifying Peaks
Identifying Peaks via Their UV Spectra (Peak Tracking)
Identifying Peaks via Their Mass Spectra (MS Tracking)
Defining Retention Times and Reference Peaks

Defining the Retention Index and the Kovats Index

Entering Amount Values

Selecting the Standard Method

Selecting the Calibration Function (Columns: Cal. Type and Int. Type)

Weighting and Averaging Calibration Points

Defining the QNT Method for Several Detectors

Entering Reference Spectra

Autogenerating the Peak Table

Also, see **How to ...: Actions in the Browser** **Creating User-defined Columns**

Identifying Peaks

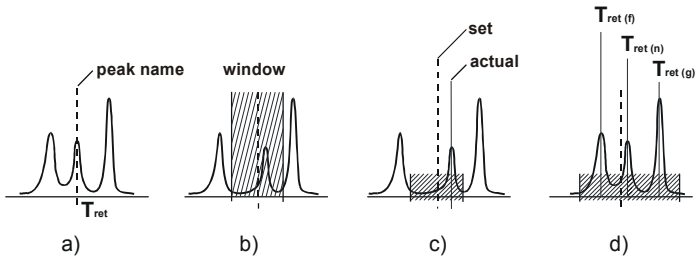
(Columns: Peak Name, Retention Time, and Window)

Most frequently, peaks are identified via the retention time.

- Enter the names of all peaks to be identified in the ⇒*Peak Name* column, line by line. Assign a nominal retention time to each peak by entering a retention time value in the corresponding peak table column (= manually creating a peak table). Or:
- Choose the **Autogenerate Peaktable** command (**Edit** menu) to automatically generate a peak table based on the current sample. In this case, the system includes all peaks integrated (!) in the current sample into the peak table. As peak name, a combination of sequence name and consecutive number is assigned. The values to be entered in the ⇒*Retention Time* and ⇒*Window* columns, are determined again using the individual peak's maxima. All other entries are replaced by default values (= automatically creating a peak table).

If a peak is detected at the specified time in an unknown sample, the peak is automatically assigned a name (fig. a).

Identification is even possible when the retention time deviates or when neighboring peaks are very close. For this, a tolerance range is defined via the **Window** (fig. b) peak table parameter. If a peak is detected in this range, it is identified even if the *nominal* and the *actual* retention time do not coincide exactly (fig. c). If several peaks are detected within this range, the data system identifies the greatest, the first, or the nearest peak to the retention time (fig. d), depending on the extension of the **Window** parameter.



The **Peak Window** can be set for each peak after pressing the F8 key or double-clicking the **Window** column. First, determine the window interpretation. Selecting **Absolute** allows you to enter the window width in minutes. Select **Relative** to define the window width in percent.

Peak Match allows selecting the peak identification criterion. If using a ➢*Photodiode Array Detector*, peak assignment is possible via the spectrum or via the spectrum and the retention time. For details, see **Identifying Peaks via Their UV Spectra (Peak Tracking)**

The window width is indicated in industry minutes in the **Window** column of the peak table (e.g. "0.25"), followed by the abbreviation for the selected window interpretation and peak match option. To identify the largest peak within a 30 second window, the column must read: "0.25 AG" (0.25 min or 15 seconds to the left and right of the retention time). Accordingly, "0.25 AN" would identify the peak nearest to the nominal retention time.

***Note**:* The retention times and window values stated in the peak table exclusively serve to identify a peak. For the retention time output within a ➢*Report*, the actual retention times (= retention time in the peak maximum) are used.

If the retention time of the same peak shifts from sample to sample due to a column trend, the peak can leave the retention time window at some point. Peak identification is no longer possible in this case. However, the Dionex Chromatography Management System offers a method to reliably identify peaks even then. (See ⇒*Use Recent Retention Time*) The option is activated via the **General** sheet of the QNT editor.

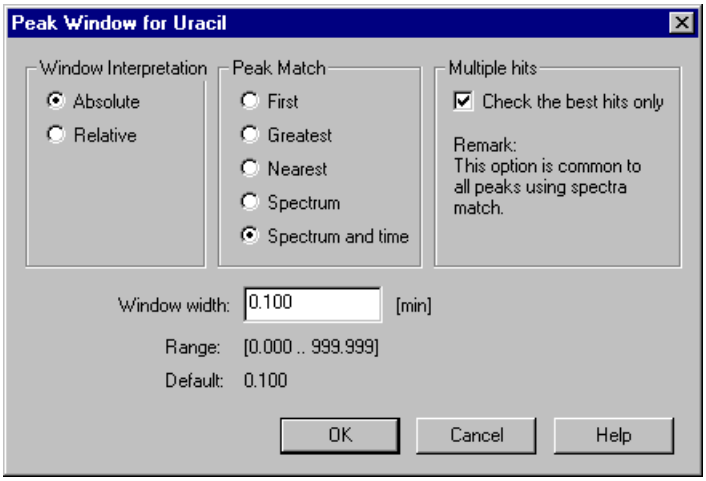
In addition to the identification via the nominal retention time, compounds can be identified via their substance spectrum.

Identifying Peaks Via Their UV Spectra (Peak Tracking)

The Dionex Chromatography Management System allows you to perform peak tracking, i.e. identifying peaks via spectra comparison. In addition to the **Reference Spectrum** column, there are further peak table columns to influence spectra comparison. These are the columns **Match Criterion**, **Check Derivative**, **Min. WL**, **and Max. WL**, **Threshold**, **Rel. Max. Deviation**, and **Check Extrema**. The values entered in these columns have the same meaning as described in the section **How to ...: Actions in the QNT Editor**  **Entering Criteria for the Spectra Library Screening**.

☞ **Tip**: If neither the minimum (**Min. WL**) nor the maximum wavelength (**Max. WL**) are set, the comparison is performed for the entire wavelength range of the reference spectrum.

Peak tracking, i.e., identifying a peak by comparing spectra, can be activated via the input in the **Window** column. In the corresponding F8 dialog box (press the F8 key or double-click in the **Window** column), select one of the options **Spectrum** or **Spectrum and time** of the group **Peak Match**.



The algorithm for peak identification via a spectra comparison can be described as follows: If (**Peak Match**) **Spectrum** or **Spectrum and time** is selected as peak match criterion in the **Window** column of the peak table, peak tracking uses the reference spectra in the corresponding column (in the case of **Spectrum and time** limited to the specified time window). Peak tracking generates a list of spectra sorted by the match factor (the peak hit list is not shown here).

Tip: Peak tracking is performed with the parameters (match criteria etc.) entered for the peak in the peak table.

The peak hit list only includes peaks with a match factor above the threshold that was entered for this peak.

An empty peak hit list indicates that no spectrum was found fulfilling the match criteria. This could be due to a very high threshold.

The peak hit list is calculated for all peaks in the peak table, for which peak tracking was activated. After that, the peak hit lists are checked for multiple hits. If the **Check the best hits only** option is activated, only the best hits are compared for the individual peaks. In the case of multiple hits, the peak with the highest match factor receives the name of the reference substance.

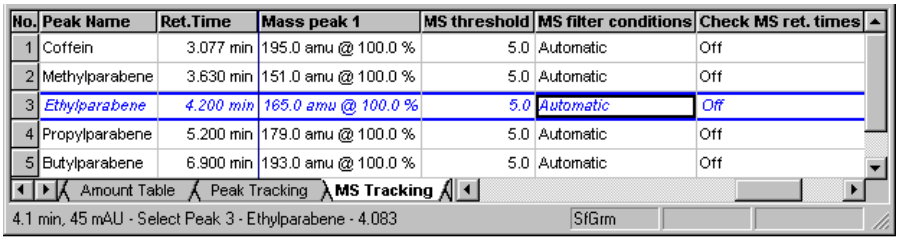
Using the match criterion Spectrum and time can usually prevent multiple hits.

All other peaks in the peak table (i.e. without activated peak tracking) are identified via the window assignment (**First**, **Nearest**, **Greatest**) as described under **Identifying Peaks**.

Identifying Peaks via Their Mass Spectra (MS Tracking)

(Column: Mass peak x, MS threshold, MS filter conditions, and Check MS ret. times)

➢*Mass Spectra* present a very reliable method for peak identification. For the available parameters, see the **MS Tracking** tab.

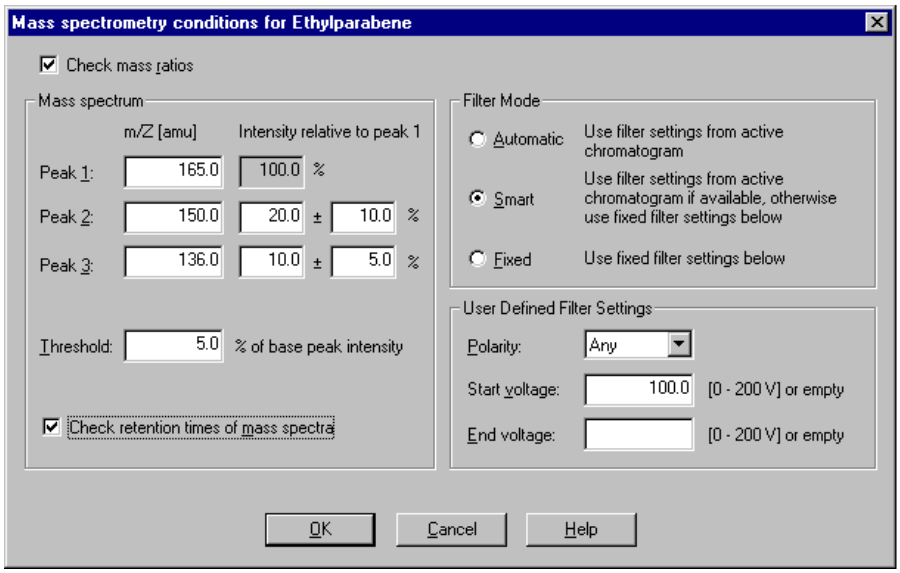


No.	Peak Name	Ret.Time	Mass peak 1	MS threshold	MS filter conditions	Check MS ret. times
1	Coffein	3.077 min	195.0 amu @ 100.0 %	5.0	Automatic	Off
2	Methylparabene	3.630 min	151.0 amu @ 100.0 %	5.0	Automatic	Off
3	*Ethylparabene*	*4.200 min*	*165.0 amu @ 100.0 %*	*5.0*	*Automatic*	*Off*
4	Propylparabene	5.200 min	179.0 amu @ 100.0 %	5.0	Automatic	Off
5	Butylparabene	6.900 min	193.0 amu @ 100.0 %	5.0	Automatic	Off

Amount Table | Peak Tracking | MS Tracking

4.1 min, 45 mAU - Select Peak 3 - Ethylparabene - 4.083 SfGrm

Double-click the respective cell or press **F8** to open the **Mass spectrometry conditions for ...** dialog box:



Peak identification via MS is enabled / disabled via the **Check mass ratios** check box.

Under **Mass Peak 1**, enter the mass of the substance, which is expected at this peak. If you expect fragmentation and can estimate the fragments, which are expected, you can enter two of them with their expected intensities under **Mass Peak 2** and **Mass Peak 3**.

Use the **MS Threshold** option to filter the noise. A mass is detected in the mass spectrum only if, compared to the ➢*Base Peak* (largest peak), its relative intensity is higher than the threshold value.

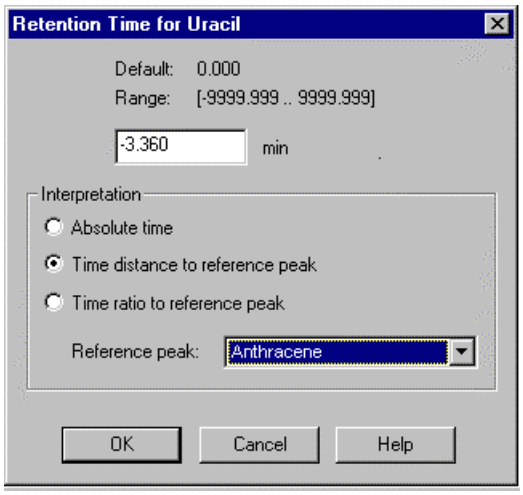
The filter settings limit the mass spectra, which are used for peak identification. This option is required if you modify the polarity and/or use a different maximum voltage for ionization of the sample.

Via the **Check retention time of mass spectra** option, you can also use the retention times of all masses for peak assignment. All retention times must be within one scan.

Defining Retention Times and Reference Peaks

(Column: Retention Time)

The **Retention Time** column allows you to select reference peaks for relative retention times and to determine how the ⇒*Retention Time* is to be interpreted for the respective peak. Open the dialog box **Retention Time for...** for the respective peaks by double-clicking or with F8 (within the **Ret. Time** column).



The display of the retention time (relative or absolute time) can be determined individually for each peak on the tab **Interpretation**. Note that relative times can be displayed either as difference or as percentage ratio to the retention time of a reference peak.

The dialog box **Reference peak** allows you to define one (or several) of the other peaks as reference peak. However, only peaks with absolute reference times can be used as reference peaks. They are indicated with a light blue background. Reference peaks cannot be deleted from a peak table.

The retention time is re-calculated automatically when the retention time interpretation is changed or a different reference peak is selected.

Besides, the retention time can be entered directly in the entry field (page **Peak Table** in the **Ret. Time** column) in the following manner:

[<Reference Peak>] <Ret. Time> [<Unit>]

You are free to choose the order in which the fields are entered.

If no name is entered for the reference peak, the time is interpreted as absolute time.

Either **min** or **%** can be selected as unit. If no entry is made, **min** is used. The unit determines whether the time given is the difference (**min**) or the ratio (**%**) to the time of the reference peak. For absolute times only **min** is permitted.

Defining the Retention Index and the Kovats Index

(Columns: Ret. Index and Kovats Index)

If you wish to generate generally comparable retention times by means of retention indexes you have to determine one or several marker peaks first in the columns ⇒*Ret. Index* or ⇒*Kovats Index*.

Enter a value between 0 and 99.999. Each peak for which a value is entered is used as marker. Incrementing values must be used, i.e. the value must be either undefined or above the value used for the predecessor peak. The default setting is "undefined."

This variable is used for calculating retention indexes or Kovats indexes, respectively, which are used, mainly in GC, to correct retention time variations. Therefore, the peak table should contain certain marker peaks, which usually have the following RI or KI values, assigned:

Retention Index: 100, 200, 300, ...

Kovats Index: 100*number of carbon atoms of the alcane.

The RI or KI values of all other peaks remain empty; they are calculated by means of interpolation.

The **Duplicate Column** command (select **Columns** in the context or **Edit** menus) allows you to duplicate the column so that different values are possible for the individual channels.

☞ ***Tip***: As the Kovats index is calculated using the adjusted retention times a ⇒*Dead Time* must be entered on the sheet **General** of the QNT editor to enable the calculation.

Entering Amount Values (Amount Column)

Standard substances are labeled by user input in the **Amount** column.

- Search the peak table for the substance name of the standard substance(s), or
- Enter the name and the retention time as described under **How to ...: Actions in the QNT Editor Identifying Peaks**.
- In this line, move to the first Amount column.
- Enter the amount value of the standard. This can be a concentration value (recommended, e.g. µg/µl) or the absolute value (e.g. µg). If a standard is available in different concentrations, the concentration of each vial *must* be entered in a separate ⇒*Amount* column. E.g. two concentrations result in two amount column entries:

No.	Peak Name	Ret.Time	Window	Standard	Int.Type	Cal.Type	Amount1	Amount2
1	Subst. A	4.400 min	0.100 AG	External	Area	Lin	50.000000	100.000000

  However, if injection is performed several times from the same sample vial (multiple injection), one amount value is sufficient. This applies even if a different volume and thus a different amount are injected, because the data system automatically considers this!
- Repeat the procedure for each substance that serves as a standard.

Inserting new Amount Columns

- From the **Edit** or the context menu, choose **Columns...**, and then **New Amount Column...**. Open the dialog box **Add Amount Column**.
- Choose **Add Standard(s**) to open the dialog box **Select Samples**.
- Select a standard sample. By pressing **OK**, the sample is included in the dialog box **Add Amount Column**.
- Press **OK** again to open the **Amount** column for the selected sample. You can now generate further Amount columns in the same way. Press **Close** to return to the peak table.

Selecting the Standard Method (Standard Column)

Via the Standard method, determine how to perform the calibration. Generally, a distinction is made between a calibration based on an *internal* or an *external* standard.

External standard means that the calibration is performed based on one or several standard samples (this is the default).

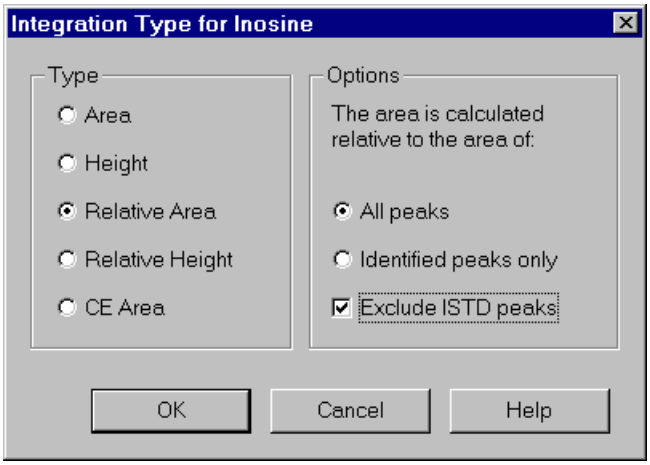
Using an **internal standard** means adding a standard to the unknown sample. This can be either before (**External/Internal**) or after (**Internal**) sample preparation. Either the standard (= ➢*Internal Standard*) can be added to all samples or it can serve as a basis for a relative area calculation. In this case, results are displayed only in relation to the amount or area of the internal standard (for further details, see **Calibration**, **Standard Methods**).

- In the **Standard** column, add the standard method for each peak to be calibrated (**external** / **internal/external Peak** / **internal Peak**).
- For the last two options, at least one peak of the peak table is used as the internal standard. This is achieved by assigning it the **Make current Peak to ISTD Peak: intern** or **Make current Peak to ISTD Peak: internal/external** option.
- Press the F8 key to enter the standard method assignment via an edit dialog box.

Selecting the Calibration Function (Columns: Cal.Type, Int. Type)

Via the **Int. Type** (⇒*Integration Type*) column, define how to evaluate the individual peaks.

To do that, press the F8 key or double-click in the **Int. Type** column. The following dialog box opens:



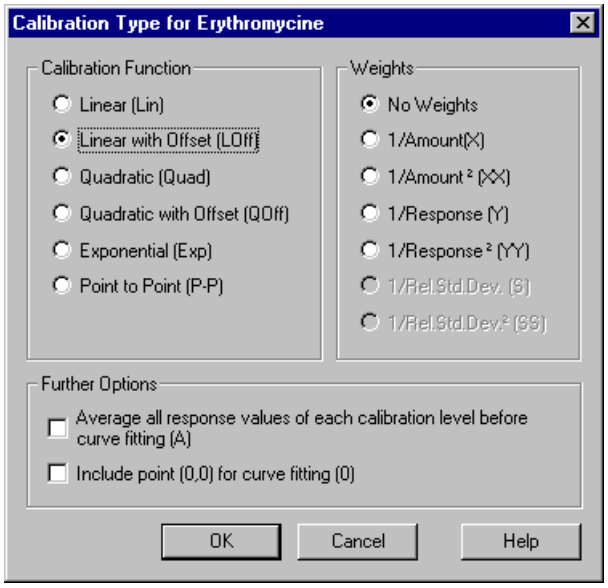
In addition to **Area**, **Height**, and **CE-Area**, you can select the relative area or the relative height as the reference for the evaluation (Integration Type).

If you select **Area**, all amount calculations refer to the area of one peak. This **Peak Area Integration** is the default setting. The peak height integration is only used in exceptional cases.

The relative height is either calculated relating to all peaks or all identified peaks. ISTD peaks can be considered for the calculation of the total area (height).

There are several peak table columns, which define the conversion of the determined area values into the calculated amount values. A separate calibration and integration type must be assigned to each calibrated peak in the peak table.

Enter a calibration function in the **Cal. Type** column. Press the F8 key to receive a list of available functions and options. Apart from few exceptions, the calibration types **Linear** or **Linear with Offset** are used.



The ⇒*Calibration Type* determines which ➢*Calibration Function* is used for deriving a valid amount/area assignment for a larger range from the calibration points of the standard samples. For detailed information on linear and non-linear calibration types, see **Calibration Types (Linear)**, or **Calibration Types (Non-linear)** in the **Calibration** section.

Via the calibration type, you can also define the weighting and averaging of calibration values (see: **How to ...: Actions in the QNT Editor Weighting and Averaging Calibration Points**.

Either the calibration curve leads through the origin (e.g., with the **Lin** and **Quad** calibration types) or the origin is not considered (e.g., with the **LOff** and **QOff** calibration types). For calibration types with offset, the origin can be treated as a calibration point via the **Include point (0,0) for curve fitting** option. In this case, the calibration curve will not be forced through the origin, but the origin will be considered nevertheless.

Normally, all other columns of the peak table can be used with the default settings. Press the F1 key to view further information. Press F8 to open an edit box.

Weighting and Averaging Calibration Points

Weighting

The Dionex Chromatography Management System generally weights calibration points of higher concentrations more strongly than lower concentrations, i.e. the course of the calibration curve is oriented towards the calibration points of higher concentration. This makes sense as smaller concentrations also cause a stronger dispersion of the determined area values, which would distort the result beyond proportion.

To undo or even reverse this type of weighting, four additional weighting functions have been introduced:

The weighting *1/Amount* (or *1/response*) virtually undoes the "normal" weighting described above, i.e. low and high concentrations are weighted similarly. The weighting *1/Amount²* (or *1/response²)* results in an over-proportional weighting of smaller amounts.

By variation of the ➢*Number of Replicates*, this weighting can be avoided. Smaller concentrations are injected more frequently than larger concentrations, more calibration points in the low concentration range support the calibration curve. **Outliers** are then less relevant.

☞ ***Tip***: The stronger weighting of higher concentrations is valid in all ➢*Calibration Functions*, with the exception of **Point-to-Point**.

Outliers can be explicitly "deactivated" by excluding a specific standard sample from the calculation on the **Calibration** sheet of the quantification method.

When calculating the calibration values **Variance**, **Var.Coeff**, **Std.Dev**, **Rel.Std.Dev**, and **Corr.Coeff**, averaging is not considered! Weighting only influences the course of the calibration curve, the values are a measure for the quality of the calibration.

Averaging

To determine the calibration curve, all available ➢*Calibration Points* are normally used. As dispersion is stronger for the lower calibration levels, many users verify the results by using a large number of calibration points. The calibration curve is thus determined by a larger number of points on the lower than on the higher level.

If all points of a ➢*Calibration Level* are averaged before calculating the calibration curve, and the subsequent calibration is performed based on these average values only; the calibration curve is based on one point of each calibration level only.

Defining the QNT Method for Several Detectors

1. If two detectors are connected in series, the retention times are delayed against each other. As the flow normally remains unchanged, the shift of the retention times is constant. The ⇒*Delay Time* parameter enables you to take this fact easily into consideration.

First, enter the name of the second detector under **Detector Name** on the **General** tab of the QNT editor. Use the arrow to select the name from the list. Then, enter the measured delay time.

2. For some applications, it might be necessary to modify the QNT method for a second detector or another channel. Therefore, you cannot use the **Delay Time** parameter when you are working with ➢*Flow Gradients*

To avoid creating a second QNT method for such or similar applications, you can duplicate the following columns and assign the duplicate to one or several channels:

⇒*Calibration Type*

⇒*Integration Type*

⇒*Kovats Index*

⇒*Left/Right Limit*

⇒*Peak Type*

⇒*Response Factor*

⇒*Retention Index*

⇒*Retention Time*

⇒*Window*

To duplicate a column, select it in the peak table (in the amount table, or in peak tracking) and select **Columns**, either in the context menu or in the edit menu. Open the respective dialog box with **Duplicate Column** and define the channel / the channels for the new column via **Add Channel**.

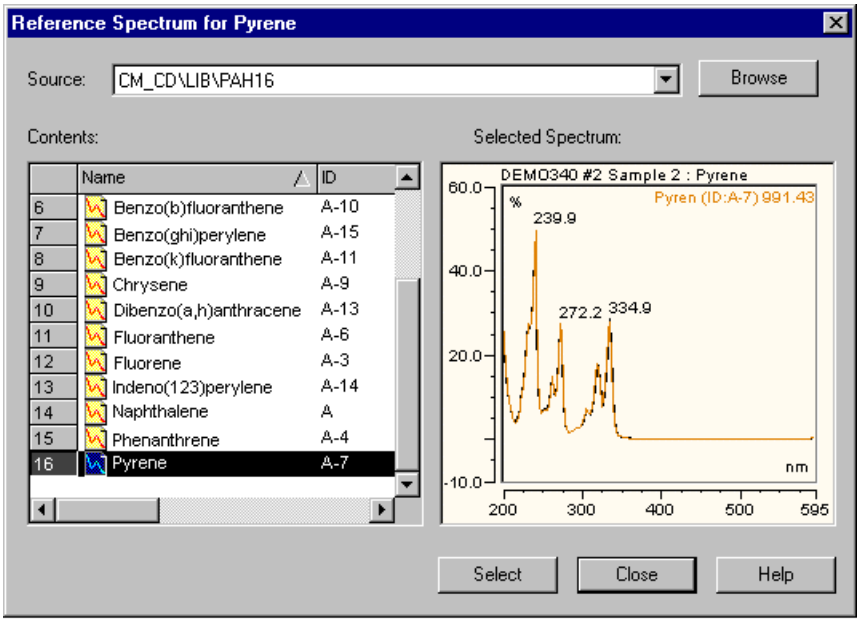
If an individual peak is not detected in a channel, the respective cell in the **Retention Time** column can be left empty. Thus, this channel will not identify this peak. If you do not wish to include a peak into the report although it was detected, just leave the **Retention Time** column empty.

In addition, you can define further detection parameters for the respective channel/channels in the **Channel** column on the **Detection** tab. Also see **How to: ...: Actions in the QNT Editor Defining Detection Parameters (Detection)**.

Entering Reference Spectra (Reference Spectrum Column)

You can enter a reference spectrum for each peak in the peak table of the QNT editor:

Position the cursor in the **Reference Spectrum** column, press the **F8** key or double-click the left mouse button to access a dialog window that allows you to select the reference spectrum of the peak. By pressing the **Browse** button, you can load any samples or spectra libraries for selecting the reference spectrum. If samples are loaded, a list of all peaks in the corresponding chromatogram is displayed. For spectra libraries, the list shows the included spectra (see figure). In the right window section, the selected reference spectrum is displayed. If the relevant peak of the peak table is identified in the current chromatogram, the spectrum is included as overlay. The corresponding match factor is shown in the upper corner of the plot frame.



After pressing the **Select** button, the selected reference spectrum is copied to the corresponding line of the peak table.

Clipboard: Spectra can copied to the clipboard from the spectra plot window or the spectra library using **CTRL**+**C** (or the **Copy** command from the **Edit** menu). In the QNT editor, the copied spectrum can be inserted in the **Reference Spectra** column as the reference spectrum via **CTRL+V** or the **Paste** command from the **Edit** menu.

Copy Peak Spectra as Reference: If one or several lines are selected in the **Reference Spectrum** column, the **Copy Peak Spectra as Reference** command allows using the spectra of the current chromatogram as the reference spectra from the **Edit** or context menu.

Overlay of the Reference Spectrum in the Spectra Plot

In the spectra plot, the current reference spectrum from the peak table can be included as **Overlay**. To do this, place the cursor in the spectrum, open the context menu, choose **Decoration**, and then choose the **Peak Spectra** tab. In the lower section, click **Reference Spectrum in corresponding peak table**. Press **OK**" to receive the spectrum from the **Reference Spectrum** column in addition to the current one.

Autogenerating the Peak Table

To save the user from having to determine the retention time of each peak, peak tables can be automatically created. Selecting the **Autogenerate Peak Table** command, either in **Edit** menu or in the context menu does this.

The Dionex Chromatography Management System automatically generates a peak table, entering the retention times of all detected peaks of the currently open chromatogram as set times. The user need only complete the table by entering component names and altering the default window and other values as necessary. Peaks, which are not of interest, can be deleted from the table. These will consequently be excluded from the report, provided the **Including all not detected peaks of the peak table** parameter in the **Integration Report Properties** (**Table Properties** command in the **Edit** or context menus) is switched to OFF.

During automatic table generation, the variables described below are set as follows:

Autogenerated Peak Table is entered as ⇒*Comment*.

The peak names (⇒*Name*) are constructed from the name of the QNT method, e.g. . in the peak table **Test**, detected peaks will be assigned the names Test-1, Test-2, Test-3, etc.

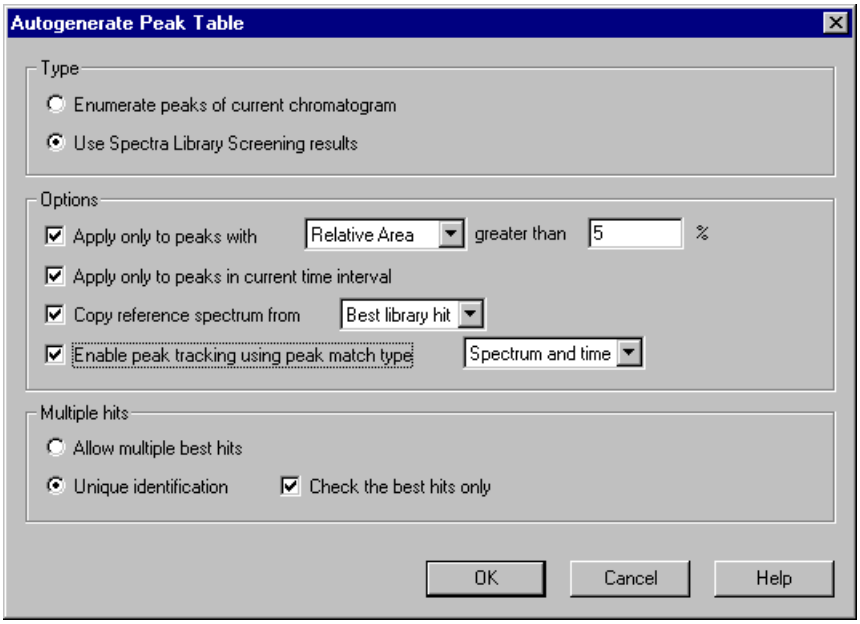
The ⇒*Window* values are entered as absolute values; they represent 1/3 of the distance from the nearest peak.

No ⇒*Group*.

The ⇒*Amount* values and the ⇒*Response Factor* at set to 1.0.

The peak type (⇒*Sample Type*) is Auto (i.e., it is determined by the Dionex Chromatography Management System).

When generating peak tables via **Autogenerate Peak Table** (Edit menu), it is possible to use the results of the spectra library screening (type: **Use spectra library screening results**) instead of enumerating all peaks in the chromatogram (type **Enumerate peaks of current chromatogram**).



In this case, library screening is performed based on the parameters entered in the QNT file. All peaks for which at least one reference spectrum was found, are included in the peak table with the name of the best hit.

The following options can also be used:

- **Apply only to peaks with ...**. With this option, only peaks exceeding a selectable absolute or relative area or height will be included in the peak table.
- **Apply only to peaks in current time interval**: Click this button to include only peaks in the currently displayed (e.g. zoomed) section of the chromatogram.
- **Copy reference spectrum from ...**: This option simultaneously includes the reference spectrum for each peak. Either the current peak spectrum (from the displayed chromatogram) or the library spectrum of the best hit from library screening can be used. For the latter, the **Use spectra library screening results** autogeneration option must be selected in the upper window section.

- **Enable peak tracking using peak match type ...**: This option allows activating peak tracking for each included peak. As with peak tracking (see **How to …: Actions in the QNT Editor** **Peak Tracking**), you can select between **Spectrum** and **Spectrum and time**.
- **Allow multiple best hits** / **Unique identification**: The results of the spectra library screening will produce a hit list of library spectra for each peak in the chromatogram. If **Unique Identification** is selected, these hit lists are handled as in Peak Tracking, i.e. multiple identical hits with smaller match factors are eliminated. In the case of **Allow multiple best hits**, each peak in the chromatogram is copied to the peak table with the best hit. If the best hits are identical, this can result in identical entries in the peak table. In this case, adding a number to the name (e.g. -2, -3) generates a unique peak.

If you have generated a new peak table via **Autogenerate Peak Table**, a note will be included automatically in the **Comment** column of the peak table:

- If you have selected **Enumerate peaks of current chromatogram**, the comment is: **Autogenerated**.
- The corresponding comment for **Use spectra library screening results** is: **Autogenerated. Spectrum:** ***Name of reference spectrum*****, Match:** ***Match factor***.

☞ ***Tip***: The **Use spectra library screening results** option automatically enters the settings made on the **Spectra Library Screening** tab in the peak table (**Peak Tracking** tab).

Defining Detection Parameters

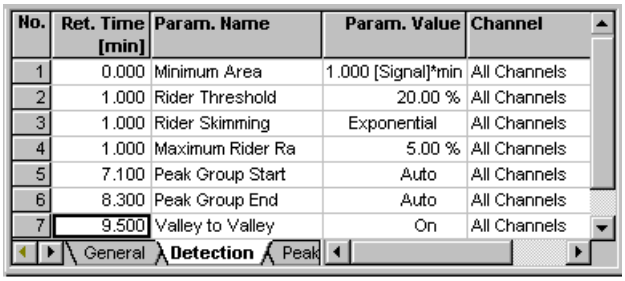
The detection parameters define how to integrate the chromatograms, which are evaluated with the respective QNT method, where to suppress peaks, how to recognize peak start and peak end, etc. This enables the user in many ways to define the integration and to minimize the re-integration effort for individual chromatograms.

You can either enter the detection parameters in the table on the **Detection** tab or define them graphically in the chromatogram.

In order to enter the parameters in the table on the **Detection** tab of the QNT editor, express the desired conditions via the columns **Parameter Name** and **Parameter**. They influence the integration of all chromatograms to which the respective QNT method applies. There are 22 different parameters, which can assume a new value at any time and whenever desired. Only the value, which was defined, last will take effect, however, only for the time of the chromatogram. The parameters are then reset to their default values. If a parameter assumes a new value at a specified time (**Retention Time** column), this is called an **Event**. You do not have to enter these events in chronological order. They will be sorted automatically when being saved. The **Channel** column allows you to define whether this applies to an individual channel only or to all channels (default) of a sample.

Each detection parameter has a default value assigned. Thus, in general about 90% of all chromatograms are automatically integrated correctly by the system. However, for critical applications (e.g. **wavelength switching**) the user can influence the baseline or the peak type (e.g., rider or main peak) or switch off the detection for defined periods.

Many parameters can only assume the values **ON** or **OFF**. They are called **switches**. All other parameters are called **variables**. Parameter tables can include up to 100 lines. For an example on how to enter detection parameters in the table of the **Detection** tab, see the following illustration:



No.	Ret. Time [min]	Param. Name	Param. Value	Channel
1	0.000	Minimum Area	1.000 [Signal]*min	All Channels
2	1.000	Rider Threshold	20.00 %	All Channels
3	1.000	Rider Skimming	Exponential	All Channels
4	1.000	Maximum Rider Ra	5.00 %	All Channels
5	7.100	Peak Group Start	Auto	All Channels
6	8.300	Peak Group End	Auto	All Channels
7	9.500	Valley to Valley	On	All Channels

General | Detection | Peak

In many cases it may be easier to enter the detection parameters graphically in the chromatogram (see **How to ...: Actions in the Chromatogram** **Defining Detection Parameters Graphically**

In addition, the QNT editor offers further detection parameters. The following sections describe how to edit the default values together with the respective possibilities and advantages. Use the detection parameters for:

- **Reducing the Number of Evaluated Peaks**
- **Excluding Certain Peaks**
- **Inhibiting Peak Integration**
- **Modifying the Baseline**
- **Modifying the Peak Recognition Algorithm**
- **Defining the Peak Start/End**
- **Defining Rider Peaks**
- **Defining the Area for PPA**

Reducing the Number of Evaluated Peaks

To limit the integration report to a manageable size, only the most important, i.e., normally the largest peaks should be included in the evaluation. Define either the ⇒*Minimum Height* or the ⇒*Minimum Area*. Proceed as follows (the following example refers to the minimum peak height):

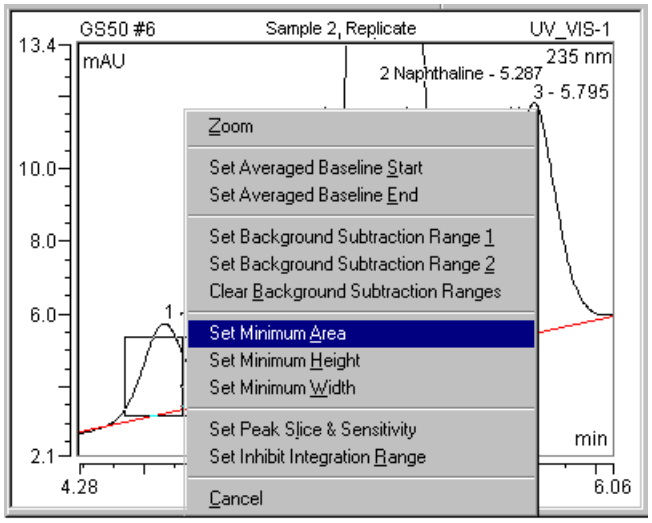
- Open a QNT file (select **Open** in **File** menu) and click the **Detection** tab.
- Look at the chromatogram and determine the minimum peak height to be evaluated. You may also click the smallest peak to be integrated. Then open the corresponding **Peak Properties** via the context menu. The dialog box then indicates the width, height, and area of the peak.
- Enter the name of the parameter to modify, e.g. the ⇒*Minimum Height* in the **Parameter Name** column of the quantification method.
- Assign the smallest possible signal value (e.g. in mAU) as the new parameter value in the **Parameter Value** column.
- In the **Time** column, determine from which time (relative to injection time) the parameter becomes valid.
- Alternatively, you can open an edit dialog box (press the **F8** key) to enter the parameter name, value, and time.

All peaks with an area smaller than the indicated %-value will not be displayed.

As the parameters affect peak recognition and thus the baseline, you must consider a tolerance of approx. 5% to ensure that all desired peaks are recognized.

Another way to define, e.g., the minimum area, is to graphically define the corresponding parameter. Proceed, e.g., as follows:

- In the chromatogram, find the smallest peak just no longer to be displayed.
- Enlarge this peak to be clearly visible.
- In the chromatogram, use the right mouse button to select an area whose area is a slightly smaller than that of the selected peak.
- In the context menu, select the **Set Minimum Area** command.



This action enters the selected area as minimum area together with the time of its left edge into the QNT method. Enter the 0.000 as time into the **Detection** tab or move the parameter in the chromatogram with the **Detection Parameter Tool** so that the minimum area is valid for the entire chromatogram.

Note: You can undo the graphical input of detection parameters. Click into one of the tables of the QNT editor and select the **Undo** command of the **Edit** menu. (In the chromatogram itself, you can only undo the modifications of the currently open chromatogram.)

Tip: If you just want to make the report clearer, proceed as follows:

- Select any cell in the report (integration tab) and choose **Table Properties** from the **Table** menu.
- Select the **Reject peaks with smaller area than ...%** check box and specify below which size not to include a peak in the report.

Excluding Certain Peaks

Spikes

Sometimes, very narrow peaks (so-called "Spikes") occur in chromatograms due to, e.g., air bubbles in the HPLC system. In such a case, the problem (e.g. the air bubbles in the HPLC system) should be solved first, of course. However, to use the chromatogram, nevertheless, the identification of these narrow peaks can be suppressed with the QNT method.

Select the ⇒*Minimum Width* parameter to define the minimum width for the peaks to be integrated. Proceed as when entering the minimum height (see **Reducing the Number of Evaluated Peaks**).

Peaks above the Detector Maximum

Sometimes peaks occur whose absorption maximum is above the detector maximum so that integration does not make sense. You can then include these peaks as unidentified peaks into the peak table by using the ⇒*Maximum Peak Height* parameter.

Broad Peaks

If an unusually broad peak occurs in the chromatogram, it may be from a previous sample. Use the ⇒*Maximum Width* parameter to define this peak as being unidentified.

Inhibiting Peak Integration

The ⇒*Inhibit Integration* parameter can be activated at the time t1 and can be deactivated at the time t2. The peaks within the time window t1 - t2 are not integrated. Whether this applies to all channels or to only one channel is specified via the **Channel** column.

To prevent the integration of all peaks in the range from 0 to 1.0min (especially the injection peak), the following input is necessary in the quantification method.

No.	Ret. Time [min]	Param. Name	Param. Value	Channel
1	0.000	Inhibit Integration	On	All Channels
2	1.000	Inhibit Integration	Off	All Channels

General | **Detection** | Peak Table | Amount Table

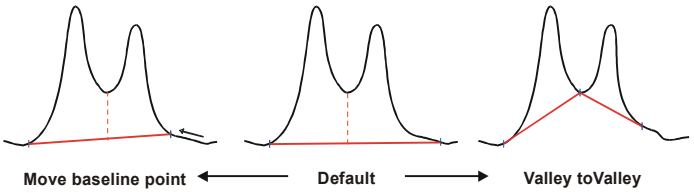
Peaks detected in this time span will not be integrated and will not be included in an integration report.

Modifying the Baseline

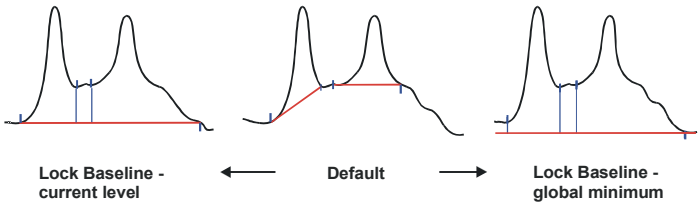
Modifying the baseline can be necessary especially for non-resolved peaks. The baseline is normally defined via a mathematical procedure. For calculating the individual peak areas, a perpendicular is dropped to the baseline from each local minimum (standard).

If you think the integration is started too early or the peak end is delayed, a better peak start or peak end can be forced by inserting a baseline point (⇒*Baseline Point* detection parameter).

If a series of non-resolved peaks can be recognized on an "absorption mound," e.g. due to an increased solvent absorption, the baseline can be forced from minimum to minimum using the ⇒*Valley to Valley* detection parameter.



If single peaks are piled on a recognizable "absorption mound," these are integrated individually. To be able to integrate the entire area, the baseline can be fixed. The parameter ⇒*Lock Baseline* extrapolates the baseline horizontally to the intersection with the signal curve. The **Global Minimum** option searches for the absolute minimum in the direction of the peak end or until the next **Lock Baseline**. Both parameters deactivate the **Valley to Valley** option!



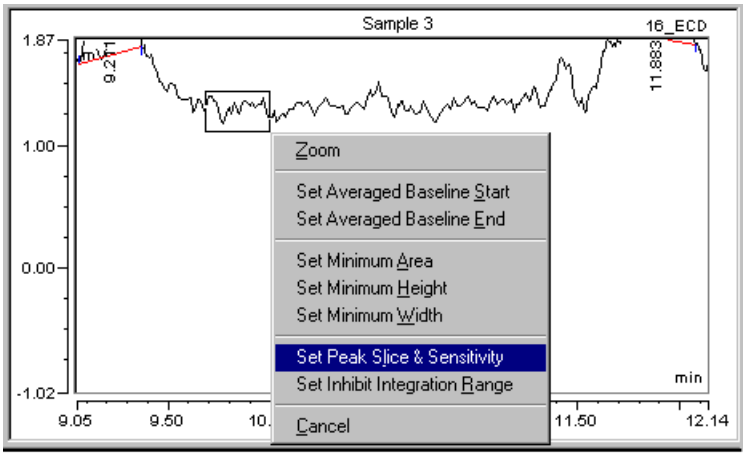
☞ ***Tip***: In all of these actions, the classification criterion **Peak Type** of the peak table has priority! For a peak of the type **Baseline-Main-Baseline**, the peak limits always have baseline contact!

Modifying the Peak Recognition Algorithm

Whether signal variations are interpreted as peaks or not, is usually set automatically. Manual modification of this "recognition sensitivity" is possible via the combination of the ⇒*Peak Slice* and ⇒*Sensitivity* detection parameters. Changing the parameters is required, for example, in chromatograms with unusually wide (many minutes) or very narrow (< 0.1sec) peaks.

Another way to define the peak recognition algorithm is to define both parameters graphically. Proceed as follows:

- Enlarge a baseline section so that the noise is clearly visible.
- In the chromatogram, use the right mouse button to select an area from which the baseline runs out neither at the top nor at the bottom.
- In the context menu, select the **Set Peak Slice & Sensitivity** command.



The width of the selected area is entered into the QNT method as peak slice and the height is entered as sensitivity at the time of the left edge of the area. Enter 0.000 as time onto the **Detection** tab or move the parameters in the chromatogram with the **Detection Parameter Tool** so that this peak recognition algorithm applies to the entire chromatogram.

Note: You can undo the graphical input of detection parameters. Click into one of the tables of the QNT editor and select the **Undo** command of the **Edit** menu. (In the chromatogram itself, you can only undo the modifications of the currently open chromatogram.)

The peak recognition algorithm considers signal variations only beyond the adjusted sensitivity values. Peaks below this threshold are interpreted as noise.

Both parameters affect peak recognition only, not integration! The area calculation (integration) is not affected.

Defining Peak Start / Peak End

Depending on the chromatogram type, the peak start or the peak end can be detected too early or too late. There are several ways to prevent this:

If, in your opinion, the integration is started too early or if the peak end is delayed too much, use the **Fronting Sensitivity Factor** parameter for the peak start and the ⇒*Tailing Sensitivity Factor* for the peak end. The entered value multiplied with the left or right peak width determines the peak start or the peak end. Depending on the chromatogram type different values may make sense. Therefore, you should try which value is best for your chromatograms. Often, the value **2** is an appropriate starting point for finding the best **Fronting/Tailing Sensitivity Factor**.

You can also set a new ⇒*Baseline Point* to force the peak to start later or to end earlier.

Caution: However, when setting a baseline point keep in mind that this point will be valid for all chromatograms, which are evaluated with the respective QNT method. If in one of these chromatograms a peak maximum occurs by coincidence at the time of your hard entered baseline point, the peak maximum will be defined as base point and the peak will not be detected.

To correct too late a peak start or too early a peak end (the latter can occur, e.g., with heavy baseline noise), proceed as follows:

1. In recorded chromatograms: Select a higher ⇒*Peak Slice* (= about 20% of the smallest peak width) and, in addition, a higher ⇒*Sensitivity*, if necessary.
2. For samples that have not been processed yet: In the program file, change the data acquisition ⇒*Step*. Select the step so that only about 20 data points are recorded for the smallest peak.

Defining Rider Peaks

The detection parameters ⇒*Rider Threshold* and ⇒*Maximum Rider Ratio* allow you to define which peaks shall be detected as ➢*Rider Peaks* and which shall be detected as main peaks. The following applies:

The smaller the rider threshold, the smaller the peaks that can be detected as rider peaks. (Peaks below the rider threshold are always regarded as main peaks. For peaks above the rider threshold, the Maximum Rider Ratio defines whether a peak is a rider peak or a main peak.) The larger the maximum rider ratio, the larger the peaks that can be defined as rider peaks.

☞ ***Tip***: When defining rider peaks with these parameters please keep in mind that the same peak may be detected in two different chromatograms as main peak and as rider peak. This would result in considerable deviations, e.g. in the calibration. To prevent this, select the peak type **Rider** (or **Main**) for the respective peak in the peak table. Thus, the peak is a rider peak, if possible (or always a main peak).

In addition, you can define how to skim rider peaks by using the ⇒*Rider Skimming* parameter. With the two options **Tangential at lower peak end** and **Tangential at both peak ends** the peak is skimmed by a tangent. Usually, there is hardly any difference between the results of the two options.

With the **Exponential** option, the course of the baseline is approximated by an exponential function, i.e., the peak is skimmed by the exponential function. This option clearly distinguishes from the two others. In most of the cases, **Exponential** maps the actual baseline course very accurate. With this option, the rider peak will usually receive a more realistic larger area. A sufficient number of data points must be available to ensure that this option can be used.

Defining the Area for PPA

When using ➢*Photodiode Array Detectors* and recording ➢*3D-Fields*, you may check the peak purity with the ➢*Peak Purity Index (PPI)*.

Define the most expressive area of you spectrum by means of the ⇒*Peak Purity Start/End Wavelength* parameters and limit the examination to this area only.

The detection limit becomes especially apparent with very small peaks. The influence (i.e., noise, drift and limits of the measuring method) on the peak spectrum is strongly developed at the peak start and peak end because, in these areas, the concentration of the peak substance in the flow cell is very low. Setting the ⇒*Peak Purity Threshold* parameter allows you to reduce the influence on the PPI and the match factor and, thus, to prevent that contaminated substances are indicated falsely. The PP threshold value defines the percentage of the peak height starting as of which the spectra will be considered for the respective purity examination.

If you work close to the detection limit, use higher PP threshold values to reduce the influence of the detection limit on the purity examinations. If you are mainly interested in the purity of large peaks, use lower PP threshold values to examine the purity over the largest possible area of the peaks.

Grouping Peaks

If you are interested in the sum parameters for two or more peaks, you can 1. define these peaks as a peak group (that is treated as one single peak) or 2. define them as a group of peaks.

1. If the peaks lie close together and are not baseline separated (e.g. with overloaded columns), define the peak group start and the peak group end via the ⇒*Peak Group Start/End* parameters on the **Detection** tab. The baseline will then be drawn from the start of the peak group to its end. Such a peak group is treated as one single peak.
2. If you wish to define a peak group in which the peaks do not necessarily succeed one another (e.g., to determine the amount/concentration of an entire class of substances), several steps must be taken:

- **Identified peaks**: Use the **Column** and **Display Column** commands of the context menu to insert the ⇒*Group* column into the peak table if the column is not yet displayed. For those peaks that should belong to this group, type the desired group name into this column.
- **Unidentified peaks**: Under **Unidentified peaks** on the **General** tab, define the time for which this group shall be valid in case of unidentified peaks. The baseline will be drawn as for individual peaks.
- Add the **Group Amount** column to the **Report** and the ➢*Printer Layout*. This column shows the desired ⇒*Amount* value. In the report, open the dialog box **Insert/Add Report Column** via the **Insert Column** or **Add Column** commands of the context menu. Choose the **Peak Results** category and select **Group Amount** as variable.

☞ ***Tip***: If the selected calibration type is e.g. **LOff** instead of **Lin**, the value in the **Group Amount** column will not be identical to the sum of the amount values of the individual peaks even if the group includes all peaks of the chromatogram.

Subtracting a Blank Run Sample

The section **Blank Run & Matrix Blank** on the **General** sheet of the QNT editor allows the user to consider absorption values of a ➢*Blank Run Sample*, a ➢*Matrix Blank Sample* or any other sample (➢*Blank Run Subtraction*).

- Select **No Blank Run Subtraction** if no correction is to be performed.

If the absorption values of a specific sample are to be considered in the sample evaluation, determine which sample is to be used as Blank Run Sample.

- Select **Subtract Recent Blank Run Sample in Corresponding Sequence** if a processed Blank Run Sample (sample type: **Blank**) of the current sequence is to be used.
- Select **Subtract a Fixed Sample** to perform the correction with a specific Blank Run Sample. Choose **Browse** to search for the sample.

When subtracting a blank run sample, the chromatogram of the blank sample is subtracted point by point from the current chromatogram. If the current sample is a standard sample, the difference between the two chromatograms is used for the calibration.

☞ ***Tip***: Although sample types other than "blank" can be subtracted as well, this usually does not make sense because often-negative peaks would occur in the resulting chromatogram.

- **Enable Matrix Blank Subtraction** activates the subtraction of matrix blank samples. Contrary to the other options, the resulting peak areas or peak heights are subtracted.

Disabling Standard Samples

On the **Calibration** tab, different calibration information is given and, in addition, you can define the standard sample to be used.

Click the box in the **Enabled** column to open the dialog box **Disable (Enable) Standard xyz** and define whether or not the respective standard sample shall be used for calibration purposes. You can exclude the respective standard from the calibration for all peaks and all channels (default) or for the selected peak and/or channel only. For further information on how to use this option, see the following examples:

The standard sample was contaminated

Exclude the entire standard from the calibration. Keep the default setting: Disable the standard for **All Peaks** and **All Channels**.

By mistake, too much of a substance was added to the standard

In this case, do not exclude the entire standard from the calibration, but disable the calibration for this substance, instead. Click on the peak and select **Selected Peaks** and **All Channels** in the **Disable (Enable) Standard xyz** dialog box.

Contamination in the standard that, however, is detected in one channel only

In this case, too, you do not need to exclude the entire standard from the calibration. Select the channel that detects the contamination and choose **All Peaks** and **Selected Channel** in the **Disable (Enable) Standard xyz** dialog box.

For information on calibration, also see: **How to ...: Actions in the QNT Editor Calibration**

Calibration

The following examples (see topics below) give a detailed description of both, the theory and the practical use of the available calibration possibilities. The first examples describe different applications

- **Introduction and Example: 1 Standard and 1 Substance (Mode: Total)**
- **Several Standards with Several Substances Each (Mode: Total)**
- **Multiple-Point Calibration Using 1 Single Standard (Mode: Total)**
- **Calibrating Using Standards of an Old Sequence (Mode: Fixed)**
- **Calibrating Unstable Substances (Mode: Bracketed)**
- **No Pure Substance Available - Known Extinction Coefficient (Response Factor)**

For a detailed description of the different ⇒*Calibration Modes* and the calibration with different types of ⇒*Standards* including calibration curve calculation see the examples below:

- **External Calibration (Mode: Total)**
- **External Calibration (Mode: Additional)**
- **External Calibration (Mode: Group)**
- **External Calibration (Mode: Bracketed)**
- **External Calibration (Mode: Fixed)**

Internal / External Calibration

Internal Calibration

Calibration with Variable Internal or Internal/External Standard

Note: Please note that the procedure is described for the **Total** mode. All other examples point out the differences of the individual calibration modes, only.

For information on validation, see the following topics:

Entering the Concentration/Amount of the Validation Sample

Validating the Calibration Curve

Note: To apply an existing calibration to a new sequence consisting of one or several **Unknown** samples, use the ⇒*Calibration Mode* **Fixed**. Always perform the calibration manually (**Calibrate**). The **Auto-Recalibrate** option is not available.

Introduction and Example: 1 Standard and 1 Substance

Most calibrations in HPLC and IC are performed using external standard samples. In the simplest case, the accompanying peak area for a known amount of a substance in one standard sample only is determined. From the ratio of amount and peak area, the data system calculates the slope (c1) of the ➢*Calibration Function* (in this case only linear without offset is possible). By means of this slope, the data system calculates the ⇒*Amount* value of this substance in unknown samples.

Short Example:

The amount of substance A shall be determined in two samples (Sample 1 and Sample 2). A standard sample (Standard) is available. For each samples a sampler injects an injection volume of 20 µl each. The samples are located at the sampler positions 1 (standard), 2, and 3 (unknown samples), respectively.

Sample List

In the **Browser** (see **Basic Operation** section), create the following sequence using the Sequence Wizard

No.	Name	Type	Pos	Inj. Vol.
1	Standard	Standard	1	20.0
2	Sample 1	Unknown	2	20.0
3	Sample 2	Unknown	3	20.0

Note: For detailed information on how to create a sample list, see **How to ...: Actions in the Browser Creating a Sample List (Sequence Table)**.

QNT Method / General Tab

The standard sample contains substance A in a concentration of 12 mg/l. A linear calibration curve (calibration type: Lin) that runs through the origin shall be created for substance A. After processing this sequence, the QNT method must be created for performing the calibration. In the **General** tab dialog box of the ⇒*QNT Editor*, enter the unit for all further entries under ⇒*Dimension of Amounts* (in this case "mg/l"). Keep the ⇒*Calibration Mode* setting **Total** under **Global Calibration Settings**.

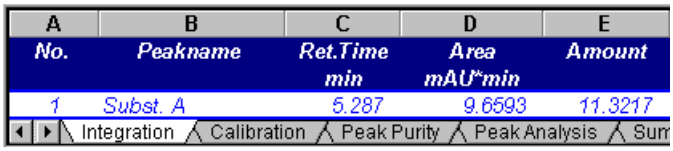
QNT Method / Peak Table Tab

Do not change the defaults in the **Standard** (External) and ⇒*Calibration Type* (Lin) columns on the **Peak Table** tab either. The Dionex Chromatography Management System automatically creates a "default" amount column. If, as in this case, only one standard sample is available, this can be kept as well. Enter the concentration in the amount column:

No.	Peak Name	Ret.Time	Window	Standard	Int.Type	Cal.Type	Amount
1	Subst. A	5.342 min	0.100 AG	External	Area	Lin	12.000000

Note: If more than one substance is available in the samples, append a new line to the table via the **Lines > Append Line** commands of the context menu and enter the corresponding concentration in the respective cell of the **Amount** column.

The Dionex Chromatography Management System calculates automatically the amount for the two unknown samples. Afterwards, you can view the results in the report on the **Integration** page:



A	B	C	D	E
No.	Peakname	Ret.Time min	Area mAU*min	Amount
1	Subst. A	5.287	9.6593	11.3217

Integration | Calibration | Peak Purity | Peak Analysis | Sum

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Several Standards with Several Substances Each

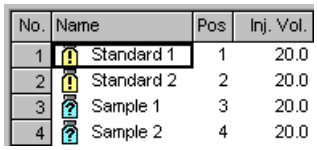
Usually calibrations are performed using several standards that very often contain more than once substance to be calibrated. In the simplest case, these are two standard samples containing two substances each, allowing you to determine not only the slope but also the offset and/or curvature of the calibration curve (depending on the number of acquired data points).

Example:

The amount of the substances A and B shall be determined in two samples (Sample 1 and Sample 2). Two standard samples (Standard 1 and Standard 2) which both contain substance A and substance B are available. For each sample, an injection volume of 20 µl is injected by an autosampler. The samples are located at the sampler positions 1 and 2 (Standard 1 and Standard 2) and 3 and 4 (unknown samples).

Sample List

The sequence appears as follows (also, see **How to ...: Actions in the Browser Creating a Sample List (Sequence Table)**):



No.	Name	Pos	Inj. Vol.
1	Standard 1	1	20.0
2	Standard 2	2	20.0
3	Sample 1	3	20.0
4	Sample 2	4	20.0

QNT Method / Peak Table Tab

The concentration of e.g. substance A in Standard 1 is 10.2 mg/l and of substance B 20.1 mg/l. Standard 2 contains 30.5 mg/l of substance A and 49.7 mg/l of substance B. Thus, for the calibration the following peak table must be created in the ⇒*QNT Editor*:

No.	Peak Name	Ret.Time	Window	Cal.Type	Amount 1	Amount 2
1	*Substance A*	*1.310 min*	*0.100 AG*	*Lin*	*10.200000*	*30.500000*
2	Substance B	2.450 min	0.100 AG	Lin	20.100000	49.700000

Remove the default ⇒*Amount* column and add new amount columns (one for each standard) for this example:

- Select **Columns...** in the **Edit** or context menu and then **Remove Amount Column**. Click on the indicated **Default** column and confirm with **OK**. The amount column is deleted and a warning is issued that the amount columns for your standards are missing.
- Open the **Add Amount Column** tab dialog box again via **Columns...** and **New Amount Column...**. Select **Add Standard(s)** to open the **Select Samples** dialog box.
- Select a standard. Press **OK** to enter this sample into the **Add Amount Column** dialog box.
- Pressing **OK** again creates the amount column for the selected sample. You may now create further amount columns in the same way. **Close** returns you to your peak table where you can now enter the corresponding values.

Note: If one of the substances is not available in the standard sample, the respective cell in the Amount column will be left empty.

If you are using several standards for calibration, you can select a ⇒*Calibration Type* other than Lin (linear without offset), if necessary.

Based on these settings, the Dionex Chromatography Management System automatically calculates the concentrations of substance A and substance B in the two unknown samples.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Multiple-Point Calibration Using 1 Single Standard

If you want to perform a multiple-point calibration (see ➢*Single-Point and Multiple-Point Calibration*) using only one standard sample, you can inject different injection volumes (= quasi ➢*Dilution Series*).

Sample List

For example, if you inject 10, 20, and 40 µl of one single standard, the sample list will appear as follows:

No.	Name	Type	Pos	Inj. Vol.
1	Standard1_1	Standard	1	10.0
2	Standard1_2	Standard	1	20.0
3	Standard1_3	Standard	1	40.0
4	Sample1	Unknown	2	10.0
5	Sample2	Unknown	3	10.0

For the Dionex Chromatography Management System, each injection is an individual sample. To distinguish between different injections made from the same standard sample vial, you may append the sample number and the injection number (see example above).

QNT Method / General Tab

The standard sample contains e.g. 10 ml/l Uracil. As all injections of such a dilution series are made from the same sample vial with the same concentration, you cannot represent the concentration in the calibration curve. Instead, enter the actually injected amount in the ⇒*Amount* column and choose a dimension of amount as unit. Thus, in the **General** tab dialog box of the ⇒*QNT Editor*, choose **ng** as **Dimension of amounts**.

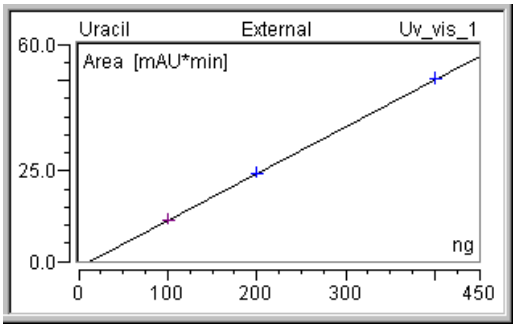
QNT Method / Peak Table Tab

As in the introduction example (see: **Introduction and Example)**, you do not need to change the default amount column setting on the **Peak Table** tab.

No.	Peak Name	Ret.Time	Window	Standard	Int.Type	Cal.Type	Amount
1	*Uracil*	*1.323 min*	*0,040 AG*	*External*	*Area*	*LOff*	*100.000000*

If, as in the example below, the calibration line does not run through the origin, you can **select Linear with Offset** (= LOff) as ⇒*Calibration Type*.

These settings will then result in the following calibration line:



For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor** **Calibration**.

Calibrating Using Standards of an Old Sequence

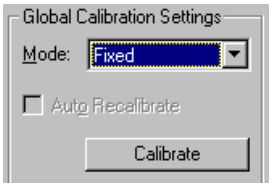
Calibration standards are often quite expensive. Thus, if the calibration curve remains constant for weeks or months, the standards of a sequence can be used for calibration for several weeks before the calibration constancy needs to be checked again.

Sample List

In this case, the new sequence will neither contain standards nor ➢*Validation Samples* but unknown samples only (perhaps plus ➢*Blank Run Samples* and/or ➢*Matrix Blank Samples*).

QNT Method / General Tab

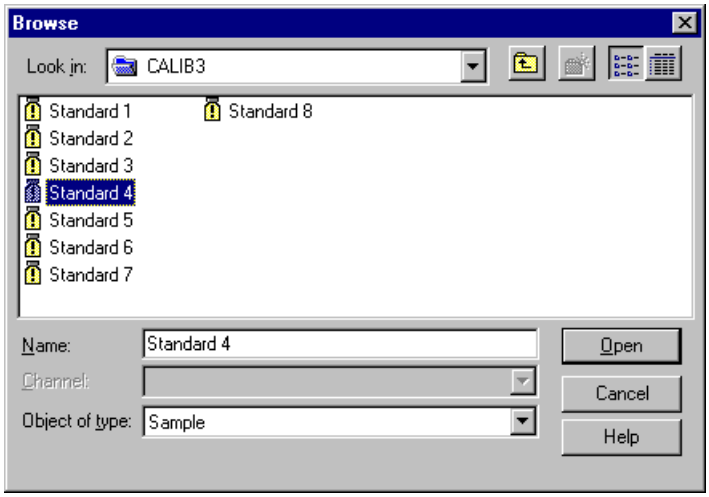
Under **Global Calibration Settings**, set the ⇒*Calibration Mode* **Fixed**:



In **Fixed** mode, manual calibration is possible only, i.e., after adding standards on the **Calibration** sheet (see below) press the **Calibrate** button on the **General** sheet to include the newly entered standards in the calibration.

QNT Method / Calibration Tab

With the calibration mode **Fixed** being selected, the **Calibration** table is empty at first. Use the **Append Standard** command of the context menu to add the desired standard(s). This command opens the **Browse** dialog box for selection of the desired standard sample from any sequence:



The **Calibration** sheet then contains the desired standards:

No.	Enabled	Name	Sequence	Smp.No.	Pos.	Inj. Vol.	Inj. Date/Time
1	☑	Standard 1	Parabenes\CALIB3.SEQ	1	6	4.0	04.12.00 12:51:27
2	☑	Standard 2	Parabenes\CALIB3.SEQ	2	6	8.0	04.12.00 13:03:25
3	☑	Standard 3	Parabenes\CALIB3.SEQ	3	6	12.0	04.12.00 13:15:24
4	☑	Standard 4	Parabenes\CALIB3.SEQ	4	6	16.0	04.12.00 13:27:24
5	☑	Standard 5	Parabenes\CALIB3.SEQ	5	6	20.0	04.12.00 13:39:23
6	☑	Standard 6	Parabenes\CALIB3.SEQ	6	6	24.0	04.12.00 13:51:24
7	☑	Standard 7	Parabenes\CALIB3.SEQ	7	6	28.0	04.12.00 14:03:22
8	☑	Standard 8	Parabenes\CALIB3.SEQ	8	6	32.0	04.12.00 14:15:24

Having entered all standards, press the **Calibrate** button on the **General** sheet to perform the calibration with those standards. Following each change (e.g., excluding a standard by disabling the **Enabled** checkbox or correcting the injection volume in the sample list) you have to press the **Calibrate** button again!

Note: If you later edit the name of the sequence from which the standards were added or the name of the directory that houses the sequence, the reference becomes invalid. Then, you have to add the standards again on the **Calibration** sheet.

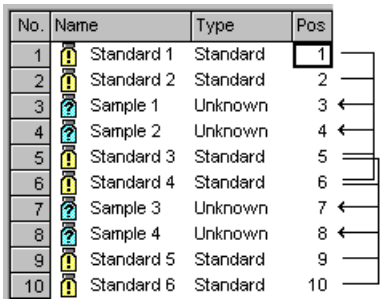
For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Calibrating Unstable Substance

If you want to calibrate unstable substances, the concentration in the samples that are analyzed later, may be considerably lower than the concentration in those samples that are analyzed first although originally the concentration was the same. The instability of the substance makes calibrating more difficult. The Dionex Chromatography Management System offers two possible solutions:

Sample List

In order to allow for the instability of substances every now and then one or several standard samples are added to a series of unknown samples. The sequence will appear e.g. as follows:



No.	Name	Type	Pos
1	Standard 1	Standard	1
2	Standard 2	Standard	2
3	Sample 1	Unknown	3
4	Sample 2	Unknown	4
5	Standard 3	Standard	5
6	Standard 4	Standard	6
7	Sample 3	Unknown	7
8	Sample 4	Unknown	8
9	Standard 5	Standard	9
10	Standard 6	Standard	10

QNT Method / General Tab

The bracketed calibration illustrated in the above figure has been achieved via the ⇒*Calibration Mode* **Bracketed** (set under **Global Calibration Settings**). The four less decayed standards 1-4 (from positions 1, 2, 5, and 6) are used for calibrating the less decayed unknown samples (samples 1 and 2 from positions 3 and 4). Calibrating the higher decayed samples 3 and 4 from positions 7 and 8 is via the more decayed standards 3-6 (from positions 5, 6, 9, and 10). The calibration curve shows the corresponding ➢*Calibration Points*, only.

For details on the mode Bracketed, see **External Calibration (Mode: Bracketed)**.

☞ ***Tip***: Knowing the half-life of an unstable substance (this is especially true with radioactive substances) offers you a clever way to calculate the chromatogram as it would be without the decay. Record all chromatograms in this special channel via a ➢*Virtual Channel Driver* as if the substance would not decay. For a program example, see **How to ...: Device Control Program Examples for Virtual Channels**. Having recorded these ➢*Virtual Signals,* perform the calibration as described in the above examples for stable substances.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

No Pure Substance Available - Known Extinction Coefficient

If you wish to quantify substance A although the pure substance A is not available, calibration can be performed nevertheless provided the ratio of the extinction coefficient to the extinction coefficient of a different substance B is known. First, create the corresponding sample list following the description under **Several Standards with Several Substances Each**.

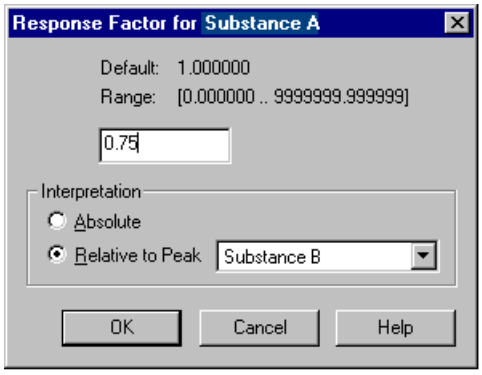
Then, create the ⇒*Amount* columns for your standards. As the pure substance A is not available and thus is not contained in the standards, the cells for substance A remain empty in the amount table:

No.	Peak Name	Ret.Time	Window	Cal.Type	Resp.Fact.	Amount Sample 1	Amount Sample 2	Amount Sample 3	Amount Sample 4
1	*Substance A*	*9.144 min*	*0.065 AG*	*Lin*	*0.750000 Substance B*				
2	Substance B	9.772 min	0.078 AG	Lin	1.000000	0.983000	2.034000	4.051000	7.890000

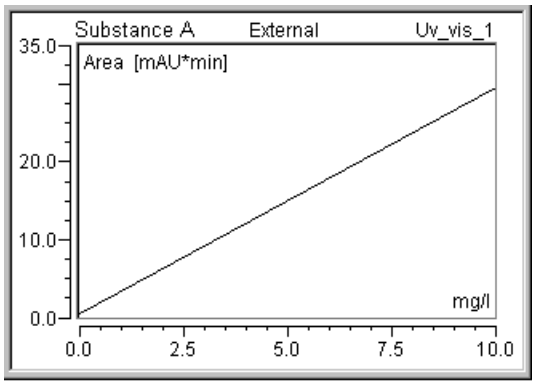
The decisive entry is the entry made in the ⇒*Response Factor* column. This column allows using the calibration of substance B for substance A. Double-click the selected cell (see above) to open the **Response Factor for Substance A** dialog box and enter the factor of the extinction coefficient at the measuring wavelength between the two substances:

$$Resp.Fact. = \frac{Ext.Coeff_{Subst.A}}{Ext.Coeff_{SubstB}}$$

Set the interpretation to "Relative to Peak" and select substance B:



The resulting calibration curve is 75% of the ➢*Calibration Function* of substance B. No calibration points are indicated in the calibration curve as no points were acquired for substance A:



Note: The calibration type that was entered in the peak table for substance A is not relevant. Although, Lin (without offset) was entered in the above example the calibration curve does not lead through the origin as LOff (linear with Offset) has been selected as calibration type for substance B.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Mode: "Total"

If more than only one standard sample exists, the calibration coefficients c0 (offset), c1 (slope), and c2 (curvature) can be calculated via the ratio between amount and peak area using the selected ➢*Calibration Function*. The resulting values are entered in the ➢*Formula for Amount Calculation*, together with the area values of the substance of an unknown sample. As the result, the data system provides the ⇒*Amount* value of substance A in the unknown sample.

Example:

In two samples (I,II), the concentration of substances A and B should be determined. One standard solution (STD 1) is available. It contains A in a concentration of 12 mg/l and B in a concentration of 17 mg/l. For A and B, a

linear calibration curve through the zero point (calibration type: linear) is created with two calibration points each. As only one standard solution is available, two different volumes (10 and 20 µl) must be injected (➢*Dilution Series*). Two ➢*Calibration Points* are resulting. The sampler injects a volume of 10 µl. The standard and analysis samples occupy the sampler positions 1 or 2, and 3, respectively.

a) User Input

Sample List

	Name	Type	Pos	Inj.Vol	Program	Method	Status
1	STD 1	Standard	1	10.0	Control1	QNT1	Single
2	STD 1	Standard	1	20.0	Control1	QNT1	Single
3	Sample I	Unknown	2	10.0	Control1	QNT1	Single
4	Sample II	Unknown	3	10.0	Control1	QNT1	Single

For how to proceed and what you must note, see **How to ...: Actions in the Browser** **Creating a Sample List (Sequence Table)**.

QNT Method / "Peak Table" Sheet

No.	Peak Name	Ret.Time	Window	Standard	Int.Type	Cal.Type	Amount1	Amount2
1	Subst. A	1.500 min	0.400 AG	External	Area	Lin	12.000000	
2	Subst. B	2.600 min	0.400 AG	External	Area	Lin	17.000000	

Regarding this example, note the following:

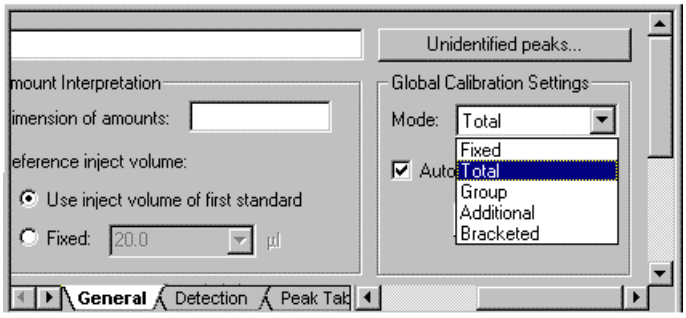
- In the **Standard** column, choose the standard method **External** via the F8 edit box. And:
- As only one standard concentration (STD 1) is available for calibrating substances A and B, exactly one amount value is entered in the **Amount** column of the peak table. The same applies if several sample list entries are generated by analyzing the same standard several times (two in this case). If the same injection volume is used for these, a 1-point calibration with several replicates is performed. If the injection volume is varied (10 and 20 µl), this is a multiple-point calibration, i.e. 2-point calibration, a special case of the ➢*Dilution Series* ("concentration series"). The Dionex Chromatography Management System automatically calculates the amount value of the second calibration point (double injection volume).

If, however, two separate standards with different concentrations are available (two vials, different sampler positions), two amount values should be entered in the peak table. In *this* case, the data system *cannot* simply calculate the concentration by considering the injection volume from the concentration of the other standard.

All other entries in the peak table are based on the criteria described under **How to ...: Actions in the QNT Editor Creating a Peak Table**.

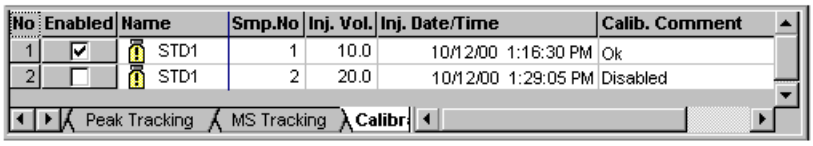
QNT Method / "General" Sheet

As all samples (here samples I and II) are calibrated with the same standard samples, the user selects the ⇒*Calibration Mode* **Total**.



QNT Method / "Calibration" Sheet

This sheet shows all standard samples (of a sequence) that are used for calibrating the current sample.



Press F4 or SHIFT+F4 to successively open all samples of a sequence. For each sample, the standard samples that are used for calibrating the sample are shown.

If you notice that an error occurred during the analysis of the standard sample, you can remove this standard. This is via the **Enable** column on the **Calibration** sheet in the QNT editor. Only the standard samples labeled **X** are included in the calibration.

b) Analysis Structure

Injection is four times. During the first run, the first calibration point of the calibration curves of the substances A and B is determined on the basis of the determined area values. In the second run, the second point is determined accordingly. Run three serves to determine the area values of the substances A and B of sample I. Correspondingly, in the fourth run, the area values of A and B of sample II are determined.

The following area values are resulting:

Name	Area Subst. A	Area Subst. B
STD 1 (first run)	150	200
STD 2 (second run)	300	400
Sample I	175	150
Sample II	95	180

c) Calculation of Missing Amount Values (of the second standard sample)

To perform the required calibration of each substance via two calibration points, two more area values must be determined after the first run.

This could be done with another standard solution of a different concentration. As no other standard solution is available, the second injection is again from the standard sample of known concentration. In this case, however, a different (the double) volume is injected. Thus, the double amount of the first run reaches the column. From the single amount value of the peak table (Amount(Peak Table)), the missing amount can be calculated considering the new volume.

$$Amount = Amount_{(Peak-Tab)} * \frac{Inj.Vol_{unknown\ Amount}}{Inj.Vol_{unknown\ Amount.}} * \frac{Smp.Wght}{Dil.Factor}$$

Evaluation of the formula (with ⇒*Weight* (sample weight) and ⇒*Dil. Factor* (dilution factor) = 1) results in the following amount values:

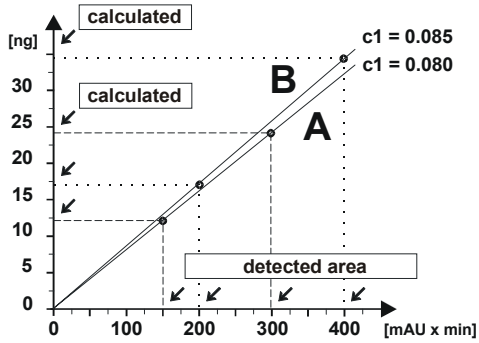
Amount (peak table)	Calculation of the second amount
A = 12.000	12 x (20/10) = 24
B = 17.000	17 x (20/10) = 34

d) Calculation of the Calibration Coefficients

From the area values of the standard samples and the corresponding amount values, the four value pairs can be determined. The intersection of each value pair represents a calibration point. Based on the selected calibration type (in the example: **Calibration Type (Linear)**), the Dionex Chromatography Management System calculates the optimum course of the calibration curve, i.e. tempts to find a course with four calibration points on or near the curve. If the course of the curve is established, the corresponding calibration coefficients (c0, c1, c2) can be calculated.

Substance	y/x-value pair	c1
A	12/150	0.08
A	24/300	0.08
B	17/200	0.085
B	34/400	0.085

With a linear course through the zero point, the calibration curve can be described by one single coefficient (c1). C1 expresses the slope of the curve. If all calibration points are located exactly on the calibration line, the resulting calibration coefficient c1 is the direct y/x-quotient of each value pair.



If the calibration points are not located exactly on one line, the data system calculates an optimized, approximate c1 value for each substance from the ➢*Calibration Function*.

If a different **Calibration Type (Non-Linear)** is used, the data system also calculates the remaining calibration coefficients (c0 and c2).

e) Amount Calculation

If the calibration coefficients of a substance A are known, each area value from an unknown sample for substance A can be converted into an amount value by inserting the values in the calibration function. When inserting this value into the ➢*Formula for Amount Calculation*, the actual amount value will result.

When performing this for the peak areas of the substances A and B in samples I and II (the correction factors of the formula for amount calculation are assumed with 1.0), the following amount values are calculated:

Sample	Calculation	Amount. A	Amount B
I	175 x 0.08	14.00	
I	150 x 0.085		12.75
II	95 x 0.08	7.60	
II	180 x 0.085		15.30

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor**  **Calibration**.

Mode: "Additional"

The following example illustrates the difference between the ⇒*Calibration Modes* **Total** and **Additional**.

Independently from the standard method, this mode determines which standard samples are used for evaluating a specific unknown sample. The position of the unknown sample in the sample list is decisive here.

Extending the Example: External Calibration / Mode: "Total"

After two unknown samples, two standard samples are injected again. An alternating list of two standard samples, two unknown samples, two standard samples etc. is resulting. All other settings are maintained, i.e., a two-point calibration is performed. The calibration is verified by additional replicates.

a) User Input:

Sample List

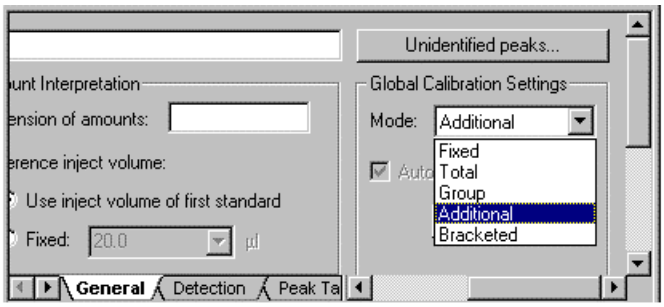
	Name	Type	Pos	Inj.Vol	Program	Method	Status
1	STD 1	Standard	1	10.0	Control 2	QNT2	Single
2	STD 1	Standard	1	20.0	Control 2	QNT2	Single
3	Sample I	Unknown	2	10.0	Control 2	QNT2	Single
4	Sample II	Unknown	3	10.0	Control 2	QNT2	Single
5	STD 1	Standard	1	10.0	Control 2	QNT2	Single
6	STD 1	Standard	1	20.0	Control 2	QNT2	Single
7	Sample III	Unknown	4	10.0	Control 2	QNT2	Single
8	Sample IV	Unknown	5	10.0	Control 2	QNT2	Single
9	STD 1	Standard	1	10.0	Control 2	QNT2	Single
10	STD 1	Standard	1	20.0	Control 2	QNT2	Single
11	Sample V	Unknown	6	10.0	Control 2	QNT2	Single
12	Sample VI	Unknown	7	10.0	Control 2	QNT2	Single

QNT Method / "Peak Table" Sheet

No.	Peak Name	Ret.Time	Window	Standard	Int.Type	Cal.Type	Amount1	Amount2
1	Subst. A	1.500 min	0.400 AG	External	Area	Lin	12.000000	
2	Subst. B	2.600 min	0.400 AG	External	Area	Lin	17.000000	

QNT Method / "General" Sheet

If the user selects the **Additional** mode, each unknown sample is evaluated based on the standard samples analyzed so far.



This means:

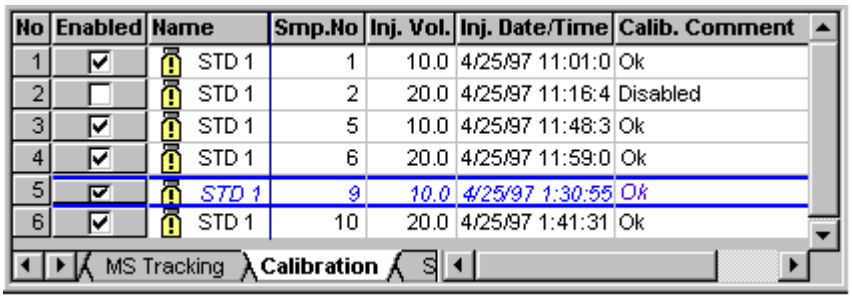
As before, samples I and II are evaluated via a two-point calibration. However, four analyzed standard samples are available for the samples III and IV. The result is a two-point calibration with two replicates each. Finally, the samples V and VI are evaluated via a two-point calibration with three replicates each.

QNT Method / "Calibration" Sheet

The sheet shows all standard samples (of one sequence) that can be used for calibrating the current sample.

Via F4 or SHIFT+F4, the samples are successively opened. For each sample, the standard samples are shown based on which the sample is currently calibrated.

Two standard samples are displayed for the samples I and II, four standard samples are displayed for the samples III and IV, and six standard samples are displayed for the samples V and VI six standard samples (see figure).



No	Enabled	Name	Smp.No	Inj. Vol.	Inj. Date/Time	Calib. Comment
1	☑	STD 1	1	10.0	4/25/97 11:01:0	Ok
2	☐	STD 1	2	20.0	4/25/97 11:16:4	Disabled
3	☑	STD 1	5	10.0	4/25/97 11:48:3	Ok
4	☑	STD 1	6	20.0	4/25/97 11:59:0	Ok
5	☑	*STD 1*	*9*	*10.0*	*4/25/97 1:30:55*	*Ok*
6	☑	STD 1	10	20.0	4/25/97 1:41:31	Ok

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If the user notices that an error occurred when analyzing the standard sample, the standard can be "excluded." This is performed via the **Enable** column on the **Calibration** sheet of the QNT editor. Only the standard samples labeled **X** are evaluated for the calibration.

b) Evaluation:

Evaluation is analogous to the example with external calibration (mode: **Total**). The only difference is:

Creating the calibration curve for different samples is created based on a different number of replicates.

This can affect the calculated calibration coefficients and thus the result, but does not necessarily do so. Normally this type of calibration is used to adapt to changed column conditions. Thus, it is possible that after a number of samples, a specific substance cannot be eluted 100 percent from the column. As this will also be the case with the standard substance, the result is automatically corrected.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor** **Calibration**.

Mode: "Group"

The ⇒*Calibration Mode* **Group** completes the modes **Total** and **Additional**. The mode is used when there are time-dependent modifications during the analysis, e.g. decomposition of the analyzed substance.

Again, the mode is described using the example of the **Additional** mode (sample list of alternating sample pairs (2 standards / 2 samples / 2 standards etc.)).

a) User Input:

Sample List

	Name	Type	Pos	Inj.Vol	Program	Method	Status
1	STD 1	Standard	1	10.0	Control 3	QNT 3	Single
2	STD 1	Standard	1	20.0	Control 3	QNT 3	Single
3	Sample I	Unknown	2	10.0	Control 3	QNT 3	Single
4	Sample II	Unknown	3	10.0	Control 3	QNT 3	Single
5	STD 1	Standard	1	10.0	Control 3	QNT 3	Single
6	STD 1	Standard	1	20.0	Control 3	QNT 3	Single
7	Sample III	Unknown	4	10.0	Control 3	QNT 3	Single
8	Sample IV	Unknown	5	10.0	Control 3	QNT 3	Single
9	STD 1	Standard	1	10.0	Control 3	QNT 3	Single
10	STD 1	Standard	1	20.0	Control 3	QNT 3	Single
11	Sample V	Unknown	6	10.0	Control 3	QNT 3	Single
12	Sample VI	Unknown	7	10.0	Control 3	QNT 3	Single

QNT Method / "Peak Table" Sheet

No.	Peak Name	Ret.Time	Window	Standard	Int.Type	Cal.Type	Amount1	Amount2
1	Subst. A	1.500 min	0.400 AG	External	Area	Lin	12.000000	
2	Subst. B	2.600 min	0.400 AG	External	Area	Lin	17.000000	

QNT Method / "General" Sheet

If the user selects the **Group** mode, each sample is evaluated based on the immediately previous standard sample in the sample list.

QNT Method / "Calibration" Sheet

This sheet indicates all *standard samples* (of a sequence) that are used for calibrating the current sample.

Press F4 or SHIFT+F4 to successively open each sample of a sequence. For each sample, the standard samples forming the basis for calibration are shown.

In the example, this means that in the **Group** mode the standard samples from the lines 1 and 2 are shown for the samples I and II. For the samples III and IV, the standard samples from lines 5 and 6, and for the samples V and VI, the standard samples from lines 9 and 10 are displayed.

b) Evaluation:

Evaluation is analogous to the examples with the external calibration (modes: **Total** and **Additional**). The only difference is that the calibration curve is constantly updated without considering the previously analyzed standard samples.

For the example, this means:

Evaluation of the samples I and II is via two-point calibration of the standard samples in the lines no. 1 and 2.

In contrast to **Additional**, the samples III and IV are also evaluated via two-point calibration. However, only the standard samples STD 1 from lines no. 5 and 6 are used.

Correspondingly, the samples V and VI are evaluated via the standard samples STD 1 in the lines no. 9 and no. 10.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Mode: "Bracketed"

In a bracketed calibration, a standard sample is included in a series of unknown samples so that modifications, e.g. column or detector drift, can also be considered in the calibration function. Amount calculation of an unknown sample is always via the calibration coefficients of the surrounding standard samples.

New Example

The concentration of substance A is to be determined in four samples (I-IV). Two standard solutions (STD 1, STD 2) of the substance A with different concentrations (50 and 100 ng/µl) are available for external calibration. At the beginning, after the second and after the fourth sample, a two-point calibration is to be performed. To receive more results that are exact, a bracketed calibration is performed. The basis for calibrating the samples I and II is provided by the standards STD 1 and STD 2 from lines no. 1, 2, 5, and 6, while the samples III and IV are calibrated on the basis of the standards no. 5, 6, 9, and 10.

a) User Input:

Sample List

	Name	Type	Pos	Inj.Vol	Program	Method	Status
1	STD 1	Standard	10	20.0	Control 4	QNT4	Single
2	STD 2	Standard	11	20.0	Control 4	QNT4	Single
3	Sample I	Unknown	1	10.0	Control 4	QNT4	Single
4	Sample II	Unknown	2	10.0	Control 4	QNT4	Single
5	STD 1	Standard	10	20.0	Control 4	QNT4	Single
6	STD 2	Standard	11	20.0	Control 4	QNT4	Single
7	Sample III	Unknown	3	10.0	Control 4	QNT4	Single
8	Sample IV	Unknown	4	10.0	Control 4	QNT4	Single
9	STD 1	Standard	10	20.0	Control 4	QNT4	Single
10	STD 2	Standard	11	20.0	Control 4	QNT4	Single

QNT Method / "Peak Table" Sheet

The external calibration (**Standard** = External) is performed via two standard samples (sampler positions 10 and 11) of different concentrations. In contrast to the **Total**, **Additional**, and **Group** examples, two different ⇒*Amount* values must be entered in the corresponding amount columns [1] and [2] of the peak table.

No.	Peak Name	Ret.Time	Window	Standard	Int.Type	Cal.Type	Amount1	Amount2
1	Subst. A	4.400 min	0.100 AG	External	Area	Lin	50.000000	100.000000

QNT Method / "General" Sheet

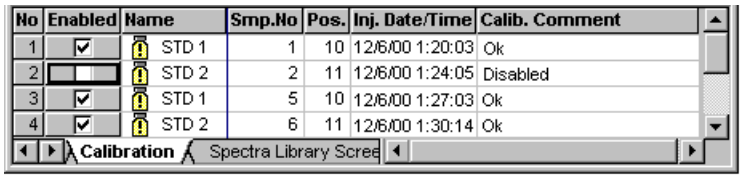
If the user chooses the ⇒***Calibration Mode*** **Bracketed**, each sample is evaluated based on the surrounding standard samples in the sample list.

QNT Method / "Calibration" Sheet

This sheet shows all *standard samples* (of a sequence) that are used for calibrating the current sample.

Via F4 or SHIFT+F4, each sample of a sequence can be opened successively. For each sample, the standard samples used for calibrating will be displayed.

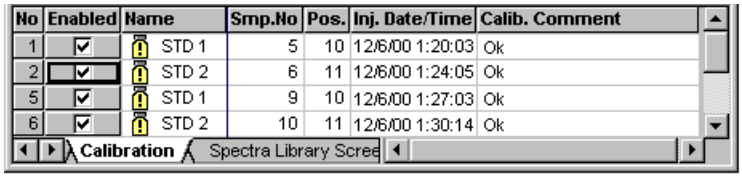
For the samples I and II, the display is as follows:



No	Enabled	Name	Smp.No	Pos.	Inj. Date/Time	Calib. Comment
1	☑	STD 1	1	10	12/6/00 1:20:03	Ok
2	☐	STD 2	2	11	12/6/00 1:24:05	Disabled
3	☑	STD 1	5	10	12/6/00 1:27:03	Ok
4	☑	STD 2	6	11	12/6/00 1:30:14	Ok

Calibration | Spectra Library Scree

For the samples III and IV, the sheet will look as follows:



No	Enabled	Name	Smp.No	Pos.	Inj. Date/Time	Calib. Comment
1	☑	STD 1	5	10	12/6/00 1:20:03	Ok
2	☑	STD 2	6	11	12/6/00 1:24:05	Ok
5	☑	STD 1	9	10	12/6/00 1:27:03	Ok
6	☑	STD 2	10	11	12/6/00 1:30:14	Ok

Calibration | Spectra Library Scree

Note that the standards in line 5 and 6 are determined only once.

b) Analysis Structure:

Injection is eight times. The following area values are determined:

Name	Area substance A
STD 1 (conc.1)	218
STD 2 (conc.2)	439
Sample I	167
Sample II	152
STD 1 (conc.1)	224
STD 2 (conc.2)	442
Sample III	283
Sample IV	305
STD 1 (conc.1)	219
STD 2 (conc.2)	441

c) Calculation of the Calibration Coefficients

From the determined area values of the standard samples and the amount values from the peak table, the value pairs of the six calibration points can be listed. Note that, depending on the standard (STD 1 or STD 2), the amount value is once taken from the peak table column **Amount [1]** and once from the column **Amount[2]**.

No.	Substance	y/x-value pair	y/x	c1 (K1)	c1 (K2)
1	STD 1 (conc.1)	50/218	0.2294	0.2267	
2	STD 2 (conc.2)	100/439	0.2278	0.2267	
5	STD 1 (conc.1)	50/224	0.2232	0.2267	0.2261
6	STD 2 (conc.2)	100/442	0.2262	0.2267	0.2261
9	STD 1 (conc.1)	50/219	0.2283		0.2261
10	STD 2 (conc.2)	100/441	0.2268		0.2261

If all calibration points would be used simultaneously, a two-point calibration with three replicates of the same calibration level would result.

As the amount determination of samples I and II or III and IV is only according to the surrounding standard samples, this means that there are two calibrations for substance A instead of one. Each one is a two-point calibration with two replicates each. Therefore, Dionex Chromatography Management System calculates two different sets of calibration coefficients.

If, as in the previous examples, a linear calibration function without offset is assumed, the Dionex Chromatography Management System determines two different c1-values. One value (K1) is calculated for the numbers 1, 2, 5, and 6, and another value (K2) is calculated for the numbers 5, 6, 9, and 10.

d) Amount Calculation

If the calibration coefficients of a substance A are known, the amount of substance A contained in each sample can be calculated by inserting the peak areas determined from the unknown samples in the calibration function. By inserting this value in the ➢*Formula for Amount Calculation*, the actual amount value will result.

If this is performed for the determined peak areas of substance A in the samples I and II (taking account of K1), the following amount values are calculated (the correction factors of the formula for amount calculation are assumed to be 1.0):

Sample	Calculation	Amount A
I	167 x 0.2267	37.86
II	152 x 0.2267	34.46

For the samples III and IV, there is the following result (taking account of K2):

Sample	Calculation	Amount A
III	283 x 0.2261	63.99
IV	305 x 0.2261	68.96

☞ ***Tip***: Calculation of the amount values is *continuously*, i.e. after analyzing an unknown sample, values are calculated based on the standard samples calculated so far!

Calculation of the area values of samples I and II is performed depending on the current processing status, first with one, then with two, three and finally with four standard samples. The same applies to the samples III and IV that are evaluated based on the standard samples in the lines 5,6,9, and 10 of the sample list.

If, for example, a ➢*Report* is generated after each sample, it will only include the results from the samples analyzed so far. The result may differ from the result. Therefore, the results of a calibration with the **Bracketed** mode should be printed after completing all standard samples.

In the "Bracketed" ⇒*Calibration Mode*, processing of all standard samples should be completed before printing the results.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor**  **Calibration**.

Mode: "Fixed"

Calibration based on the **Fixed** ⇒*Calibration Mode* allows using any desired standard samples of an existing calibration for determining current unknown samples.

Caution: Always perform the calibration manually (**Calibrate**). The **Auto-Recalibrate** option is not available.

a) User Input:

Sample List

Only unknown samples are entered.

If the sample list is generated via the Sequence Wizard, decide whether to refer to an existing QNT file (which is recommended) or whether to leave out this information. When closing the Wizard, the Dionex Chromatography Management System recognizes that the sequence does not contain any standard samples and copies the QNT file with the entire information to the sequence directory. The **Fixed** mode is selected at the same time.

If no QNT file is defined in the Sequence Wizard, its name must be entered in the **Method** column of the sample list after creating one.

QNT Method / "Peak Table" Sheet

If an existing QNT file is copied, a peak table already exists. Change it according to your requirements.

If, however, a new, i.e. empty QNT file is used, a new peak table must also be created. Only entering the ⇒*Amount* value is not necessary, as calibration is based on an existing calibration.

QNT Method / "General" Sheet

If an existing QNT file is copied in which the calibration mode **Fixed** is selected, changing to this mode is automatic.

If a new QNT file was generated, select the **Fixed** mode. Determine the standard samples to be used for calibration on the **Calibration** sheet.

QNT Method / "Calibration" Sheet

If a QNT file was copied, this sheet lists all standard samples to which the QNT-File originally referred.

With each newly created QNT file, no standard samples are listed. Choose the **Insert Standard** or **Append Standard** commands of the context menu to insert the standard samples to be used for calibration and to evaluate the current samples according to their results.

The standard samples listed here always apply to all samples of a sequence. Press F4 or SHIFT+F4 to display the same, maximum number of standard samples.

b) Analysis and Evaluation

Performing the analysis and the evaluation of the individual samples is analogous to the previous examples.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Internal/External Calibration

In a calibration with the internal/external method, the external calibration is corrected by an ➢*Internal Standard* (= ISTD):

The exact quantity of an internal standard is added to each standard sample and each unknown sample so that the internal standard has the same concentration in each vial. The internal standard and the substance to be determined are calibrated via known standard solutions, i.e. the ➢*Calibration Coefficients* are determined from the ⇒*Amount* values of the standard sample and the corresponding peak area values via the ➢*Calibration Function*. Thus, the amounts of all substances (including the ISTD) can be determined. As the concentration of the internal standard is identical in all samples, the same ISTD amount should result.

If this is not the case, an error occurred in the chromatography system (sample preparation, injection, carry-over etc.). The deviation of the actual ISTD amount from the nominal ISTD indicates the extent of the error. It can be assumed that the values of the remaining contents of the sample deviate in the same way, i.e., they are incorrect. A correction by the set/actual deviation of the internal standard supplies the actual values.

Example:

In two patient samples, the concentration of alanine and glycine is to be determined. One standard sample is available. The internal standard norvaline is added to all three sample vials, so that a final concentration of 10 mmol/l is reached. During the subsequent pre-column derivatization, 10 µl sample + 20 µl OPA reagent + 20 µl stop reagent are pipetted together. A constant concentration of 2 mmol/l is added from the norvaline. The chromatographic separation follows the derivatization of the amino acids in OPA derivatives. 10 and 20 µl of the standard solution (➢*Dilution Series*) and 10 µl of each sample (sampler position 2 and 3) are injected.

a) User Input:

Sample List

No.	Name	Type	Pos	Inj. Vol.	Program	Method
1	STD 1	Standard	1	10.0	ALA_GLY	QNT_ALA
2	STD 1	Standard	1	20.0	ALA_GLY	QNT_ALA
3	Sample I	Unknown	2	10.0	ALA_GLY	QNT_ALA
4	Sample II	Unknown	3	10.0	ALA_GLY	QNT_ALA

QNT Method / "Peak Table" Sheet

No.	Peak Name	Ret.Time	Window	Standard	Cal.Type	Amount1	Amount2
1	Alanine	5.400 min	0.400 AG	Int/Ext Norvaline	Lin	50.000000	
2	Glycine	7.800 min	0.400 AG	Int/Ext Norvaline	Lin	50.000000	
3	Norvaline	13.600 min	0.400 AG	STD: Int/Ext	Lin	20.000000	

As the calibration of alanine and glycine is performed with only one (STD 1) standard concentration (same sampler position in the sample list), only one amount value is be entered for each peak.

Proceed as follows to define the **Internal Standard**:

- In the **Norvaline** line, select the Standard column and open the F8 edit box.
- Choose **Use this peak as internal Standard** and thus define norvaline as the Internal Standard.

The correct assignment is indicated by the light yellow background of the line as well as by the **ISTD: Internal** entry.

- In the **Alanine** line change to the **Standard** column and open the F8 edit box again.
- Choose the **Internal/External** option. In the field **Associated ISTD Peak**, select the standard substance serving as **Internal/External Standard** (here: norvaline).
- Repeat this operation for each peak that should be calibrated based on the Internal/External method (here: glycine).

After completing the input, the following occurs: In the **Standard** column, alanine and glycine are labeled **Int/Ext Norvaline**. In addition, norvaline is labeled as the internal standard for an Internal/External calibration. The description **ISTD: Internal** is changed to **ISTD: Int/Ext** and the yellow coloring of the norvaline line is intensified.

Note: After a color changes from light yellow to dark yellow, there are two possible colors more. If the retention time is expressed depending on a selected reference peak (see ⇒*Retention Time*), a light blue background highlights this reference peak. If this reference peak is also used as the internal standard peak, the corresponding line is displayed in green (blue + yellow = green).

QNT Method / "General" Sheet

The mode **Total** is selected. This ensures that the calibration of all samples (Samples I and II) is performed based on *all* standard samples (STD 1).

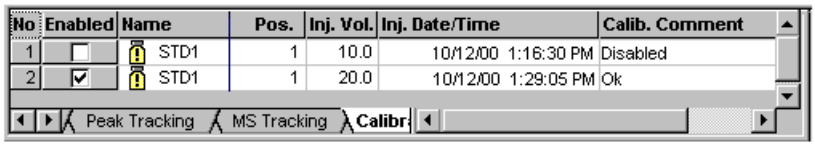
QNT Method / "Calibration" Sheet

The sheet shows all *standard samples* (of a sequence) that are used for calibrating the current sample.

Via F4 or SHIFT+F4, successively open each sample of a sequence. For each sample, the standard samples currently used for calibrating the sample are shown.

Due to the selected mode, samples I and II have the following appearance:

In the **Standard** column, the internal standard is labeled **ISTD Peak: Int/Ext**. All other peaks receive the label **Internal/external Peak ...**. Proceed as follows:



If you discover that an error occurred during the analysis of a standard sample, this standard can be excluded from the above list. This is by disabling the corresponding sample in the **Enabled** column on the **Calibration** sheet in the **QNT Editor**. Only selected samples only are included in the calibration.

b) Analysis Structure:

Injection is four times. During the first run, the first calibration point of the calibration curve is determined, and during the second run, the second point is determined. Run three serves to determine the concentration of alanine and glycine in sample I. Correspondingly, in the fourth run, the concentration of alanine and glycine in sample II are determined.

The data system determines the following area values:

Name	Area Alanine	Area Glycine	Area Norvaline
STD 1 (first run)	55	80	40
STD 1 (second run)	110	160	80
Sample I	45	75	39
Sample II	80	150	41

The determined area values of the internal standard norvaline reflect (except for minor inaccuracies) the ratio of the injected volumes (amounts).

c) Calculation of Missing Amount Values

The second calibration point is determined by injecting different volumes of the same standard sample. The data system calculates the missing amount value directly via the following formula:

$$Amount = Am._{(Peak-Tab.)} * \frac{Inj.Vol._{unknown\,Amount}}{Inj.Vol._{known\,Amount}} * \frac{Smp.\,Wght}{Dil.\,Factor}$$

With the ⇒*Dil. Factor* (dilution factor) and the ⇒*Weight* (sample weight) = 1, the result is as follows:

Peak Name	Calculation	Amount [2]
Alanine	50 x (20/10) =	100
Glycine	50 x (20/10) =	100
Norvaline	20 x (20/10) =	40

d) Calibration Points

From the known (Amount 1) or calculated (Amount 2) amount values and the determined area values of the standard samples, the value pairs of the individual calibration points can be established:

Substance	Area value	Amount value [1]	Amount value [2]
Alanine	45	50	
Alanine	90		100
Glycine	80	50	
Glycine	160		100
Norvaline	40	20	
Norvaline	80		40

The data system determines all calibration coefficients, depending on the selected calibration function.

e) Calculation of the Calibration Coefficients

A linear calibration curve through the zero point (calibration type **Linear**) can already be described by one calibration coefficient (c1). If the example is chosen so that the calibration point in each calibration curve are located exactly on a straight line (e.g. in an exact measurement), c1 results as the y/x-quotient of each value pair (= slope of the calibration curve).

Substance	y/x-Value pair	c1
Alanine	50/45	1.111
Alanine	100/90	1.111
Glycine	50/80	0.625
Glycine	100/160	0.625
Norvaline	20/40	0.500
Norvaline	40/80	0.500

If the calibration points are not located exactly on one line, the data system calculates an optimized c1 approximate value for each substance. If a different calibration type were selected, the data system would also calculate the remaining calibration coefficients (c0 and c2) according to the calibration function.

f) Amount Calculation: Internal Standard in the Unknown Samples

If the area values of the internal standards from samples I and II are known, the amount of the internal standard (norvaline) can be determined in the two samples via the calibration coefficient c1 (here = 0.5) established for the calibration curve of the norvaline.

Sample	Calculation	Amount (ISTD)
I	39 x 0.5	19.50
II	41 x 0.5	20.50

The ratio between the (nominal) amount value entered in the peak table and the ⇒*ISTD Amount (Amount of the Internal Standard)* of the internal standard in the corresponding sample is referred to as ISTD factor.

$$ISTD - Factor = \frac{Amount_{ISTD(Peak-Tab.)}}{Amount_{ISTD(Sample)}}$$

The following values are resulting:

Sample	Calculation	ISTD Factor
I	20 / 19.5 =	1.026
II	20 / 20.5 =	0.976

The result states that an error was made by 1.026 (sample 1) or 0.976 (sample 1). As the actual amounts of alanine and glycine deviate (in all probability) by 2.6 / 2.4% from the "real" values. They are corrected by this amount as follows.

g) Amount Calculation: Alanine and Glycine

Calculation of the amount values of glycine and alanine is via the ➢*Formula for Amount Calculation*. In contrast to an external calibration, the term **ISTD Factor** is now unequal 0, i.e., the results are corrected by the calculated ISTD factor.

Sample	Calculation (Area x c1 x ISTD Fact. =)	Amount
I	45 x 1.111 x 1.026 =	51.30 (Alanine)
I	90 x 0.625 x 1.026 =	54.90 (Glycine)
II	80 x 1.111 x 0.976 =	86.75 (Alanine)
II	160 x 0.625 x 0.976 =	97.60 (Glycine)

The alanine or glycine amount values corrected by the norvaline deviation are resulting.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Internal Calibration

In the pure internal standard method, calibrating is via the ➢*Internal Standard*, only. Calculation is with area and amount ratios instead of absolute areas and amounts. In the ➢*Formula for Amount Calculation*

$$Amount_p = a_p(x_p) * \mathrm{Re}sp.Fact._p * ISTD - Fact. * \frac{Dil.\ Fact_n.}{Smp.Wght_n}$$

the ratio of the peak area to the peak area of the Internal standard (**x**(p rel.)) is used instead of the peak area (xp) for this purpose.

$$x_{(prel)} = \frac{Area_p}{Area_{ISTD}} \qquad Amount_{(p,rel)} = \frac{Amount_p}{Amount_{ISTD}}$$

Instead of an ⇒*Amount* (Amount p), the result is the ratio to the internal standard (Amount p rel).

$$\frac{Amount_{Peak}}{Amount_{ISTD}} = Am._{p.rel} = a_p * \frac{Area_{Peak}}{Area_{ISTD}} * Resp.Fact._p * \frac{Dil.Fact._n}{Smp.Wght._n}$$

If the result is multiplied with the amount of the internal standard, the amounts of the sample substances to be determined are resulting.

Example

In a clinic lab, prepared urine samples of two patients are examined for the catechol level. Adrenaline and dopamine are to be determined. Two standard solutions of different concentrations are available (STD 1: 50 ng/µl each; STD 2: 100 ng/µl adrenaline/dopamine each). To check the precise dosing of the sampler, catechol is added. The internal standard method is selected. 20 µl of each sample and each sample is mixed with 20 µl of the catechol solution. As the concentration of the added catechol solution is 10ng per µl, each vial (40 µl) contains 10 x 20 = 200 ng catechol. This means that exactly 200/4 = 50 ng catechol is injected with each 10 µl injection.

a) User Input

Sample List

No.	Name	Type	Pos	Inj. Vol.	Program	Method
1	STD 1	Standard	1	10.0	ADR_DOPA	QNT_DOPA
2	STD 2	Standard	2	20.0	ADR_DOPA	QNT_DOPA
3	Sample I	Unknown	3	10.0	ADR_DOPA	QNT_DOPA
4	Sample II	Unknown	4	10.0	ADR_DOPA	QNT_DOPA

In contrast to the examples in the external and internal/external calibration, the second calibration point is not determined via the modified injection volume but via a second standard sample with the double concentration. As a result, two different sampler positions are used (1 and 2).

QNT Method / "Peak Table" Sheet

No.	Peak Name	Ret.Time	Window	Standard	Cal.Type	Amount1	Amount2
1	Adrenaline	3.400 min	0.400 AG	Internal Catechol	Lin	50.000000	100.000000
2	Dopamine	5.500 min	0.400 AG	Internal Catechol	Lin	50.000000	100.000000
3	Catechol	9.600 min	0.400 AG	ISTD: Internal	Lin	50.000000	50.000000

As the calibration of adrenaline and dopamine is performed with two standard concentrations (STD 1, STD 2, different autosampler position in the sample list), two amount values are entered for each peak.

Then, the **Internal Standard** is labeled. Proceed as follows:

- Select the **Standard** column in the **Catechol** line and open the F8 edit box.
- Choose **Use this peak as internal Standard** and thus define catechol as Internal Standard.

The yellow coloring of the line and the **ISTD: Internal** entry indicate the correct assignment.

- Change to the **Standard** column in the **Adrenaline** line and open the F8 edit box again.
- Choose the **Internal** option and select the standard substance serving as Internal Standard (here catechol) in the field **Associated ISTD Peak**.
- Perform this operation for each peak that should be calibrated with the **Internal** method (here dopamine).

After completing the input, the following occurs: In the **Standard** column, alanine, and dopamine are labeled **Internal Catechol**. In addition, catechol is indicated as the internal standard by a darker shade of yellow.

Note: After the color changes from light yellow to dark yellow, two more colors are possible. If the retention time is expressed depending on a selected reference peak (see ⇒*Retention Time*), a light blue background highlights this reference peak. If this reference peak is also used as the internal standard peak, the corresponding line is displayed in green (blue + yellow = green).

QNT Method / "General" Sheet

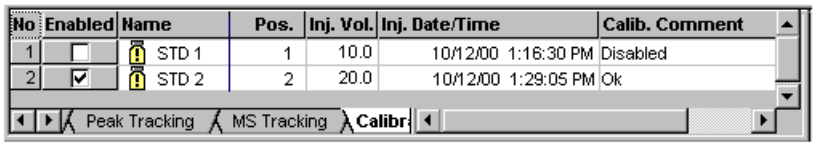
The mode **Total** is selected. This ensures that the calibration of all samples (Sample I and II) is performed based on *all* standard samples (STD 1, STD 2).

QNT Method / "Calibration" Sheet

This sheet shows all *standard samples* (of a sequence) that are inserted for calibrating the current sample.

Via F4 or SHIFT+F4, each sample of a sequence can be opened successively. For each sample, the current standard samples for calibrating the sample are indicated.

Due to the selected mode, sample I and II appear as follows:



If you discover that an error occurred during the analysis of the standard sample, this standard can be excluded from the above list. This is by disabling the corresponding sample in the **Enabled** column on the **Calibration** sheet in the **QNT Editor**. Only selected samples are included in the calibration.

b) Analysis Structure

Injection is four times. During the first run, the first calibration point of the adrenaline and dopamine calibration curve is determined via STD 1, and

during the second run the second point is determined accordingly via STD 2. Run three serves to determine the concentration of adrenaline and dopamine in sample I. Correspondingly, in the fourth run, the concentrations of adrenaline and dopamine in sample II are determined. In addition, the area of the added catechol is determined in each run.

The data system determines the following area values:

Name	Area Adrenaline	Area Dopamine	Area Catechol
STD 1	125	200	250
STD 2	250	400	250
Sample I	223	150	245
Sample II	178	380	255

The area values determined for catechol reflect the ratio of the injected volume or amounts (except for minor inaccuracies).

c) Calculation of (Amount p, rel). and x (p, rel)

The Area (Peak) to Area (ISTD) ratio results in x (p, rel):

$$x_{(prel)} = \frac{Area_p}{Area_{ISTD}}$$

Substance	Area	Area (ISTD)	x (p, rel)
Adrenaline (STD 1)	125	250	0.5
Adrenaline (STD 2)	250	250	1.0
Dopamine (STD 1)	200	50	0.8
Dopamine (STD 2)	400		1.6

The Amount (Peak) to Amount (ISTD) ratio results in (Amount p, rel).

$$Amount_{(p,rel)} = \frac{Amount_{Peak}}{Amount_{ISTD}}$$

Substance	Amount	Amount (ISTD)	Amount (p, rel)
Adrenaline (STD 1)	50	50	1.0
Adrenaline (STD 2)	100	50	2.0
Dopamine (STD 1)	50	50	1.0
Dopamine (STD 2)	100	50	2.0

d) Calculation of the Calibration Coefficients

A linear calibration curve through the zero point (calibration type **Linear**) can already be described by one calibration coefficient (c1). If the example is chosen so that the calibration point in each calibration curve are located exactly on a straight line (e.g. in an exact measurement), c1 results as the y/x-quotient of each value pair **Amount p rel** to **x p rel**:

Substance	Amount (p rel) / x (p rel)	c1
Adrenaline	1.0/0.5	2.000
Adrenaline	2.0/1.0	2.000
Dopamine	1.0/0.8	1.250
Dopamine	2.0/1.6	1.250

If the calibration points are not located exactly on one line, the data system calculates an optimized c1 approximate value for each substance.

If a different calibration type is selected, the data system calculates the corresponding calibration coefficients (c0, c1, and c2).

e) Amount Calculation

Via the ➢*Formula for Amount Calculation*, the relative amount (=relative to the amount of the ISTD) of the sample contents adrenaline and dopamine can be calculated from the known c1 and from the ratio peak area (sample) to peak area (ISTD). If the correction factors ⇒*Dil. Factor* (dilution factor) and ⇒*Weight* (sample weight) are assumed to be 1, the following Amount / Amount ISTD values result:

Sample I	Calculation: Amount /Amount ISTD
Adrenaline	2.000 x (223/245) = 1.820
Dopamine	1.250 x (150/245) = 0.765

Sample II	Calculation: Amount /Amount ISTD
Adrenaline	2.000 x (178/255) = 1.396
Dopamine	1.250 x (380/255) = 1.863

By multiplication with the amount values of the internal standard, the actual amount values for adrenaline and dopamine in the analysis samples can be calculated.

Sample I	Calculation: Amount
Adrenaline	1.820 x 50 = **91.00** [ng]
Dopamine	0.765 x 50 = **38.25** [ng]

Sample II	Calculation: Amount
Adrenaline	1.396 x 50 = **69.80** [ng]
Dopamine	1.863 x 50 = **93.15** [ng]

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to...: Actions in the QNT Editor** **Calibration**.

Calibration with Variable Internal or Internal/External Standard

The method itself or the properties of the ➢*Internal Standard* make it sometimes impossible to add exactly the same amount of the ISTD. To solve this problem, the Dionex Chromatography Management System offers the **use sample amount as reference (Variable)** option (see F8 box of the **Standard** column in the peak table).

In this case (**Internal/External** or **Internal**), the amount of the internal standard is not entered in the ⇒*Amount* column of the peak table (not possible at this point), but in the **ISTD Amount** column of the sample list. For each sample, it is thus possible to enter the amount of internal standard separately.

a) User Input

Sample List

No.	Name	Type	Pos	Inj. Vol.	Program	Method	Amount
1	STD 1	Standard	1	20.0	ADR_DOPA	QNT_D	49.5000
2	STD 2	Standard	2	20.0	ADR_DOPA	QNT_D	51.3000
3	Sample I	Unknown	3	20.0	ADR_DOPA	QNT_D	48.8000
4	Sample II	Unknown	4	20.0	ADR_DOPA	QNT_D	50.3000

The amount of internal standard is now entered directly in the **Amount** column of the sample list.

QNT Method / "Peak Table" Sheet

No.	Peak Name	Ret.Time	Window	Standard	Cal.Type	Amount1	Amount2
1	Adrenaline	3.400 min	0.400 AG	Internal Catechol	Lin	50.000000	100.000000
2	Dopamine	5.500 min	0.400 AG	Internal Catechol	Lin	50.000000	100.000000
3	Catechol	9.600 min	0.400 AG	ISTD: Internal	Lin	1.000000	1.000000

Except the substance serving as internal standard, all amount values are entered as before. Then, the **Internal Standard** is selected as follows:

- In the **Catechol**" line, select the **Standard** column and open the F8 edit box.
- Choose **Use this peak as internal standard** and thus mark Catechol as the internal standard.
- Select **Use sample amount as reference (Variable Internal Standard)** to use a variable internal standard.

The correct assignment is indicated by the yellow coloring of the line and by the entry **ISTD: Var. Internal**. The corresponding **Amount** column fields are set to 1.

All other QNT file entries are performed as before.

b) Evaluation

Evaluation is analogous to the corresponding evaluation without variable internal standard. However, slightly different calibration and evaluation formulas are used.

For a detailed description of the differences between standard methods, see **Evaluation with Various Standard Methods** in the **Calibration** section.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to...: Actions in the QNT Editor Calibration**.

Entering the Concentration/Amount of the Validation Sample

➢*Validation Samples* are used to check the calibration. They correspond to standard samples in as much as the amount of analyte is known. However, they are not used to determine the calibration curve but only to validate the calibration.

The known concentration (or amounts) of the different analytes in the validation samples is entered in the QNT editor. Please note the following difference:

1. Validation Sample = Standard Sample

All individual concentrations/amounts corresponds to the concentrations/amounts of a standard sample that has already been used for the calibration curve, especially if the validation sample is injected from a vial containing standard sample.

In this case, an ⇒*Amount* column for the corresponding standard sample is already available in the QNT editor. If you wish to use this column for a validation sample, proceed as follows:

- On the **Amount Table** tab, place the cursor in the **Amount** column of the corresponding standard sample.
- Select the **Columns** option in the context menu (right mouse click) and **Amount Column Properties...** to open the **Amount Column Properties** dialog box.

- Press **Add Standard(s)...** to open the **Select Sample(s)** dialog box.
- Select **Validation samples** to list the available validation samples in the right window. Select the desired validation sample(s) from the list.
- Press **Ok** to accept the selection and press Ok once again in the **Amount Column Properties** dialog box.

All amount values of the respective standard sample now also apply to the validation sample(s).

2. Validation Sample ≠ Standard Sample

Using a validation sample whose composition is different from all standard samples (if only in its concentration of amount of one analyte) requires a separate **Amount** column for this validation sample. Proceed as follows:

- In the QNT editor, go to the **Amount Table** tab.
- Select the **Columns** option in the context menu. Select **New Amount Column...** to open the **Add Amount Column** dialog and proceed as described under **Validation Sample = Standard Sample** above.

In this way, a separate column was created for your validation sample. If this column shall be valid for other validation samples or for standard samples, proceed as described under **Validation Sample = Standard Sample**.

For information on how to use the validation sample for checking the calibration curve, see **Validating the Calibration Curve**.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Validating the Calibration Curve

If you wish to check the calibration using the respective values of the ➢*Validation Samples* (perhaps of the standard sample as well) you have to compare the expected concentration or amount values to the measured/calculated values either numerically by means of the Amount Deviation report variable or visually by means of the calibration function.

1. Numerically, by means of the Amount Deviation report variable:

The determined (actual) area values are converted to concentration or amount values by means of the ➢*Calibration Function* and compared to the expected (nominal) values of the ⇒*Amount* table.

- Add a new column to a report or a ➢*Printer Layout* page or change the assignment of an existing column as described under **How to ...: Actions in the Report**  **Defining the Contents of a Report**.
- Select the **Amount Deviation** variable in the ⇒*Peak Results* report category. Use the **Parameter** button to define whether the result of the variance comparison shall be expressed as absolute amount value or as deviation in percent (**Relative in % of the expected Amount**).

2. Visually, by means of the Calibration Curve

For checking the calibration curve visually, the validation samples can be displayed (specially marked) in the curve:

- Select the **Decoration** command in the context menu of the calibration curve (the **Properties Calibration Plot** command in the Printer Layout, respectively).
- Select the **Draw validation sample points** checkbox on the **Options** tab.

 ***Note**:* Even if this action is performed in the QNT editor these validation samples will not be considered for the calibration. If, nevertheless, you wish to use a validation sample as standard sample later and consider it for calculating the calibration curve, set its ⇒*Type* (Sample Type) to **Standard** in the sample list of the Browser.

In addition, the confidence region can be made visible in the calibration curve. Selecting the **Draw upper and lower confidence limit** checkbox on the **Options** tab and defining the desired confidence region allows you to check whether your validation and standard samples are within the corresponding confidence interval.

For information on how to enter the concentration/amount, see **How to ...: Actions in the QNT Editor Entering the Concentration/Amount of the Validation Sample**.

For an overview on the different calibration possibilities offered by your Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Calibration**.

Spectra Library Screening

The **Spectra Library Screening** sheet of the **QNT Editor** allows you to search spectra libraries for reference spectra. The spectra search is also possible from the spectra plot, as described in **How to ...: Actions in the UV Spectra and Mass Spectra Starting a UV Spectra Search**.

For further information, see the following topics:

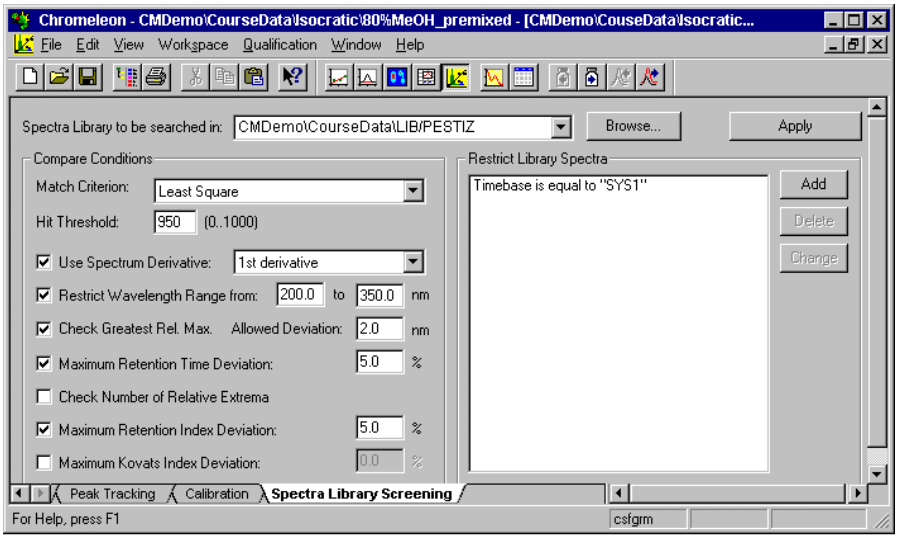
Entering Criteria for the Spectra Library Screening

Starting Library Screening and Viewing Results

Integrating Screening Results in Reports and Peak Labels

Entering Criteria for the Spectra Library Screening

Enter the criteria for a spectra library search on the **Spectra Library Screening** (= **SLS**) sheet of the QNT editor:



- Select a spectra library (LIB file) from the field **Spectra Library to be searched in ...**. If the required LIB file is not included, press the **Browse** button to search for the file.
- In the **Match Criterion** field, select the method (see ⇒*Match Criterion*) used for comparing the original spectrum and the library. The best search results are usually received via the setting **Least Square**.
- In the **Hit Threshold** field, enter a ➢*Match Factor* between 0 and 1000, e.g. 950. Only spectra with a match value above 950 will be shown. Spectra with less similarity will not be included. Unless derivatives of spectra are compared with each other, reference spectra with a match value below 900 are usually spectra of other substances. Exceptions to this rule are only acceptable, if the signal to noise ratio is low.

Note: To be able to compare UV spectra, the spectrum and the reference spectrum should be recorded under identical conditions. For best results, create your own library of spectra you recorded yourself.

Additional conditions are possible to perform a more exact search:

Usually, the **Use Spectrum Derivative** option is deactivated, i.e. the comparison of spectra is based on their actual curve. If the **1st derivative** option is selected, the comparison of two spectra is based on the first derivative. As a result, the curve characteristics increase (shoulders become extrema), allowing a more exact comparison of extrema. However, the signal to noise ratio will considerably decrease; and sections with lower signals will be less significant.

Restrict Wavelength Range allows you to limit the spectra comparison to the relevant spectral range.

Select **Check Greatest Rel. Max.** to use only spectra with the greatest relative maximum at the same position. Select **Allowed Deviation** to specify a tolerance range. The range should not exceed 10 nm, otherwise the criterion will lose significance.

Click the field **Maximum Retention Time Deviation** to determine the maximum retention time deviation of the reference spectrum in percent. This prevents including substances with very similar spectra that are eluted at different retention times.

If you select **Check Number of Relative Extrema**, the Dionex Chromatography Management System checks the number of relative extrema of the reference spectrum. This option allows excluding spectra that are very similar but show an additional maximum.

Select **Maximum Retention Index Deviation:** or **Maximum Kovats Index Deviation:** to include only those spectra in the comparison for which the retention index or, respectively, the ⇒*Kovats Index* is identical with the index of the sample substance. The respective tolerances are defined in the right field.

⚠ ***Caution***: If noise is very strong, noise peaks can be considered extrema. In this case, it is recommended to deactivate **Check Number of Relative Extrema**.

On the right side of the window, you can further restrict the resulting library spectra. Open the dialog box **Restrict Library Search** with **Add**. Via **Field Name**, you can then select type of parameter to be determined from the following search criteria:

Solvent Composition	**Detector Serial Number**
Control Program	**Timebase**
Substance Name	**Sequence Name**
Unique ID	**Sample Name**
Comment	**Extract Operator**
Detector Name	

These items can be linked (partly) via the following operators (**Conditions**) with a freely selectable value:

Operator	Restricts the search to spectra with parameters that
is equal to:	fulfill the specified condition.
starts with:	start with the entered string.
does not start with:	do not start with the entered string.
ends with:	end with the entered string.
does not end with:	do not end with the entered string.
contains:	contain the entered string.
does not contain:	do not contain the entered string.

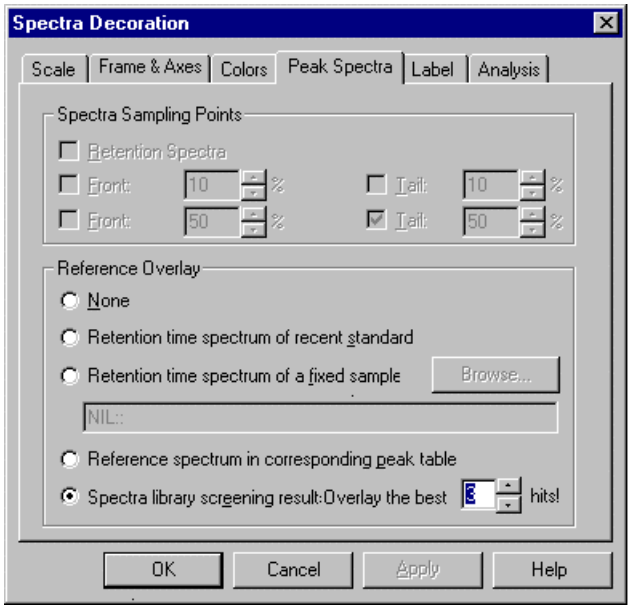
Note: If you want to search all libraries in a directory, simply enter the character ***** as the file name. The wildcard characters (known from MSDOS) ***** and **?** are valid. Example: LIB::\CMDATA\LIB\D* searches all libraries starting with the letter **D** in the directory **LIB** of the datasource CMDATA.

Starting Library Screening and Viewing the Results

Press the **Apply** button to use the entered search parameters. This command starts the library search for each peak in the current chromatogram.

The spectra plot is displayed in addition to the chromatogram. The reference spectrum (hit) with the corresponding match criterion will be shown. The displayed spectrum is the reference spectrum of the selected peak. You can view the search results for the other substances by clicking the corresponding peaks in the chromatogram.

If more than one library spectrum fulfills the entered criteria, you can view the other hits. Place the cursor on the spectrum, open the context menu, and open the **Spectra Decoration** sheet. The **Peak Spectra** tab allows you to enter the number of reference spectra to overlay:



In this example, you will receive a list of three reference spectra. The first spectrum has the highest match value and thus the greatest similarity to the original spectrum.

Inserting Screening Results in Reports and Peak Labels

If you save the search parameters in the QNT file, the results of the **Spectra Library Screening** can be used for the peak label or in report tables or templates (➢*Printer Layout*).

Inserting Screening Results in ➢*Report Definition Files*

To view the screening results in the report, the report category **Peak Purity** offers the following variables:

Number of SLS Hits calculates the number of library screening hits for a peak.

SLS Hit opens the ⇒*Hit Spectrum* report category that includes all variables of the corresponding library spectrum:

Designation	Description
Substance Name	
Match Factor	➢*Match Factor*
Library Name	Name of the spectra library
Library Record	Opens the ⇒*Spectra Library* category
Number of rel. Extrema	
Solvents	
Comment	➢*Comment*
Sequence Name	
Sequence Header Record	
Sample Name	
Sample Record	Branches to the ⇒*Sample* category
Acquisition Time	Acquisition date and time
Timebase	➢*Timebase*
Program	➢*PGM File*
Sample Rate	
Retention Time	⇒*Retention Time*
Lambda Min.	Minimum wavelength
Lambda Max.	Maximum wavelength
Lambda Range	Wavelength range
Lambda Resolution	Spectral wavelength resolution
Detector Name	
Detector Serial Nr.	
Extract Time	Time when the sample was added to the library
Extract Operator	User who added the sample to the library
Retention Index	Linear ⇒*Retention Index*
Kovats Index	⇒*Kovats Index*

The **Formula** field shows a short version of your selection, e.g. **peak.hitSpec(1).name** for the spectra name of the best hit. The digit indicates the hit: 1 is the best, 2 is the second best hit, etc.

Including Screening Results in the Peak Label

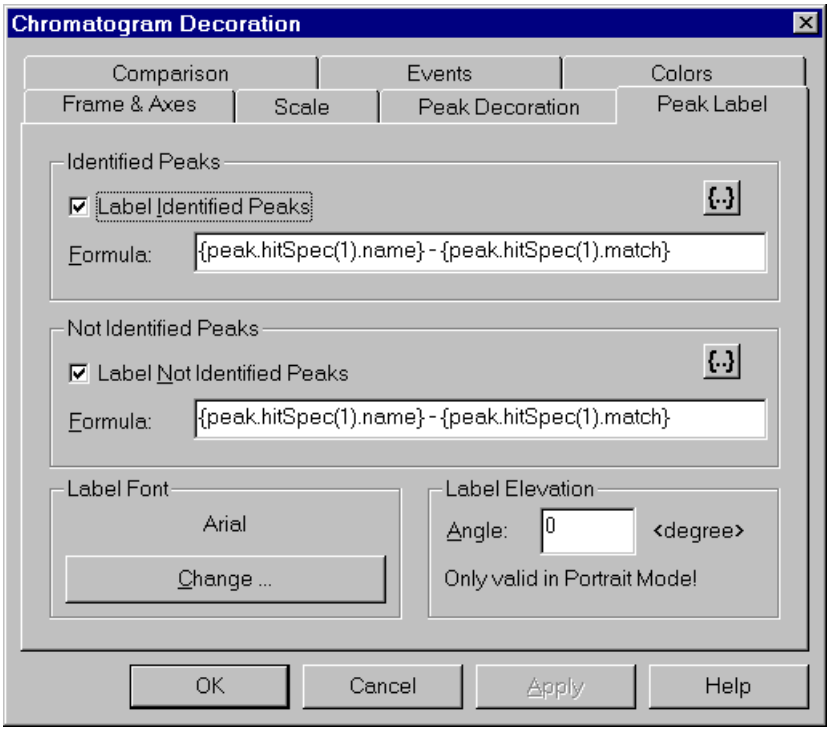
To include the screening results in the chromatogram, perform the following steps:

- Position the cursor in the chromatogram.
- Select **Chromatogram Decoration** from the context menu.
- On the **Peak Label** tab of the **Chromatogram Decoration** dialog box, press **{...}** to reach the **Insert Variable into Peak Label Formula** dialog box. From the category **Peak Purity**, you can choose the **Number of SLS Hits** and **SLS Hit** variables (see **Report** above).

Example

To label each peak in the chromatogram with the name of the best hit and the corresponding match factor, perform the following steps:

- From the category **Peak Purity**, choose **Substance Name** under **SLS Hit**.
- In the **Formula** field, enter " - " after the formula, then click **Match Factor** under **SLS Hit**.
- Press **OK**. You will receive the following "**Formula** input on the **Peak Label** sheet of the **Chromatogram Decoration** dialog box:



☞ ***Tip***: If you have saved the search parameters in the QNT file, it is sufficient to activate **Spectra library screening results**, e.g. in the spectra plot. Just open the context menu and select the option via **Spectra Decoration** and **Peak Spectra**. In this case, you do not need to open the **Spectra Library Screening** dialog and press **Apply**.

Defining the System Suitability Test

The **SST** tab (see ➢*System Suitability Test (SST)*) of the ⇒*QNT Editor* allows you to check your system's performance for individual samples. Any number of tests (limited only by the capacity of your computer) is possible. Each single test is given in an individual line. Use the arrow key ↓ to append additional lines to the bottom line. This action automatically opens the SST Wizard that guides you through the process of entering the SST conditions.

***Tip*:** If you want to perform a System Suitability Test, ensure to enter the QNT file into the sample list before starting the analysis. Otherwise, the ➢*Batch* cannot be aborted in case of **Fail Action - Abort Batch** because the SST will not yet be performed during the batch run!

For further information, see

Inserting a New SST: SST Wizard

Modifying the System Suitability Test

Inserting SST Results in the Printer Layout

Inserting a New SST: SST Wizard

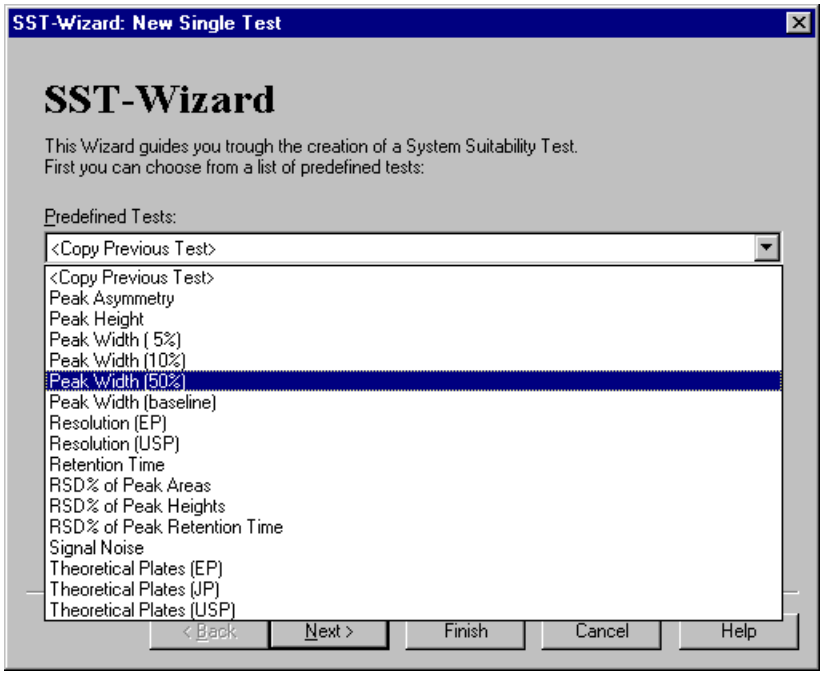
The SST Wizard supports you in inserting a new ➢*System Suitability Test (SST)*. Double-click a cell or press F8 to open the SST Wizard. The Wizard opens automatically via the **Append Line** and **Insert Line** commands of the context menu or via the ↓ key (note: to open the SST Wizard via the ↓ key, the cursor must be placed in the bottom line).

The SST Wizard includes the following pages:

- **Start**
- **Sample Condition**
- **Test Condition**
- **Aggregated (optional)**
- **Peak & Channel Condition (optional)**
- **N.A. & Fail Action**

Start

On the **Start** page, you can choose from a list of predefined tests:



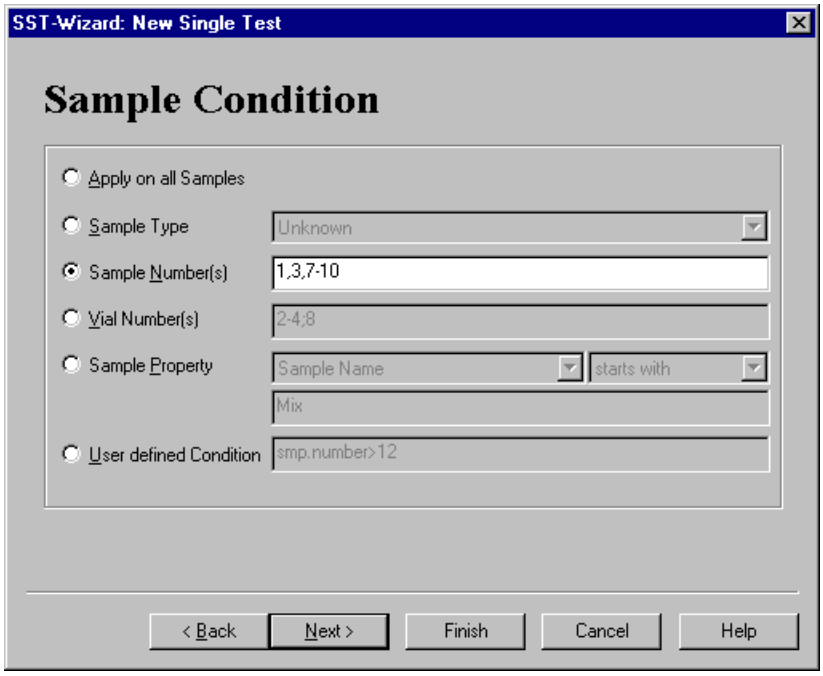
All predefined values on the following pages depend on the selection made here.

The special entry **<Copy Previous Test>** copies the previous test. If the test is the first within a list (i.e., there is no previous test), the test that was previously at this position will be copied.

As no other conditions are required, the Wizard can be terminated here. Pressing **Next** proceeds you to the following Wizard pages where you can check and, if necessary, modify the predefined conditions.

Sample Condition

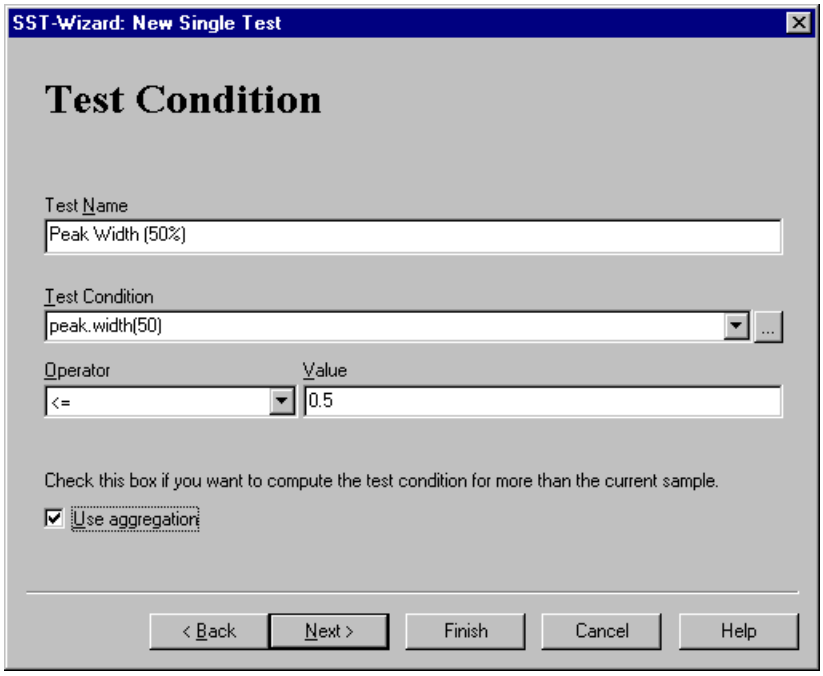
Here you can modify the sample conditions. There are five possible choices:



Apply on all Samples performs the test for each sample. Select **Sample Type** to perform the test for a certain sample type only. Under **Sample/Vail Number(s)** define the sample numbers for which to perform the test (e.g. 5,17;4-6;13,11). With **Sample Property** being selected, the test is performed for samples with the specified property only. The property is entered below. The **User defined condition** option is for advanced users and allows you to enter any kind of formula in the report format. The test is then performed for samples only for which this condition is true.

Test Condition

This Wizard page allows you to enter the basic conditions for the SST:



First, enter a unique name under **Test Name** before specifying the **Test Condition**. Use the Browse button "**...**" to select the desired variable in the report variable dialog. Via the **Compare Operator**, the selected variable is then compared with the **Compare Value**. The **Compare Value** can either be a value or a report variable / formula. Check the **Use aggregation** box to aggregate the test conditions over several samples and to open the **Aggregate** page.

Aggregate

This page of the SST Wizard serves to define the function, sample(s), and condition for sample aggregation. (For further details, see *Aggregate* in the Online Help).

Peak & Channel

This page is optional and opens only if the test condition requires a peak or channel to be entered. (For further details, see *Peak & Channel* in the Online Help).

N.A. & Fail Action

Define the test result if the test condition cannot be checked (**N.A.**) and decide whether the server shall abort the batch if the test condition is not fulfilled (**Fail Action**).

Modifying the System Suitability Test

Double-click a cell or press F8 to modify an existing ➢*System Suitability Test (SST)*. The following tabs are available in the opening **SST Properties** dialog:

- **Sample Condition**
- **Test Condition**
- **Aggregate**
- **Peak & Channel Condition**
- **N.A. & Fail Action**

The tabs correspond to the individual SST Wizard pages. For further details, see **How to ...: Actions in the QNT Editor Inserting a New SST: SST Wizard**

Inserting SST Results in the Printer Layout

If you save the SST parameters in the QNT file, the results of the ➢*System Suitability Test (SST)* can be used for the peak labels or as individual variables in the ➢*Printer Layout* (not in tables).

In the Printer Layout:

The **Report** category **System Suitability Test** allows you to view the SST results in the printer layout. The following variables are available:

Variable	Description
Number	Number of the SST
Name	Name of the SST
Sample Condition	Sample Condition for the SST
Test Condition	
Aggregate	Aggregate function
Operator	
Value	
Channel	
Peak	
N.A.	User-defined test result if checking of the condition is not possible
Fail Action	
Aggregated Samples	
Sample Condition Results	
Test Results	
Aggregated Sample List	
Aggregated Sample Result List	
Result of Test Condition or Aggregate	
Result of Compare Value	

The **Formula** field indicates your selection in short, e.g., **sst.test_condition** for the test condition.

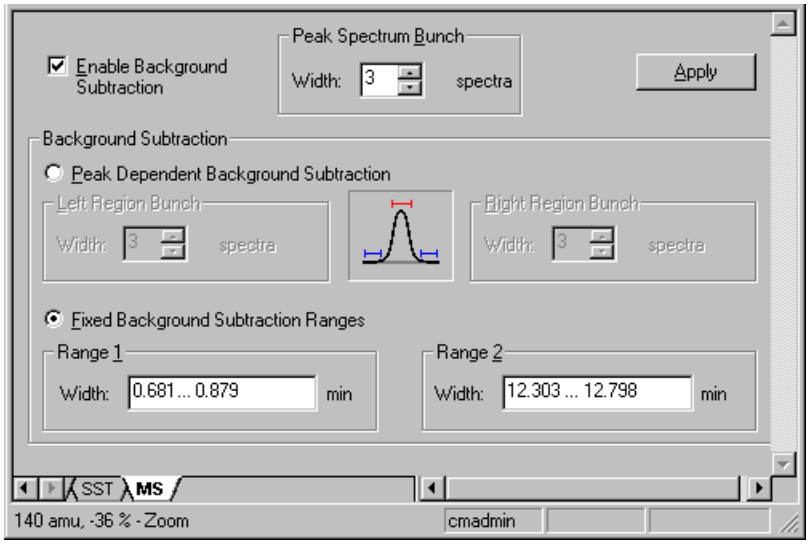
Processing Mass Spectra

➢*Mass Spectra* have a relatively high noise level. Therefore, they must be processed before being used further. The Dionex Chromatography Management System uses the following algorithm:

- First, the spectrum of the peak maximum is determined by averaging several spectra on both ends.
- Then, the background spectra of both peak ends are determined. Averaging several spectra also does this.

- The background peak spectrum (normally at the peak maximum) is then determined via linear interpolation of these two background spectra and is finally subtracted from the single spectrum (normally of the peak maximum).

The **MS** tab of the ⇒*QNT Editor* allows you to specify how to form mass spectra from individual spectra. Check the **Enabled** box to activate spectrum enhancement:



Under **Peak Spectrum Bunch**, indicate the number of single spectra that shall be aggregated to the spectrum at the peak maximum. It is possible to average max. 99 single spectra. For symmetry reasons, odd numbers can be entered only.

Activate **Peak Dependent Background Subtraction** to allow automatic background subtraction for each peak individually.

Use the **Left/Right Region Bunch** fields to select up to 99 single spectra each for forming the two background spectra. Zero and even numbers are permitted as well.

The **Fixed Background Subtraction Ranges** option allows defining two fixed ranges for the entire chromatogram that are then used for background subtraction. Usually it makes sense to set one range at the beginning and the other one at the end of the chromatogram.

Press **Apply** to accept the settings and calculate the resulting mass spectrum. With enabled view, the newly calculated mass spectrum will be displayed at once.

Note: Defining the background subtraction manually in the chromatogram affects the settings on the **MS** tab. Setting **Background Subtraction** e.g. to **Fixed Background Ranges** in the context menu of the chromatogram activates the corresponding option on the MS tab of the QNT editor.

Actions in the Calibration Curve

The **Calibration Curve** window displays the ➢*Calibration Curve* calculated from the ➢*Calibration Points*. The **Calibration** tab of the **Report** allows you to view the calibration data of the peaks of the current chromatogram.

If, in the **Calibration** settings in the **QNT Editor**, a single standard was excluded from the calculations (**Enabled** column), the corresponding calibration point is red. Calibration points of this type will not be used for calculating the calibration curve for which they were disabled. The display color of the calibration points of the current sample is purple.

In the **Calibration Curve**, the **Disable Standard** command of the context menu allows you to exclude standards, completely or in part, from the calibration. The **Disable (Enable) Standard xyz** dialog box opens for the selected calibration point. (This point refers to the selected peak in the current chromatogram. Double-clicking a different calibration point allows you to select a different standard.) Define whether the corresponding standard sample shall be used for calibration purposes. You can exclude the respective standard from the calibration for all peaks and all channels (default) or for the selected peak and/or channel only. (Also, see **How to ...: Actions in the QNT Editor**  **Disabling Standard Samples**).

In addition, the following options are available:

- From the context menu, choose **Next Peak / Prev.Peak** to view the calibration curve of the next/previous peak.
- Choose **Decoration** to change the caption, color, and axes.

Actions in the Printer Layout

The Printer Layout allows preparing your data for the printout. It is part of the ⇒*Report Definition File* (= RDF). To assist you in preparing the first printout and in creating your own report definition files (also called report templates in the following), the Dionex Chromatography Management System offers some default RDF templates.

To printout further data that is not included in the default report definition files, the Dionex Chromatography Management System offers the possibility to create individual worksheets via the ➢*Printer Layout* window. These worksheets can be combined and saved as a report template. The results of sample processing can thus be printed in a number of layouts.

For further information, see the topics below:

Creating a Worksheet

Inserting a Chromatogram

Inserting a Table

Inserting Individual Variables

Inserting Text

Saving/Loading a Report Template

Specifying the Printout

Printing the Results of a Single Sample

Printing the Results of a Sequence / Sample Batch

Setting Print Area / Print Title(s)

Saving the Contents of a Report Template

Users who have the ➢*Report Publisher* add-on product installed can use the following additional features:

How to ...: Actions in the Printer Layout

Entering User-defined Formulas

Entering User-defined Formulas (Practice-oriented Example)

Creating Charts

For assistance to change the page format and to create headers and footers, see **How to ...: Actions in the Printer Layout**:

Changing the Page Format

Notes on the Page Setup

Creating a Worksheet

The worksheet represents an area that is unlimited in horizontal and vertical direction, but is divided in "n" printed pages. By inserting chromatograms, tables, diagrams, or other elements, certain areas are reserved on the worksheet. When printing one or several samples, the areas are "filled" with the values of the current sample.

To create your own worksheet, proceed as follows:

- Choose the **Insert Sheet** command in the **Edit** menu to insert an additional worksheet, or
- Select an existing worksheet and change it according to your requirements.

Inserting a Chromatogram

- Choose the **Insert Chromatogram** command to insert a chromatogram.
- Draw a rectangular frame of any size using the now visible **+** mouse. Reserve this area to display the chromatogram of the current sample.
- Click the area to select it.
- The frame can now be moved, reduced or enlarged in size.
- Choose the **Properties** command in the context menu to format the chromatogram (caption, axes, font size, etc.).
- Press the F4 or Shift+F4 key to view the chromatogram of the next or previous sample and to check whether the selected settings are appropriate for all chromatograms.

Inserting a Table

- Choose the **Insert CHROMELEON Report Table** command to include a table.

Caution: If the worksheet already contains a report table, insert the new table above or below the existing one. It is currently not possible to insert several report tables next to each other.

- Choose a method to pre-select the columns to print. On the right-hand section of the edit dialog box, the names of the columns are displayed.
- Select the columns that are to be part of the printed column. Press and hold the **Ctrl** key to select several columns simultaneously.
- Choose **OK** to complete the procedure and to insert the table in the worksheet.
- Select a column header and choose the **Properties Report Column...** command from the context menu to determine the header, the dimension, and the format of the column or of the column values.
- Select a single cell, an area or the entire table to modify the appearance of the table via the **Format** menu (font size and type, frame, color etc.).
- Select a column or a row to delete it (**Delete Row(s)/Column(s)**) or to insert additional rows or columns in front of the selected area (**Insert Row(s)/Column(s)**).

Inserting a "Total" Row

Proceed as follows to insert a **Total** row at the end of the table:

- Copy any cell from another **Total** row (e.g. from another ➢*Printer Layout* table or from an integration report).
- Select the cells of the new table where the sum of all cell values of the column should appear.
- Choose the **Insert** command.

Creating the correct cell reference

The sum value in the **Total** row must receive the correct cell reference. This is especially important, if the new table is longer than the table from which the sum value was copied.

- Activate the ➢*Layout Mode* (View menu) to display the edit line.
- Select the first sum cell value of the **Total** row. In the edit line, the corresponding formula (e.g. =SUM(C10:C22)) will appear.
- Use the mouse cursor to select the cell range in parentheses in the edit line (e.g. C10:C22).
- Then select the actual cell range within the table or enter the cell range in the edit line via the keyboard.
- Press Enter.

The sum cell value is recalculated based on the new cell range. Then perform the individual steps for the remaining sum cell values.

Note: It is not possible to move or copy an entire table. Only the current contents (=values) can be copied to the clipboard, not the underlying variables! Moving individual columns is not possible. Insert a new column where required and delete the column that is no longer needed.

Inserting Individual Variables

At the start of a printout or as an addition to a table or a chromatogram it may be necessary to include general data, e.g. the sequence name, the corresponding ➢*Datasource*, the user name, etc.

- Select a single cell and choose the **Insert CHROMELEON Report Variable** command.
- Via an edit dialog box, you can now select a single variable from different categories.
- Choose **OK** to complete the procedure and to include the variable in the previously selected cell area.
- Select the cell to modify the appearance of the variable via the **Format** menu.

Note: Cells containing an underlying Dionex Chromatography Management System variable can be recognized by the formula name that is displayed on the status bar (e.g. peak.height) whenever the cell is selected. If the selected cell contains text information, the status bar will remain empty.

Inserting Text

Text can be positioned in any cell of the worksheet. The size of the cell limits the available space. Note the following:

- As long as the following cells in the same row are not used, no line breaks are inserted when text is entered in the first column of a worksheet.
- Activate the check box **Word Wrap** (see **Format / Alignment**) to insert a line break.
- Text will always be covered if graphics, e.g. chromatograms are included in the worksheet.

Saving / Loading a Report Template

The ➢*Printer Layout* of a report template (⇒*Report Definition File*) can contain one or several worksheets. Saving or loading a report template always saves or loads all worksheets that are included in the Printer Layout. Saving a single worksheet is possible only if the report template contains only one worksheet.

- Choose the **Save Report Definition** command from the context menu to save the report template and the contained worksheets under one name.
- Choose the **Load Report Definition** command from the context menu to open an existing report template.

Tip: In addition, a report template contains various settings of the screen report such as window size, type, and number of columns in a report, axis captions, etc.

Specifying the Printout

Before you can printout your data, define the printer to be used. In addition, define the headers and footers, margins, etc. via the **Print** dialog or the **Page Setup**. Use the **Print Setup** and **Page Setup** commands of the **File** menu.

The **Print Setup** and **Page Setup** settings are stored separately for each worksheet in a report template (**Integration**, **Calibration**, **Peak Analysis**, **Summary**, etc.). Select the desired settings for each worksheet separately.

- Choose the **Print Setup** command of the **File** menu to determine the printer, the paper size, and the format (portrait or landscape). Having made these settings, a message box allows specifying whether to use these settings for either the current worksheet or all worksheets of the printer layout of the current report definition file (RDF).

☞ ***Tip***: The **Print Setup** settings selected here apply only to the report definition file of the current sequence. They do not affect the default settings for Windows. In addition, changing the default printer, paper size, and format in Windows will not affect the settings selected here.

- Choose the **Page Setup** command of the **File** menu to determine the appearance of the headers and footers, the size of the margins, the alignment etc. Here you can also set a grid, determine whether column headers are displayed and whether the printout should be in black and white or in color. For further information, see **How to ...: Actions in the Printer Layout** **Notes on the Page Setup**.

☞ ***Tip***: Due to technical reasons, direct help information for the **Print Setup** and **Page Setup** dialog boxes is not available.

Also, see: **How to ...: Actions in the Printer Layout**:

Saving/Loading a Report Template

Saving the Contents of a Report Template

Printing the Results of a Single Sample

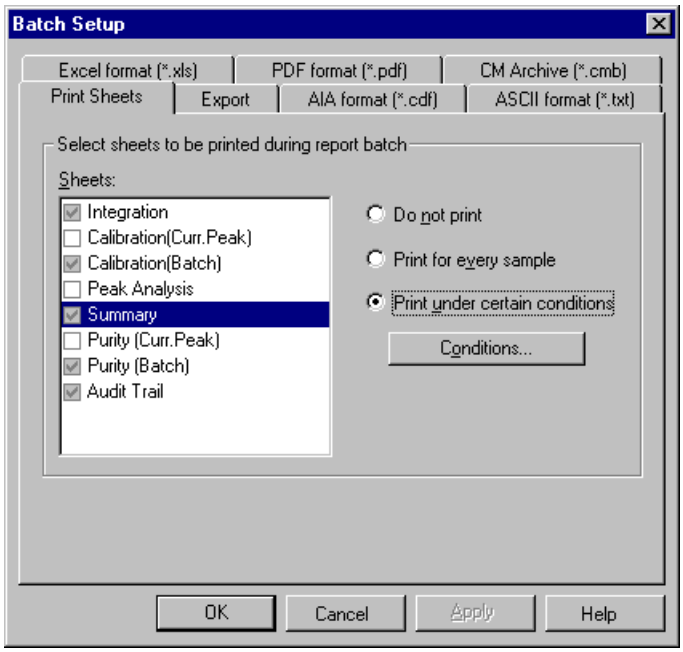
The results of single samples can be printed from either the printer layout or the screen report (integration plot).

For each printout, the pages of the ➢*Printer Layout* that are saved in the ⇒*Report Definition File* are used as template. The results of a single sample or a sequence (see the next topic **Printing the Results of a Sequence / Sample Batch**) are output in the defined way. However, the report templates and worksheets define the appearance of the printout, not its contents.

You have to specify which of the worksheets that were created in the printer layout shall be printed. Different alternatives and windows are available for doing this.

Printer Layout

The **Batch Setup** command of the **File** menu allows specifying the worksheets to be printed. The **Batch Setup** dialog box opens:

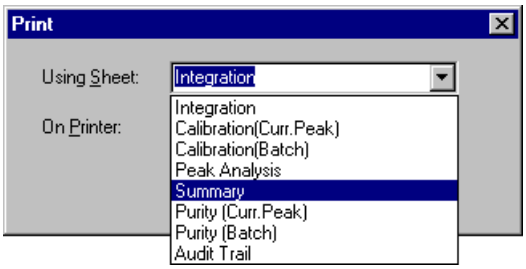


Make the corresponding settings on the **Print Sheets** tab of this dialog box. The **Sheets** field lists the available worksheets. Define which pages shall be

printed and under which conditions. Use the **Conditions…** button to specify these conditions, i.e., you can define for which samples to print a page. For example, it would be sensible to printout a summary report for the last sample of sequence only.

Report (Screen Report)

To print the results of the currently open sample from the screen report, use the **Print** command of the **File** menu.



In the dialog box, select the worksheet to be printed. The sheet will always be printed with the results that are currently displayed on the screen provided they are included in the defined view. For example, the current mass spectrum will be printed only if a mass spectrum is part of the selected worksheet.

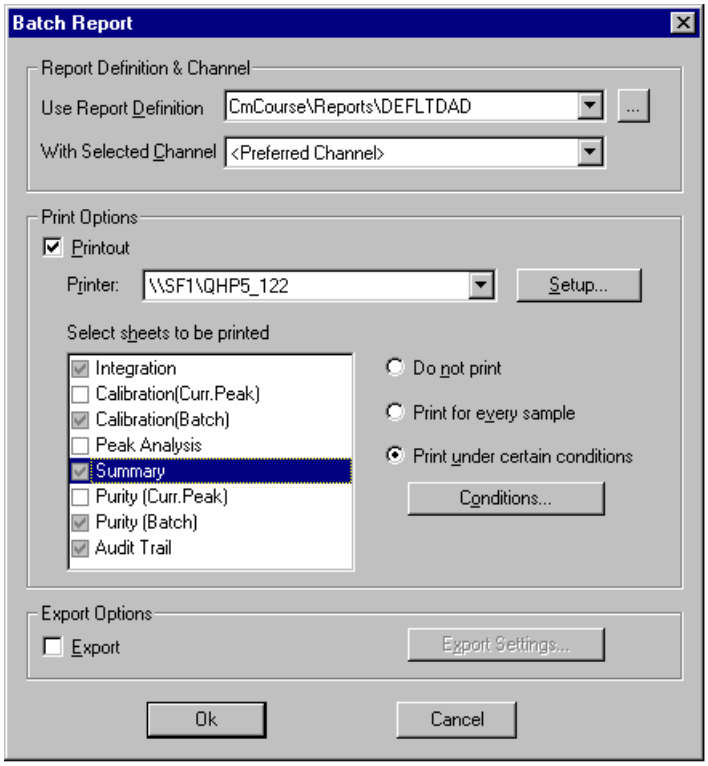
☞ ***Tip***: In the printer layout, you can select peak spectra only. Use the report if you want to print the retention time spectra. Select the desired spectrum on the screen and select a worksheet to be printed that includes a spectrum.

Printing the Results of a Sequence / Sample Batch

You may also print the results of an entire sequence, a ➢*Query* or a ➢*Batch*. If not already done, you have to specify which of the worksheets that were created in the ➢*Printer Layout* shall be printed. Different alternatives and windows are available for doing this.

Browser

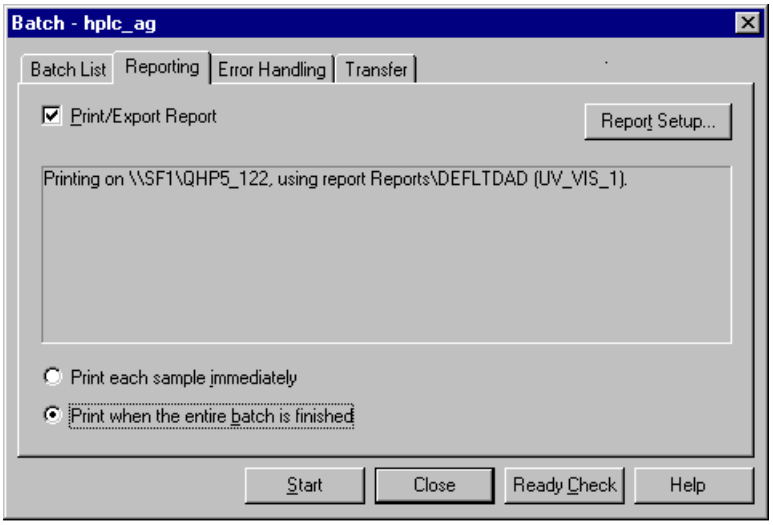
After you clicked a ➢*Sequence* or a sample in the Browser, open the Batch Report dialog box via the Batch Report command of the File menu. Select the desired report template in the **Use Report Definition** list box (via the arrow) or via the "**…**" button.



The **Select sheets to be printed** field shows the worksheets that were defined in the printer layout of the report template. Specify which pages shall be printed. Define under which conditions they shall be printed via the **Conditions…** button. Pressing **OK** then prints the entire sequence or the selected samples of a query. Select all samples of a query by clicking the **No**. field at the top left of the sample list to print the entire query.

Printing the Results Directly after Data Acquisition: Control Panel

To print the results directly after data acquisition, you can open the **Reporting** dialog box via the **Reporting** command of the **Batch** menu:



The **Print/Export Report** option opens the above dialog box (that is displayed in the Browser section) once again. Proceed as described above. The window on the tab indicates the printer, report definition file (RDF), and channel to be used for the printout. In addition, you can specify whether to print each sample separately and directly after the data acquisition or all samples when the batch is finished.

Tip: The settings made in the Browser or from the control panel are saved in the report definition file of the current sequence. They apply to all sequences that use this report definition file. They will also be used for these sequences as default for the worksheets to be signed by means of ➢*Electronic Signature*.

Also, see the previous topic:

Printing the Results of a Single Sample

Setting Print Area and Print Title(s)

If you want to print a defined area of a ➢*Printer Layout* page, proceed as follows:

- Select the desired area with the left mouse button.
- Select the **Set Print Area** command via the **Printing** option of the **Format** menu.
- Deselecting the set print area is via the **Release Print Area** command of the **Printing** option in the **Format** menu. The set print area is indicated in parenthesis behind the command.

When printing a table that exceeds one page you can have the titles printed not only on the first page but on all following pages as well:

- Select the complete lines via the left mouse button. .
- Select the **Set Print Titles** command via the **Printing** option of the **Format** menu.
- Selecting the **Release Print Titles** command of the same option allows deselecting the set print titles. These set print title area is indicated in parenthesis behind the command.

Saving the Contents of a Report Template

For the report data of the current sample, the Dionex Chromatography Management System offers various formats for saving the data.

- Choose the **Save as...** command from the **File** menu to start saving the data.
- Select the **Excel ... (*.xls)** file format to convert data into the Excel format and to save as a separate file. In addition to the values of a table, it is of course possible to include graphics and diagrams. If the ➢*Printer Layout* of the ⇒*Report Definition File* contains several worksheets, this division will be maintained in the Excel file. Please note that different file types will be available depending on the Excel version (4 or 5 or 7).
- Select the file type **HTML (*.htm)** to save the data as a HTML page. Graphics and diagrams cannot be represented.
- Select the file type **Tabbed Text (*.txt)** to save data in pure text format. The contents of individual report columns are separated by a tab stop. Graphics and diagrams cannot be represented.

Entering User-defined Formulas

Tip: The options described below require the ➢*Report Publisher* add-on product.

Creating user-defined formulas is analog to the Microsoft Excel spreadsheet. The following description is intended for users who are not familiar with entering formulas:

Example 1:

Let's assume that a table containing two columns (A and B) and three lines (1 to 3) is extended by one column (C), for which there is *no* Dionex Chromatography Management System report variable. Thus, e.g. the quotient of the cell contents of columns A and B can be included in column C.

To enter a formula in a cell, the corresponding cell must be selected first. In this example, select the cell C1. Now enter the equals sign. The entire input can be seen in the edit line above the worksheet (here indicated by blue print).

C1	**=**		
	A	**B**	**C**
1	12	5	
2	17	10	
3	13	20	
4			

Select the cell A1, enter a division sign (slash), select the cell B1, and complete your input by pressing ENTER. The edit line now shows the formula (C1=A1/B1) and the cell C1 shows the result of the operation (2.4). The cursor moves to cell C2.

C1	**=A1/B1**		
	A	**B**	**C**
1	12	5	2.4
2	17	10	
3	13	20	
4			

Proceed in the same way to output the respective results in the cells C2 and C3. Clicking the cell C1 again, grabbing the selection frame on the lower right corner, and dragging it to the required cells (C2, C3) can facilitate this procedure. For calculating the cell values, the Dionex Chromatography Management System uses the previously entered formula and automatically creates the correct reference, line by line.

C1	**=A1/B1**		
	A	**B**	**C**
1	12	5	2.4
2	17	10	1.7
3	13	20	0.65
4			

Example 1 (continued)

To form the sum of the cells of column C in the field C4, proceed as follows:

Select the cell C4 and enter an equals sign. Enter the SUM command required for adding cell values (see *SUM* in the Report Publisher Online Help). Then enter a bracket sign.

C4	**=SUM(**		
	A	**B**	**C**
1	12	5	2.4
2	17	10	1.7
3	13	20	0.65
4			

Now select all cells (C1, C2, C3) of which you want to add the values. Close the bracket after the last cell. Press the ENTER key to complete your input.

C4	**=SUM(C1:C3)**		
	A	**B**	**C**
1	12	5	2.4
2	17	10	1.7
3	13	20	0.65
4			**4.75**

In addition to the SUM command, numerous other functions are entered in the same way. Thus, you can form the average (see *AVERAGE* in the Report Publisher Online Help), express conditions (see *IF*, *True*, *FALSE* in the Report Publisher Online Help), create logical operations (see *AND*, *OR* in the Report Publisher Online Help), or enter time values (see *TIME*, *DATE*, *DAY*, *YEAR* in the Report Publisher Online Help).

☞ ***Tip***: For an alphabetically sorted list of the available formulas, see the ➢*Additional Functions* topic.

Example 1 (continued)

As a further possibility, calculating with "fixed references" is enabled. In contrast to variable value pairs described above (A1/B1, A2/B2, A3/B3), the quotient is now formed of a variable and a fixed value (A1/C4, A2/C4, A3/C4). In this example, output is in column D.

Proceed as described above to create the first cell reference (D1).

D1	**=A1/C4**			
	A	**B**	**C**	**D**
1	12	5	2.4	2.5263
2	17	10	1.7	
3	13	20	0.65	
4			4.75	

Now extend the formula by adding two **$** signs and thus convert a variable reference into a fixed cell reference.

D1	**=A1/$C$4**			
	A	**B**	**C**	**D**
1	12	5	2.4	2.5263
2	17	10	1.7	
3	13	20	0.65	
4			4.75	

If you copy the formula now, the reference to cell C4 will be retained. The fields to be calculated (D2 and D3) can then be calculated by simultaneously selecting the cells D1, D2, and D3.

D1	=A1/$C$4			
	A	**B**	**C**	**D**
1	12	5	2.4	2.5263
2	17	10	1.7	3.5790
3	13	20	0.65	2.3768
4			4.75	

For a practice-oriented example, see **How to ... Actions in the Printer Layout**  **Entering User-defined Formulas (Practice-oriented Example)**.

Entering User-defined Formulas (Practice-oriented Example)

If you use samples with ➢*Internal Standard* but wish to calculate the percentage values of the different substances in the sample (without internal standard), please proceed as follows:

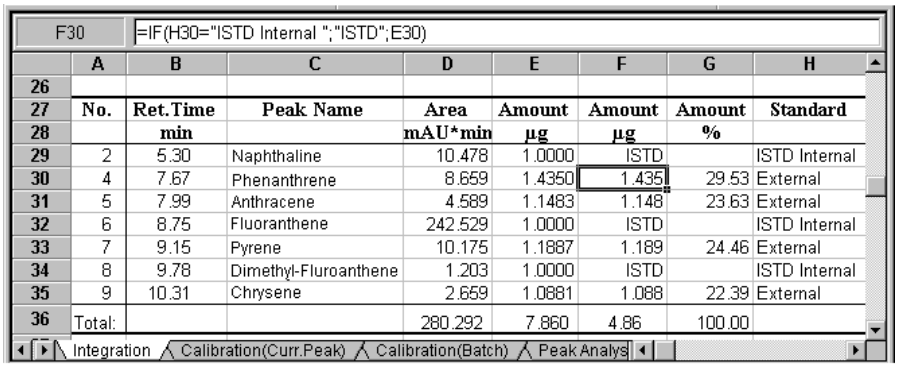
1. Insert the **Standard Method** variable of the **Peak Table** category into a column that you do not need (in the example below "H").

2. a) Select a different column which is not required. Open the dialog box with F8 and delete the entry in the field **Formula**. Afterwards delete the entries in the column (except the last line).

2. b) Enter the formula **=IF(H29="ISTD Internal ";"ISTD";E29)**, e.g. in field F29 (Caution: Do not omit the space following **Internal"**!), and copy it to the following lines.

3. a) Select another column which you do not need either. Open the dialog box with F8 and delete the entry for the field **Formula**. Afterwards delete the entries in the column (except the last line).

3. b) Enter the formula **=F30/F36*100** in field G30 and copy it to the following lines of the original substances of the sample. Excel will now place the formula **=F31/F37*100** in cell G31, etc. that you should finally correct to **=F31/F36*100**, etc.



F30 =IF(H30="ISTD Internal ";"ISTD";E30)

	A	B	C	D	E	F	G	H
26								
27	No.	Ret.Time	Peak Name	Area	Amount	Amount	Amount	Standard
28		min		mAU*min	µg	µg	%	
29	2	5.30	Naphthaline	10.478	1.0000	ISTD		ISTD Internal
30	4	7.67	Phenanthrene	8.659	1.4350	1.435	29.53	External
31	5	7.99	Anthracene	4.589	1.1483	1.148	23.63	External
32	6	8.75	Fluoranthene	242.529	1.0000	ISTD		ISTD Internal
33	7	9.15	Pyrene	10.175	1.1887	1.189	24.46	External
34	8	9.78	Dimethyl-Fluroanthene	1.203	1.0000	ISTD		ISTD Internal
35	9	10.31	Chrysene	2.659	1.0881	1.088	22.39	External
36	Total:			280.292	7.860	4.86	100.00	

Integration | Calibration(Curr.Peak) | Calibration(Batch) | Peak Analys

Creating Charts

Tip: The add-on product ➢*Report Publisher* is required for performing the options described in this section.

The CHART Wizard facilitates creating charts. Perform the steps described below:

- Select the columns and rows that you would like to present in a chart.
- Choose the **Insert ... Charts** command from the context menu. The mouse cursor will change its shape to a small **+** sign.
- Press the left mouse button and draw a rectangle frame of the size required for the chart.
- Follow the steps of the CHART Wizard to determine the style, the layout, and the axes of the chart.
- As soon as you have completed the information for the individual steps, press the FINISH button to close the CHART Wizard.

The completed (raw) chart will be displayed in the previously drawn frame. If required, you can perform various changes. You can alter the line width, the color, and pattern of lines, areas, or captions; you can smooth curves or change the chart type. You can also change the size and the position of the entire chart.

- Click individual chart elements to select them. Now double-click the element to change it. Get familiar with the numerous options the Dionex Chromatography Management System offers in various dialog boxes.
- Select the chart frame to reposition or resize the entire chart.

Changing the Page Format

In the ➢*Printer Layout*, the page format can be changed as follows:

Define the printer settings

- Select the **Print Setup** command in the **File** menu.
- Define the paper size in the Print Settings dialog box. Use the arrow of the combo box to select the desired size. The size is used for all pages of the respective printout but is accepted as default.

☞ ***Tip***: The settings are only valid for the report definition file of the current sequence. They do not overwrite the default Windows settings. Any change of the default printer, paper size, or format that is made under Windows does not affect the settings made here.

Directly printing in the desired format:

- Select the **Print** command of the **File** menu.
- Click Properties to open the corresponding dialog box.
- Select the desired paper size in the lower selection box.

Notes on the Page Setup

Headers and footers are printed at the upper and lower page margins. They are defined in the dialog box **Page Setup** that can be selected in the **File** menu.

Headers and footers can contain text and specific format codes. The syntax for entering is compatible to Microsoft Excel. The numerous possibilities include:

&L	Left-aligns the characters that follow
&C	Centers the characters that follow
&R	Right-aligns the characters that follow
&A	Prints the current sheet name
&D	Prints the current date
&T	Prints the current time
&F	Prints the ⇒*Report Definition File*
&P	Prints the page number
&P+number	Prints the page number plus number
&&	Prints an ampersand
&N	Prints the total number of pages in the document

The following font codes must precede other inputs. Otherwise, they will be ignored. After each alignment code (&L, &C, and &R), the font can be changed.

&B	Bold
&I	Italic
&U	Underline
&S	Strikeout
&"fontname"	Use the specified font
&nn	Use the specified font size

When entering headers and footers longer than one line, note that the alignment codes (&L,&C,&R) must be column-oriented. First, enter all left-aligned rows, then all centered rows and then all right-aligned rows. Press Ctrl-Enter to separate rows.

In addition to the above pre-defined variables, you can enter the variables of the Dionex Chromatography Management System. These are given in braces.

Example:

&L&BSequence: {seq.name}, No. {smp.number} of {seq.nSamples}<Ctrl-Enter>Timebase: {seq.timebase}&RDate: &D<Ctrl-Enter>Time: &T

This example produces the following header or footer (<Ctrl-Enter> is not visible!)

Sequence: AMINO, No. 1 of 99 **Date: 11.10.96**
Timebase: SYS1 **Time: 2:04 PM**

In principle, any variable of the Dionex Chromatography Management System can be included in the header. However, generally only sample and sequence variables make sense. The formulas of Dionex Chromatography Management System variables are identical with the ones generated in the dialog box for entering report variables. The number of decimal places for numerical variables can be entered after the formula, separated by ";" (default: 0). Example: {smp.inject_volume;2}. Time entries cannot be formatted.

 ***Note**:* All worksheets of the ➢*Printer Layout* that are selected for the printing are considered one single print job, i.e., page numbering is consecutive for all worksheets.

Actions in the Peak Purity Analysis (PPA) Window

The **PPA (Peak Purity Analysis)** window displays the ➢*3D-Field* of a sample, provided there is a corresponding raw data file. This is the case if the channel **3DFIELD** was selected for ➢*Data Acquisition*.

The 3D-field in the lower right-hand window section has cross-wires. With the mouse, the axes can be moved separately or together. The spectrum or chromatogram extracted along the current y and x-axis will be displayed on the left or above the 3D-field.

- Move the y-axis of the cross-wires to successively view all spectra of the current chromatogram.
- Move the x-axis of the cross-wires to view the appearance of a chromatogram at different wavelengths.
- The status bar shows the retention time, wavelength value, and signal height of the current cross wire position.

Apart from this simple spectra and chromatogram selection, use this method to perform the following operations (see topics below):

Analyzing Peak Purity

Selecting the Optimum Integration Path

Extracting Spectra, Chromatograms, and 3D-Fields

Analyzing Peak Purity

Peak purity can be evaluated using the following methods (see topics below):

Visual Check

PPI and PPI Match Factor

Normalized Spectra Overlay

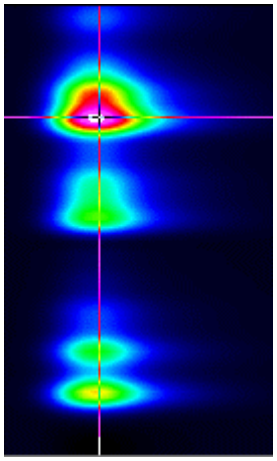
Peak Inhibition via Virtual Channels

Multiple Ratio

Visual Check of Iso-Line Plot

The Visual Check of the Iso Line Plot is a simple method to evaluate peak purity. High peak purity is indicated by:

- All recognizable absorption maxima are located vertically below one another in direction of the wavelength axis.
- The maxima are separated so that the surrounding iso lines do not touch (no overlapping).
- Pure peaks have (local) symmetry or an idealized ellipse shape in the maximum.



PPI and PPI Match Factor

In the chromatogram window of the PPA method, curves for the ➢*PPI (Peak Purity Index)* and the ➢*Peak Purity Match Factor* can be displayed:

- Double-click within the window and select the options **Draw PPI** and **Draw Match** from the tab dialog box **Chromatogram Plot**.

The peak purity index is represented by a purple curve, and the match factor is indicated by a green curve. A distinctive rectangular shape is one criterion (of many) for peak purity. The exact match value at the current mouse cursor position is shown on the status bar. The ideal value is 1000 and requires approx. 80% of the available window height.

PPI, match value, and the corresponding standard deviation (RSD) can be included in a report. The report variables are in the category **Peak Purity**.

The smaller the standard deviation, the more critical the quality of the rectangular curve should be judged, i.e., the better the two spectra will match in various points of a peak.

Normalized Spectra Overlay

In a normalized spectra overlay, single spectra of the spectra recorded for the peak are extracted and are compared with each other. Usually, extraction is at the run time of the peak and at a specific peak height in the ascending and descending flank of the peak, e.g. in 10 and 50% of the peak height. Comparing spectra, which are ➢*normalized* (!) by the same method, in the spectra window is an indication of the peak purity.

The better the spectra match, the higher the possibility that the peak is pure. The following are indications for the impurity of a peak:

- The number of relative maxima and minima of two spectra does not match
- The relative maxima are clearly offset against each other
- The height of the relative maxima strongly deviates

However, please note the following:

- Especially near peak limits, spectra have an increased noise level due to the normalization procedure. This applies in particular to the UV range.
- Despite baseline correction, the detector drift cannot be compensated completely in the case of very long peaks.
- The spectra shape depends on the solution, i.e. the spectra of a peak can only be compared if the mixing ratio was constant during detection.
- It is possible only to compare spectra with the (complete!) absorption in the dynamic validity range of the Lambert Beer Law. If the peak maximum including the baseline spectrum is considerably above 1 AU, caution is called for.

☞ ***Tip***: The normalized spectra overlay via peak height is currently only possible in the **Spectra Plot**. Within the PPA method, the "animated" extraction of spectra is possible. Pressing the CTRL key in the 3D-field extracts the current spectrum. If the y-axis of the cross-wires is moved simultaneously, all spectra existing for this range are displayed in the spectra window. The extraction period is indicated in the chromatogram by a different color. This process can be repeated (e.g. for different retention times within the peak width). If the CTRL key is released between the individual extractions, the spectra extracted per range are represented in a separate color.

Peak Inhibition via Virtual Channels

If two overlapping peaks have different spectra s1(λ) and s2(λ) the following equitation is true when the area below the baseline is ignored:

$$A(\lambda, t) = s1(\lambda)*c1(t) + s2(\lambda)*c2(t) \quad (1).$$

c1 and c2 stand for the time-dependant concentrations of the corresponding components in the flow cell. Then, two wavelengths λ1 and λ2 are selected and the following signal is created:

$$d(t) = A(\lambda1, t) - K*A(\lambda2, t) = c1(t)[s1(\lambda1) - K*s1(\lambda2)] + c2(t)[s2(\lambda1) - K*s2(\lambda2)]. \quad (2),$$

The c2 term disappears provided the appropriate expression was selected for K, i.e.

$$K = s2(\lambda1) / s2(\lambda2) \quad (3)$$

This is the channel ratio of the second peak. It can be read off the height ratio of the two peaks if they do not overlap completely. In order to be able to use this approach, the channel ratio of the first peak

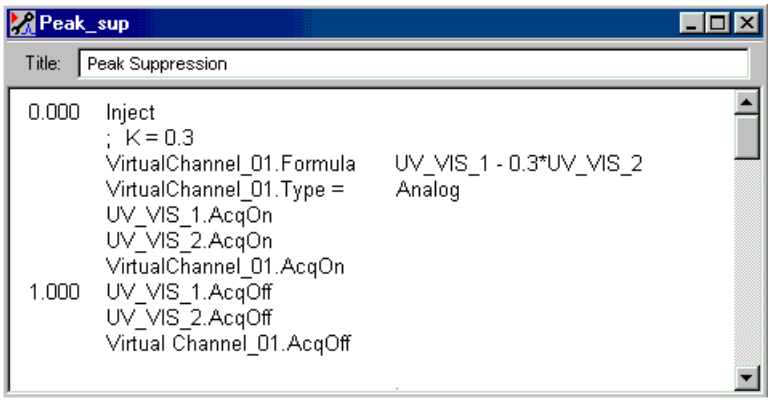
$$K' = s1(\lambda1) / s1(\lambda2) \quad (4)$$

must be different from K. If not, the first term in equation (2) will disappear as well. Select wavelengths λ1 and λ2 in such a way that the difference between K and K', i.e.

$$\Delta K = |K - K'| \quad (5)$$

is the maximum difference. The best way to determine the appropriate wavelengths is to do so in the PPA Window. After this, the virtual channel d(t) can be defined. Of course, it is possible to inhibit the first peak in the same way.

If you know the wavelengths for which ΔK is max. before you acquire the chromatogram, the two channels e.g. UV_VIS_1 and UV_VIS_2 can be adjusted to those wavelengths and the following ➢*Program* may be used:



As already mentioned in the comment line of the program, the following equation is true for this example:

$$K = 0.3.$$

Multiple Ratio

Each channel extracted from a 3D-field can be used for performing the ratio test. Especially suited are chromatograms in the range of spectral minima or maxima. If the ratio condition is met, this can indicate, but does not prove peak purity. Performing the test with a larger number of channels does not change this fact.

Selecting the Optimum Integration Path

The Dionex Chromatography Management System is capable of calculating the ➢*Optimum Integration Path* within a 3D-field. The calculation is performed automatically. The result can be displayed in the 3D-field window of the PPA method.

- Double-click within the window and select the **Draw Opt-Int-Path** option in the tab dialog box **Iso/3D-Plot**.

A green line in the 3D-field indicates the integration path. Similar to chromatograms, it can be saved as a separate channel with variable wavelength.

- Choose the **Extract: Opt. Int. Path to file** command from the View or context menu and determine the name under which the path is saved as a separate channel.
- Select the **Extract from all samples of current sequence or query** option, if the path should be extracted for all samples of the underlying sequence or query. The shape of the path is identical for all samples!

If the path should serve as a basis for a ➢*Wavelength Switch* in future samples, the switch times and the selected wavelength values must be entered in a program with exact time specifications. This can also be performed by automatically inserting the data.

- Choose **Extract: Opt.Int.Path to clipboard** from the **View** or context menu to copy the data to the clipboard.
- Select the **Name** of the channel, for which the wavelength is automatically switched in the future.
- Enter a value for the **Bandwidth** if several chromatograms should be averaged to one. The bandwidth determines the range of the path. All sections of a chromatogram within this range are averaged to one chromatogram.
- Open a ➢*PGM File* and insert the data at the beginning of the program (**Commands** view) via the **Paste** command.

The resulting PGM file could have the following appearance:

```
0.000    UV_VIS_1.Bandwidth = 0
         UV_VIS_1.Wavelength = 210
3.320    UV_VIS_1.Wavelength = 210
4.830    UV_VIS_1.Wavelength = 206
6.100    UV_VIS_1.Wavelength = 272
8.100    UV_VIS_1.Wavelength = 262
9.660    UV_VIS_1.Wavelength = 278
10.480   UV_VIS_1.Wavelength = 250
```

- Enter further commands in the program to complete it. Sort it according to ascending retention times.

Extracting Spectra, Chromatograms, and 3D-Fields

Spectra

Each spectrum extracted from a 3D-field in the method PPA or the **Spectra Plot** window can be copied (**Copy**) to the Windows clipboard. The spectrum can then be inserted in a **Spectra Library** via the **Paste** command. Perform the following steps:

- Choose the **Extract: Spectrum to clipboard** command from the View or context menu to copy the current spectrum from the 3D-field of the method PPA to the Windows clipboard.
- Open an existing Spectra Library. Choose the command by opening the corresponding LIB file via the Browser, or
- Create a new library via the **File/New/Spectra Library** command.
- Choose the **Paste Spectra** command to save the spectrum and the data in the library.

Chromatograms

In the method PPA, the chromatogram of any wavelength can be extracted from an opened 3D-field.

- Choose **Extract: Chromatogram to file** from the **View** or context menu to save the current chromatogram as a separate channel.
- Choose the wavelength and the bandwidth at which to extract the chromatogram.

The Dionex Chromatography Management System will suggest a name for the extracted chromatogram, considering the wavelength. Of course, any other name can also be used. The chromatogram is saved in addition to the raw data of the existing 3D-field. Simultaneously, the extracted chromatogram is opened via the method **Integration** to give the user an overview of the saved data.

In addition, the **Extract: Chromatogram to file** command offers a special option. Instead of saving one single chromatogram, another chromatogram of the same wavelength can be extracted and saved from all samples of the underlying sequence or query. Activate **Extract from all samples of current sequence or query**. Especially in this case, automatically naming the extracted chromatogram (see above) is very useful.

3D-Field Data

The **Export 3DFIELD** command enables including and displaying the current 3D-field raw data in other applications, e.g. Microsoft Excel. Data is converted into a general ASCII format.

- After executing the **Export 3DFIELD** command, change to the other application and insert the data via the **Paste** command. Apart from the pure raw data, additional sample and sequence information is transferred to the application.

☞ ***Tip***: In the GynkoSoft chromatography data system, the GSRAWASC.EXE user program enabled this option.

Actions Related to the aQa-MS

The Dionex Chromatography Management System allows acquiring MS data via the Finnigan aQa ➢*Mass Spectrometer*. However, before mass spectra acquisition and processing, several conditions must be fulfilled. For a detailed description on these conditions and possible actions with these data, see:

Installing MS Components

Conditions

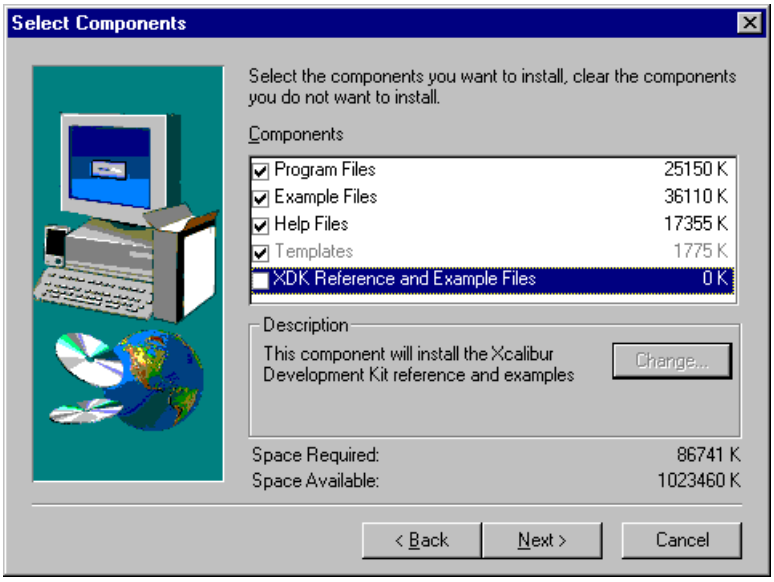
The complete ➢*Xcalibur* (= XC) system (REV 1.2) must be installed on every computer (also pure Remote Clients of the Dionex Chromatography Management System) that must be able to access MS data. Thus, the minimum system requirements for an LC/MS system are as follows:

- 400 MHz PII CPU
- 128 MB RAM
- 10 GB hard disc
- 1024 x 768 x 16 screen resolution

Individual Steps

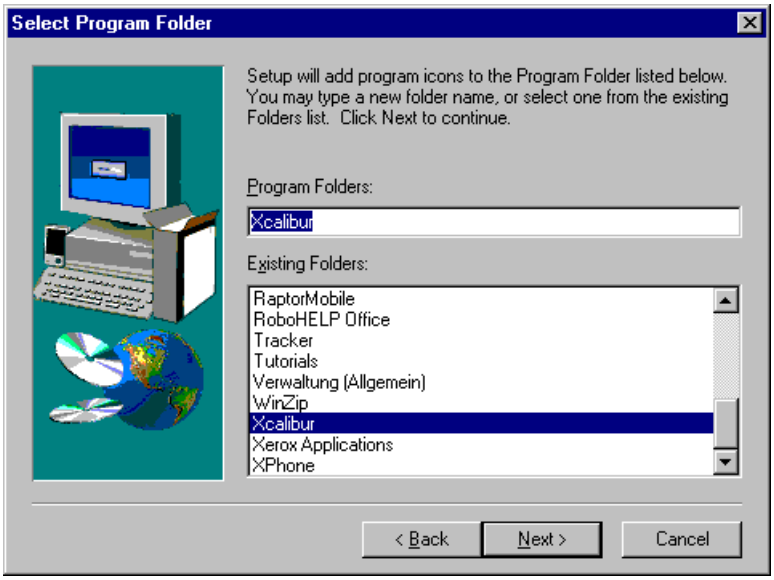
Installing the software requires the following steps:

- Run SETUP.EXE of the XC core system and install it to the local hard disk. Install the default components:



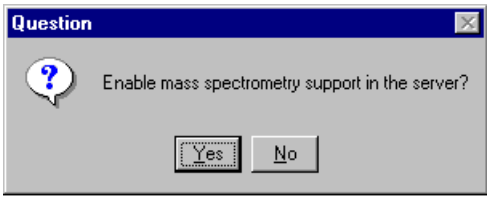
You are then prompted to restart your PC. However, installing Xcalibur under the Dionex Chromatography Management System does not require rebooting your PC now.

Execute SETUP.EXE of the XC aQa VI driver. This is also required for pure clients of the Dionex Chromatography Management System that should be able to access the XC / aQa method files (METH files).



Upon being prompted by the system, reboot your PC.

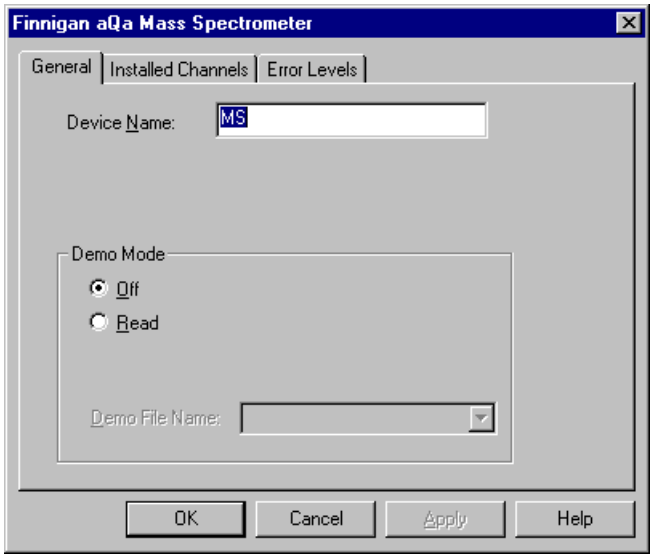
- You can now start the CM setup. During the installation process the CM setup will ask you:



- Answer this question with **Yes** if you want to control an aQa with this server installation. Answer with **No** for every other installation type (Remote Client, LC/IC Servers without an aQa).

  If your answer is **Yes**, the Dionex Chromatography Management System setup checks whether an XC installation exists. If a complete XC installation is not found (XC core + XC aQa), the setup will abort.

- To be able to control an aQa ➢*Mass Spectrometer*, ensure that the aQa driver of the Dionex Chromatography Management System is installed in the **Server Configuration**.

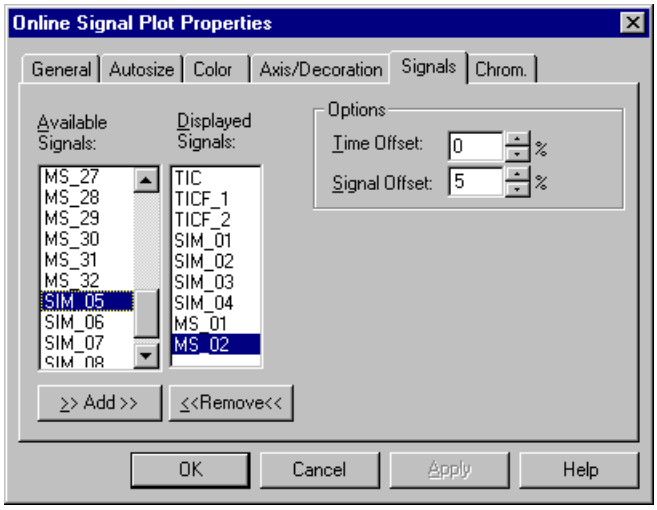


You do not need to change any of the default settings except if you want to operate the instrument in ➢*Demo Mode*.

☞ ***Tip***: For installation details, see **Controlling and Installing Third-Party Instruments** **FINNIGAN aQa-Mass Spectrometer**.

Defining the Number of MS Channels

The **Installed Channels** tab in the **Server Configuration** allows limiting the number of channels. A maximum of 69 channels (default setting) can be defined and displayed during data acquisition in the ➢*Control Panel*.



Limiting the number of channels is possible as well.

☞ ***Tip***: Bear in mind that data will be lost if more channels are defined in the program than can be recorded according to the Server Configuration settings.

A distinction is made between channels for individual ions (= ➢*SIM* channels), channels for the total ions (= ➢*TIC* channels), and TICF channels (= Total Ion Chromatogram Full scan). SIM channels are recorded in **Selected ion monitoring** (= SIM) mode, while ➢*Full-Scan* mode is required for TICF channels. In full-scan mode, you can extract ➢*Mass Traces* online during data acquisition (see **Extracting Mass Traces Online**). These **Online Mass Extract Channels (OMECs)** are designated MS_01 to MS_32.

Each mass that is recorded in the aQa method in **Selected ion monitoring** (= SIM) mode requires its own channel. See **Number of Required MS Channels - Examples** for three illustrating examples.

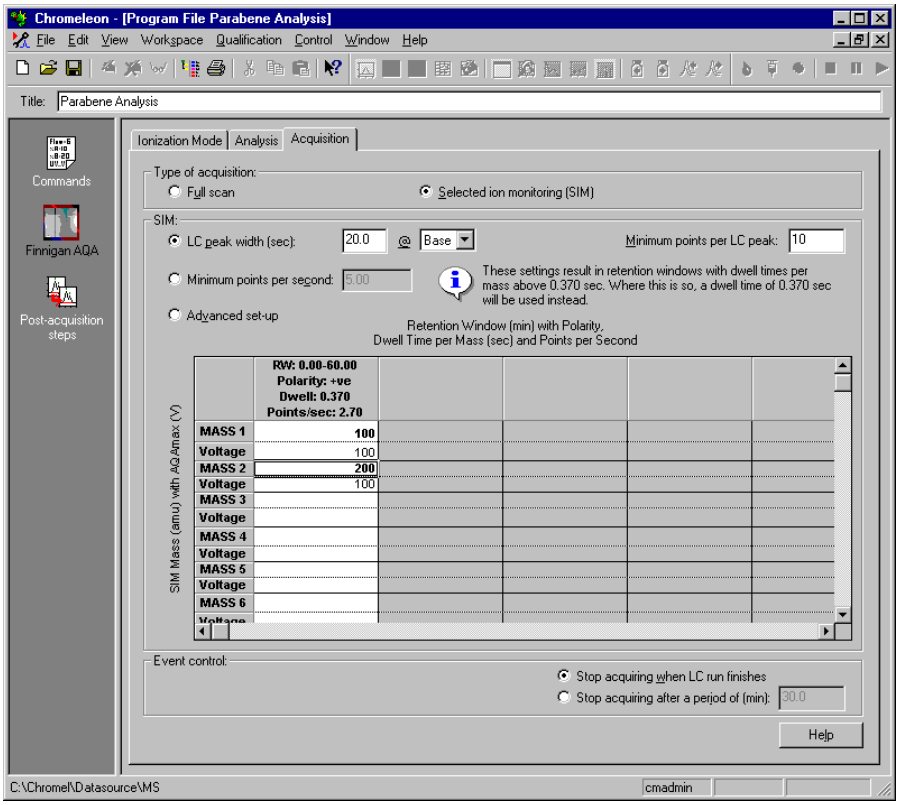
If you notice after data acquisition that a channel is missing, you can extract separate ➢*Mass Traces* (this may be mass ranges as well) from the ➢*Mass*

Spectrum and save them as new channels (see **How to ...: Actions Related to the aQa-MS Extracting Mass Traces Afterwards**).

Number of Required MS Channels - Examples

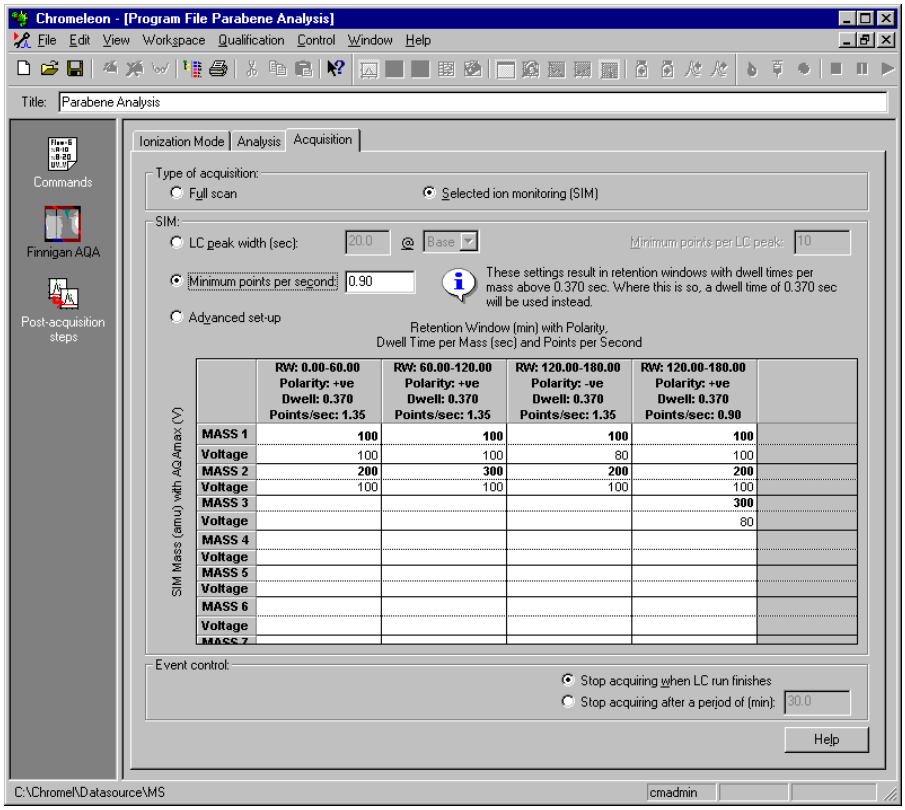
The examples below illustrate the number of channels that are required for the different types of acquisition.

The first example requires two SIM channels plus the TIC channel:



The SIM1 channel records the chromatogram at a mass of 100, the SIM2 channel records the same chromatogram at a mass of 200.

The second example requires six SIM channels and the TIC channel:



The channel assignment is as follows:

SIM_01: Mass 100, positive voltage, 100V,

SIM_02: Mass 100, negative voltage, -80V,

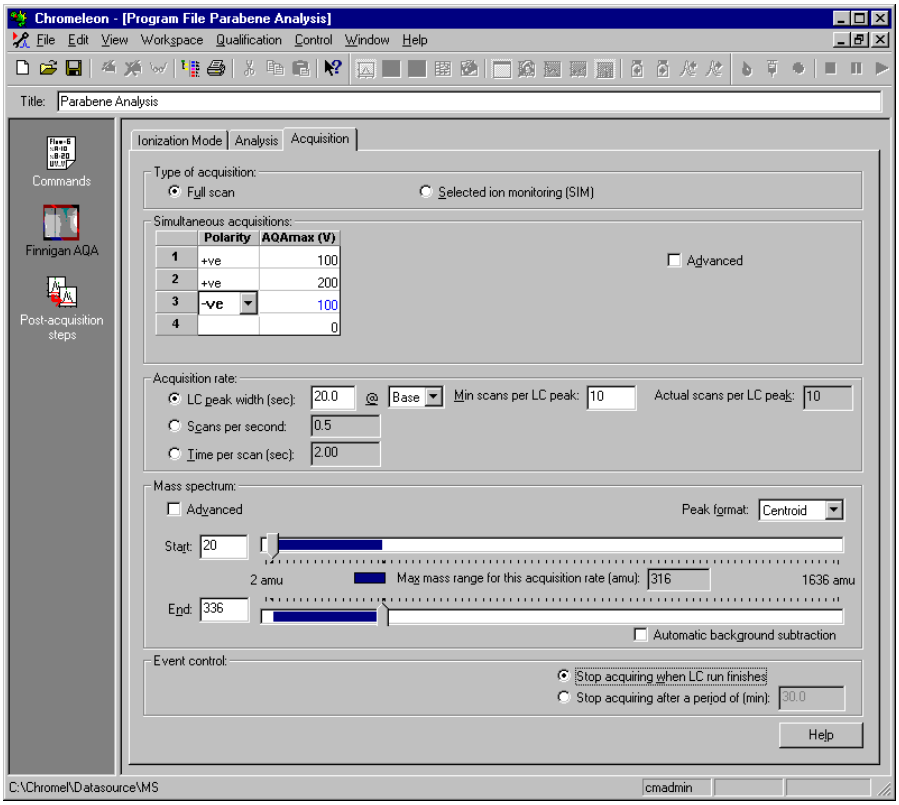
SIM_03: Mass 200, positive voltage, 100V,

SIM_04: Mass 200, negative voltage, -100V,

SIM_05: Mass 300, positive voltage, 100V,

SIM_06: Mass 300, positive voltage, 80V.

The third example requires three TICF channels and the TIC channel:



The channel assignment is as follows:

TICF1: positive voltage, 100V

TICF2: positive voltage, 200V

TICF3: negative voltage, -100V.

If you notice after data acquisition that a channel is missing, you can extract separate ➢*Mass Traces* (this may be mass ranges as well) from the ➢*Mass Spectrum* and save them as new channels (see **How to ...: Actions Related to the aQa-MS Extracting Mass Traces Afterwards**).

Creating an MS Program and Sequence

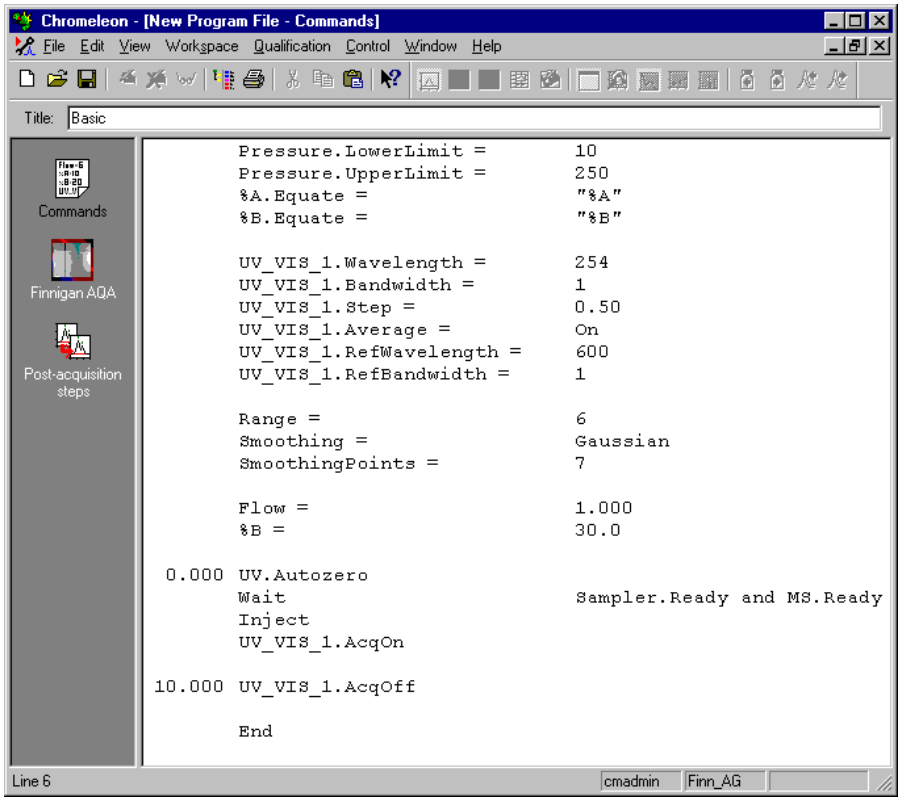
As manual data acquisition is not available for the aQa ➢*Mass Spectrometer*, you need to prepare a sequence before data acquisition can be started. Thus, a control file (➢*PGM File*) is required.

Program Wizard (PGM Editor: Commands)

Create a new PGM file using the **Program Wizard** (see **Control (Programmed)** section). If you have an aQa mass spectrometer installed on the current timebase, you can specify the data acquisition using the MS channel on the **Acquisition Options** page. This opens the page for MS specific parameters.

This page allows setting the parameters that are required for ➢*Mass Trace* processing (= MS chromatogram). The **Range** parameter is the scaling factor for the online display of mass traces in the respective panel (e.g., Range = 5 allows a maximum value of 100.000 = (1 E+5) counts in the online display). However, the stored data are not affected. The ➢*Smoothing* parameter allows selecting the smoothing filter for smoothing MS chromatograms.

Under **Points**, define the number of data points to be used for smoothing. Select the number of datapoints such that the width of the smoothing filter approximately equals the peak's half width. For example, the following program will be created:



The Wizard-generated PGM file provides no ⇒*AcqOn/Off (Data Acquisition On/Off)* commands for the aQa channels. The channels that are needed for mass trace acquisition depend on the contents of the MS method.

The Program Wizard automatically generates the **wait MS.ready** command before the inject command. This is synchronization is required between the aQa mass spectrometer and the Dionex Chromatography Management System. If you want to create your own PGM files manually, always add the **wait MS.ready** command before the inject command.

If you want to use ➢*Blank Run Samples*, ensure that the inject mode is set to **Inject**. Otherwise, the aQa mass spectrometer will not start data acquisition as no injection signal is received.

Example:

```
Wait MS.Ready
Inject Blank=Inject
```

On the last page of the Program Wizard, select the **Review the program in a new window** option. This selection automatically opens the PGM editor as soon as the new PGM file is saved. The PGM editor allows defining the aQa mass spectrometer settings for the PGM file. Select the **Finnigan AQA** view via the respective icon in the left editor section. For information on how to create a method for the aQa mass spectrometer, see **Creating a Method for the aQa-MS**.

Sequence

Then, create a sequence for your HPLC- or IC system

a) Using the Sequence Wizard:

   Enter the created PGM file under step 4.

b) From a previous sequence:

   Copy the PGM file to a new sequence and enter the PGM file into the sample list.

Tip: Ensure that the **Operation** property of the aQa mass spectrometer is in **On** state. Otherwise, the gas flow and the probe heating are switched off and data acquisition cannot be started.

Then start data acquisition as usual (see **How to ...: Device Control Starting Data Acquisition**). The current mass spectrum can be displayed in the ➢*Control Panel*.

Creating a Method for the aQa-MS

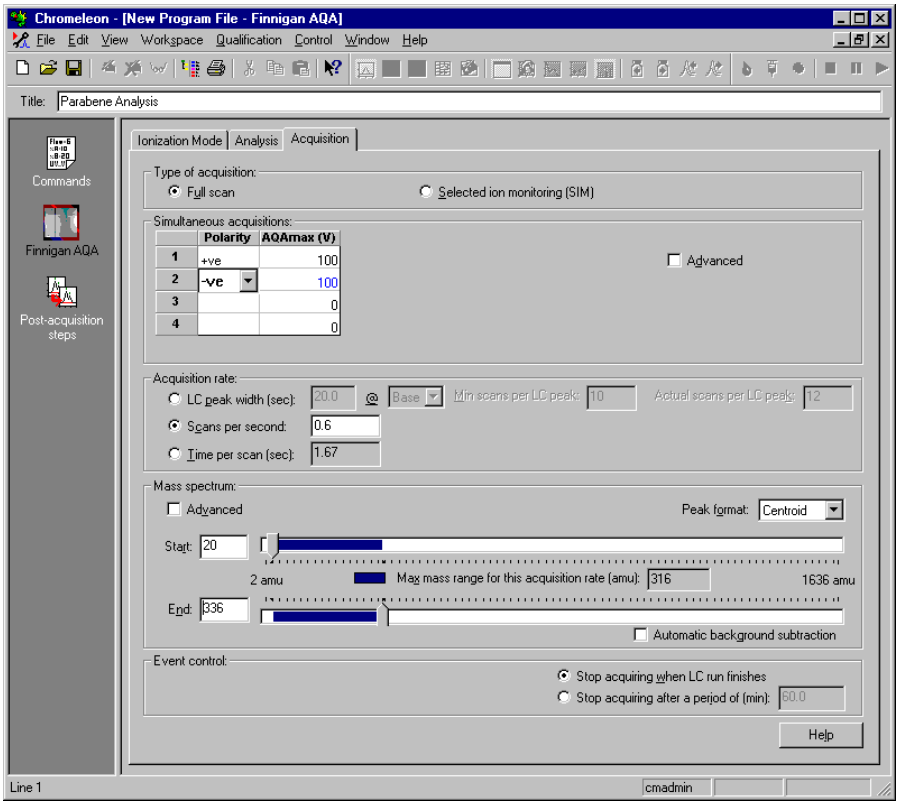
The **Finnigan AQA** view of the PGM editor allows creating a new method for the aQa ➢*Mass Spectrometer*. Open this view via the respective icon in the left PGM editor section. The view is part of ➢*Xcalibur* and serves to specify the method used by the aQa mass spectrometer.

As ionization mode, select **Electrospray** or **APCI** (chemical ionization at ambient pressure) on the **Ionization Mode** tab.

On the **Analysis** tab, set the sensitivity of the mass spectrometer via the detector voltage. Via **Advanced (from tune file)**, load a previously specified tune file or directly perform fine-tuning of the mass spectrometer via the **Tune…** button.

Caution: When using the Xcalibur method editor in the Dionex Chromatography Management System, the **Other detectors** section is irrelevant. Do **not** use this section for data acquisition with other detectors (e.g. UV detectors)! In this case, perform data acquisition as usual.

On the **Acquisition** tab, enter the aQa-specific signal parameters for ➢*Mass Spectra* acquisition:



Select the data acquisition mode first: ➢*Full-Scan* to acquire the entire mass spectrum for each analyte or ➢*SIM* to obtain MS chromatogram at a defined mass.

In Full-Scan mode, the **Simultaneous acquisitions** tab allows setting the polarity and maximum voltage at the aQa-MS for four single channels (➢*TIC*F channels). Under **Acquisition rate**, specify the rate for data acquisition; under **Mass spectrum**, specify the mass range for which to perform data acquisition.

Tip: This view of the PGM editor is part of Xcalibur. Thus, you can open the Xcalibur help via either the **Help** menu or the **Help** button. The Xcalibur help provides detailed information on mass spectra acquisition.

Acquiring MS Data in MCA Mode

The MCA (= Multi-Channel Analysis) mode allows calibrating the aQa ➢*Mass Spectrometer* and analyzing pure, low-concentration solutions of substances. Usually, the solution in question is provided to the mass spectrometer via infusion.

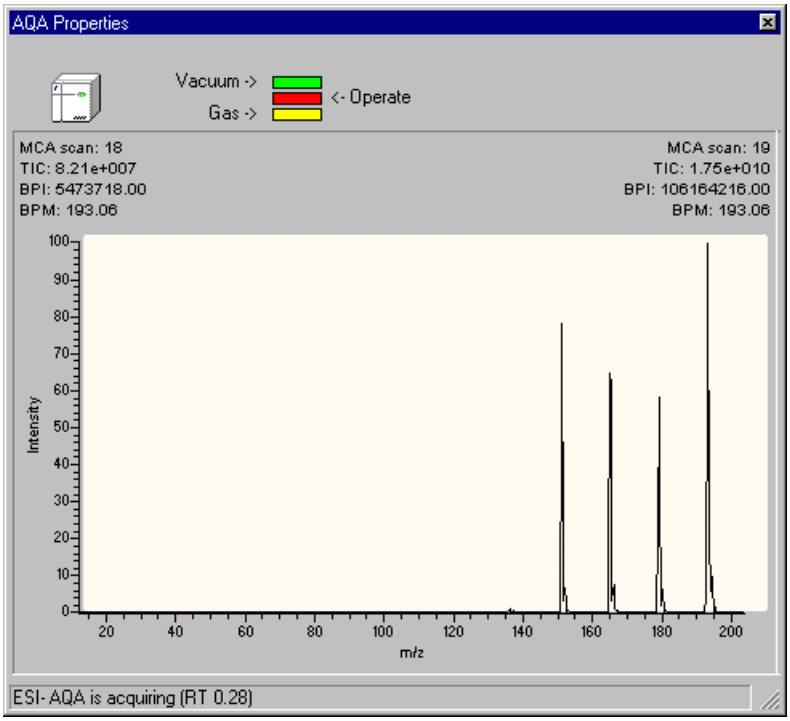
The MCA mode summarizes all ➢*Mass Spectra* of the single scans. Only the resulting mass spectra (up to four) are saved when the analysis is finished.

Caution: The MCA mode does not allow recording and showing mass spectra at a defined time of the chromatogram. Therefore, the MCA mode **is not suitable for chromatographic analyses**!

Data acquisition in MCA mode is as follows:

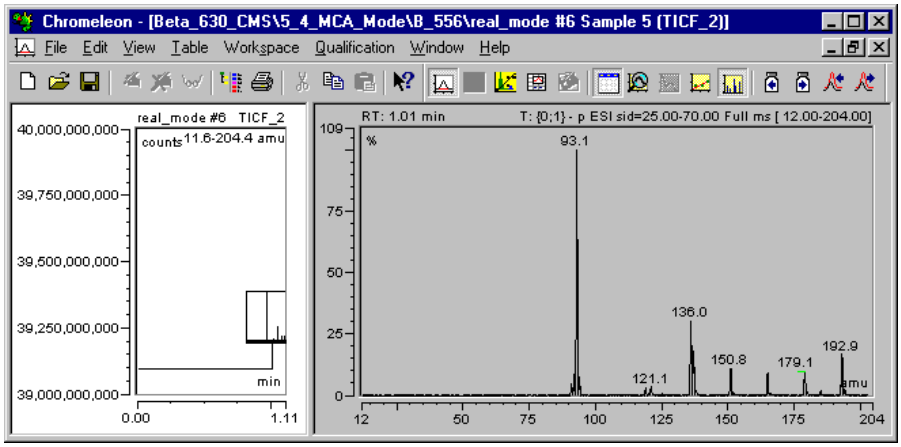
- Create a PGM file using the **Program Wizard** (see Control (Programmed) section).
- Ensure that the PGM file includes an **Inject** command even if you do not use an autosampler. Otherwise, the data acquisition cannot be started.
- In the QNT editor, open the **Acquisition** tab of the Finnigan aQa window. Under **Mass spectrum**, select **MCA** as **Peak format**.
- Save the PGM file and close the PGM editor.
- Enter the PGM file in your sequence and start the sequence in a batch.

The ➢*Xcalibur* window below opens automatically when data acquisition is started:



The status bar indicates the time that passed since the data acquisition was started. At the top left and right, the results of the last two scans are given.

As soon as the data acquisition is finished, you can view the results in the report of the Dionex Chromatography Management System. To view the results click the line at the highest retention time in the Chromatogram Plot using the Spectra Tool. This action opens the following view:



The "chromatogram" in the left pane contains one datapoint only that is at the highest retention time. To illustrate the summing up of the entire acquisition period, it shows one line in the height of the entire counts of all summed up mass spectra. In addition, only one single (entire) mass spectrum is displayed in the right window section.

Tip: As MCA mass spectra are formally retention time spectra, they cannot be inserted in the ➢*Printer Layout*. Therefore, for printing mass spectra the **Print** command of the **File** menu is available. In the opening dialog box, select the desired Printer Layout page that contains the mass spectrum.

Extracting Mass Traces Online

It is possible to extract ➢*Mass Traces* (MS chromatograms) and save them as additional channels. This is possible online during data acquisition but can be done later as well (see **Extracting Mass Traces Afterwards**).

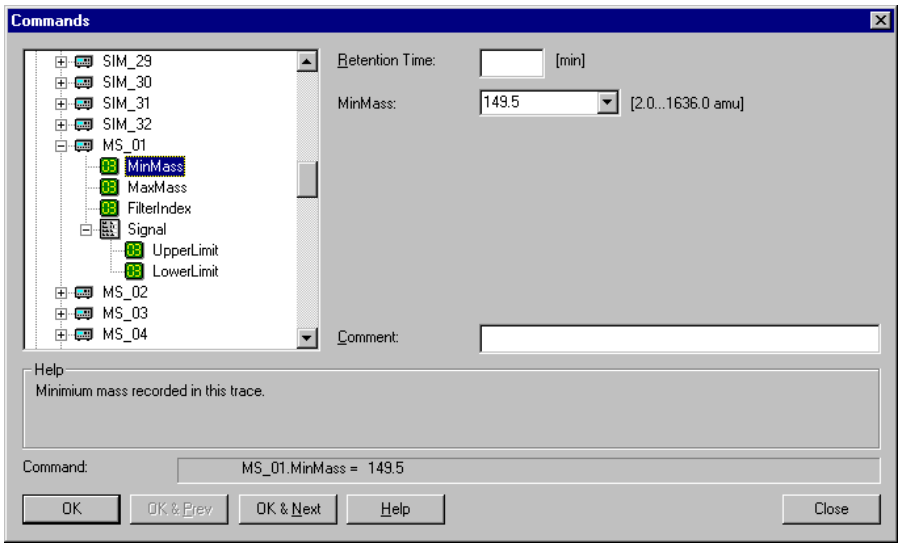
In the **Server Configuration**, define the required number of Online Mass Extract Channels on the **Installed Channels** tab. (Up to 32 channels can be defined.) These channel are automatically named MS_01 to MS_32.

Create a ➢*PGM File* for data acquisition in ➢*Full Scan* mode using the **Program Wizard** (**Control (Programmed)** section). Afterwards define the following parameters for the each single MS channel:

Parameter	Min.	Max.	Default	Usage
FilterIndex	0: NoFilter	n: TICF_n (n = number of the TICF channel configured in the Server Configuration)	0	Selects the filter for extraction. The filter indexes correspond to the four filters that can be defined in the aQa method. 0 = NoFilter means that the ➢*TIC* channel is used.
MinMass	2.0 amu	1636.0 amu		Minimum mass of interval that will be extracted.
MaxMass	2.0 amu	1636.0 amu		Maximum mass of interval that will be extracted.

As these parameters cannot be set using the Program Wizard, proceed as follows:

- Open the PGM File.
- Open the **Commands** dialog box via **Command** in the **Control** menu.
- Select your ➢*Mass Spectrometer* (listed by the name defined in the Server Configuration).
- Open the mass channel to be extracted (e.g. MS_01).
- Specify the individual parameters:



Use the **Upper/Lower Limit** parameters to specify the signal limits.

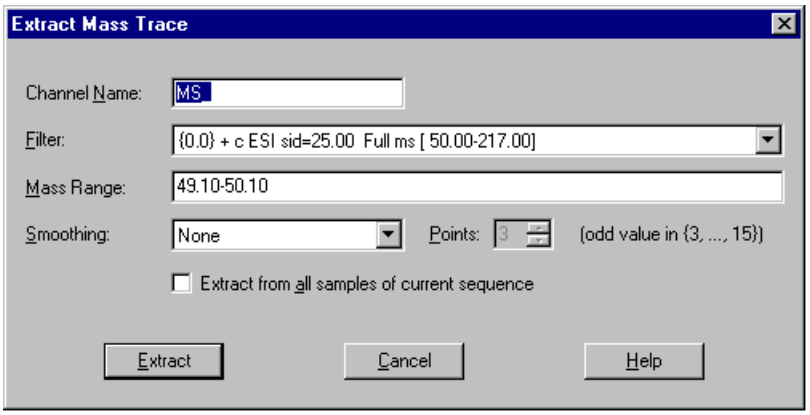
The corresponding section in the ➢*Program* could look as follows:

```
MS_01.MinMass =   149.5
MS_01.MaxMass =   150.5
MS_01.FilterIndex =  1
```

You can view these channels in the ➢*Control Panel* online during data acquisition.

Extracting Mass Traces Afterwards

If you did not extract a ➢*Mass Trace* online during data acquisition, you can do this afterwards as well (see **Extracting Mass Traces Online**). Place the mouse cursor in the respective ➢*Mass Spectrum* either of the **Integration** window or in the ⇒*QNT Editor*. Select **Extract Mass Trace/Range** from the context menu to open the following dialog box:



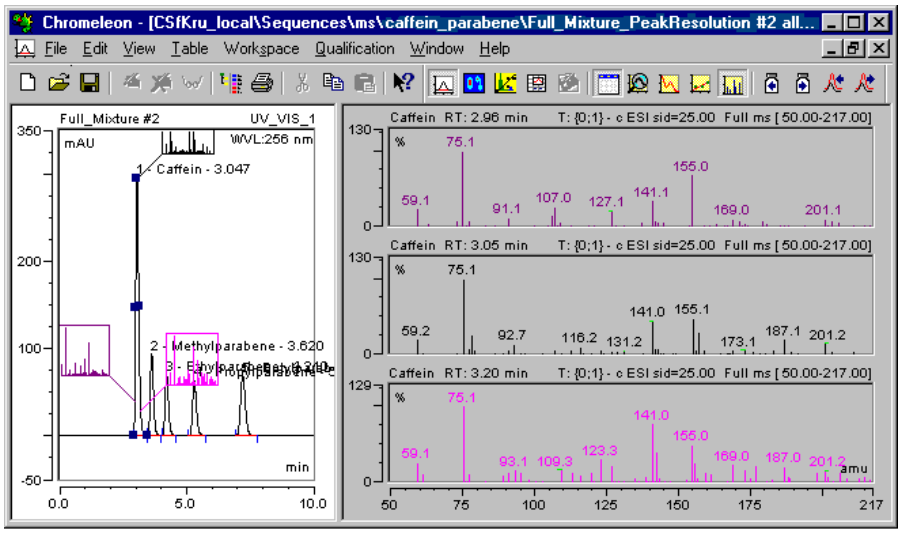
First, enter the name for the new channel. Then, select the desired filter and mass range as well as the ➢*Smoothing* type for the MS chromatograms and the number of data points to be used. Pressing **Extract** makes the new channel available for chromatogram representation.

If you know already before the data acquisition which channels you will need, you can omit this step and record the required channels right from the beginning (see: **How to ...: Actions Related to the aQa-MS Defining the Number of MS Channels**) or extract them as described above.

Showing Mass Spectra

The ➢*Mass Spectra* view can be added to almost all windows of the Dionex Chromatography Management System (Integration, ⇒*QNT Editor*, Printer Layout) provided ➢*Xcalibur* is installed. Enable the mass spectra view via the

button or the **Show Mass Spectra** command of the **View** menu. A mass spectrum can be added to the ➢*Printer Layout* via the **Mass Spectra Plot** option of the **Insert** command in the **View** or context menus.



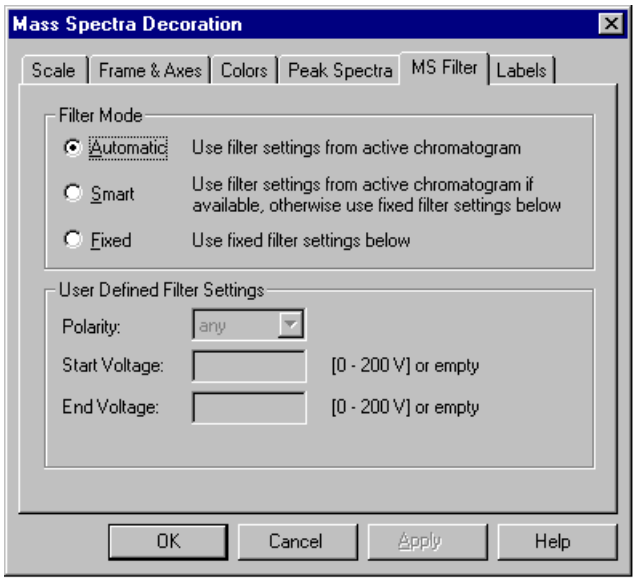
The appearance of the shown mass spectra may be quite different. It depends on the MS instrument method that was used. For details, see **How to …: Actions Related to the aQa-MS**  **Creating a Method for the aQa-MS**. For information on the parameters that should be used in this method to receive a certain mass spectrum, see the Xcalibur help.

In the captions of the single mass spectra plots, the peak name (if the mass spectrum of a peak is given) plus the retention time of the mass spectrum is given on the left. On the right, the acquisition mode is given: **Full ms** indicates ➢*Full-Scan* mode; **SIM ms** indicates ➢*SIM* mode.

In the caption of full-scan mass spectra, the entire mass range is given in parenthesis on the right. The fragmentation voltage that is given in front of the mode is important as well.

With mass spectra that were acquired in SIM mode, no entire mass spectra are available. These SIM mass spectra are extracted from single mass traces so that the resulting SIM mass spectrum usually shows gaps between the single traces. In the caption, the single mass ranges are given together with the corresponding fragmentation voltage behind the respective mass range (following a @ sign) on the right.

To set the MS specific parameters of the view proceed as follows: Place the cursor on the mass spectrum and right click to open the context menu. Select the **Decoration** option and make the desired settings on the **MS Filter** tab:



Reprocessing Mass Spectra

➢*Mass Spectra* usually include more details than UV spectra. Normally, however, they suffer from heavier noise. Especially with low signal intensity, they are considerably affected by the background spectrum. In order to use the information of mass spectra in the best possible way, reprocessing should be performed.

The Dionex Chromatography Management System offers two alternatives:

Spectra Bunching

To reduce mass spectra noise, you can bunch several single mass spectra to one entire mass spectrum. Spectra bunching can be performed both, for peak spectra and retention time spectra.

The **MS** tab of the ⇒*QNT Editor* allows bunching several single spectra to the left and the right of the chromatogram peak together with the peak maximum spectrum to one entire **peak spectrum**.

In the chromatogram, define the range for which to display the entire **retention time spectrum**. Use the **Spectra Tool** to select the desired range while pressing the left mouse button. You can perform this in a UV channel as well.

Subtracting Background Mass Spectra

Subtracting the background of mass spectra allows eliminating the influence of the background on the mass spectra. The background mass spectrum to be subtracted can be defined either for the entire chromatogram or automatically by the Dionex Chromatography Management System for each single peak.

The corresponding setting is made on the MS tab of the ⇒*QNT Editor* or in the chromatogram. The settings made in the chromatogram are saved to the QNT file of the current sample as well. Thus, your input affects all samples that are evaluated using this QNT file.

For details, see **How to…:**

Actions in the QNT Editor  **Processing Mass Spectra**

Actions in the Chromatogram  **Subtracting MS Background Spectra**

Tracking the Effects of Background Subtraction

You can track the effects of spectra subtraction directly in the mass spectra plot:

- Open the mass spectrum **Decoration** via the context menu and select **Peak Spectra** tab.
- Under **Background Subtraction Overlay**, select **Background Spectrum** to view the subtracted background mass spectrum in addition to the peak and retention time spectra.
- In addition, use **Original Spectra** to view the respective mass spectrum without subtraction.

Defining Further QNT Settings for MS

Handling the Retention Time Delay as against a second detector

Use the ➢*Delay Time* option on the **General** tab to take the retention time difference into account that is due to the time needed by the substances to travel from the first detector to the aQa ➢*Mass Spectrometer*.

For details, see **How to ...: Actions in the QNT Editor Defining the QNT Method for Several Detectors** in the **Creating a Peak Table** section.

Defining Peaks via Mass Spectra

For peak identification via mass spectra, use the six MS columns:

- Mass Peak 1 (as well as Mass Peak 2 and Mass Peak 3)
- MS threshold
- MS filter conditions
- Check MS retention times

For details, see **How to ...: Actions in the QNT Editor Identifying Peaks via Their Mass Spectra (MS Tracking) Detectors** in the **Creating a Peak Table** section.

Actions in the Server Configuration

Dionex Service connects, installs, and configures chromatography components, as well as installs the software of the Dionex Chromatography Management System.

If you need to modify the current installation, you will find useful information in the topics below:

Changing the Server Configuration

Selecting the Copy Protection Location and Entering the Key Code

Updating Moduleware

Before you connect new chromatography components to the data system or install additional PC plug-in boards and ➢*Sharable Devices*, see the information in the topics below:

Adding Timebases / Instruments

Installing a Sharable Device

If devices are connected to the Dionex Chromatography Management System via the ➢*DX-LAN*, certain built-in diagnostic and calibration ("System Wellness") functions are provided. These functions are enabled and disabled from the Server Configuration. See the following topic for details:

Enabling/Disabling System Wellness Functions

Changing the Server Configuration

Starting the "Server Configuration" Program

To start the Server Configuration, select ➢*Server Configuration* from the **Start/Programs** menu on the task bar. For example, for CHROMELEON, choose **Start/ Programs/ Chromeleon/ Server Configuration**.

Caution: Modifications to the server configuration are only possible if the corresponding ➢*Server* was started before! Normally, this is done automatically when starting the computer on which the server is installed.

Configuring the Server

Double-click the name of the server whose configuration you want to extend or change. Then enter the ➢*Key Code* and the type of **Software Protection**.

Adding Components

Select the name of the server of which you want to extend the configuration. Click the **+** character in front of the server name to view its current configuration.

Select via the **Edit** menu or in the context menu:

- **Add Timebase** to install a ➢*Timebase* on the server. Enter the name of the timebase in the **Edit** box.
- **Add Sharable Device** to install components that can be assigned to several timebases. This includes e.g. PC plug-in boards as the A/D Converter or the Pump Control Board.
- **Add Device** to add further chromatography instruments to a timebase. Select the instrument from the list. Only one instrument can be added at a time.

Note: When the timebase is created, a corresponding folder is also created in the Browser. This folder has the same name as the timebase and contains a default Sequence table and a folder for **Protocol Data** files for the timebase.

Configuring Components

Click the component to configure and select the item **Properties** from the context menu. Each configurable component has one or several tab dialog boxes for alternative settings.

Refer to context-sensitive online help for information on possible settings.

Deleting Components

Click the component to delete and select the item **Delete** from the context menu.

Note: When deleting a timebase, all instruments installed below this timebase are also deleted. The same applies to deleting single hardware components or the complete hardware. If you select a server and choose **Delete**, the components and the installation file CMSERVER.CFG are deleted.

Copying or Moving Components

Each selected component can be copied to the clipboard via the **Copy** command and can be inserted in a different place via **Paste**. It is also possible to **Cut** single components. Alternatively, both actions can be performed via **Drag & Drop.**

Access Control for Servers and Timebases

The Dionex Chromatography Management System not only allows restricting the **Access Control** for ➢*Datasources*, directories, and sequences (see **How to ...: Actions in the** ➢*Browser* **Locking Datasources, Directories, and Sequences**), but also for servers and timebases.

- Select a *server* and choose the **Properties** command (or double-click) to change the server settings.
- Select a *timebase* and choose the **Properties** command (or double-click) to change the timebase settings.

Note: Server and timebase can be accessed independently of each other. However, a timebase can only receive the rights of the corresponding server, i.e. operations prohibited on the server (e.g. Monitoring) are automatically prohibited on the underlying timebase.

- From the right list box (**List of All Groups**) on the **Access Control** tab, choose the ➢*Access Groups* that should receive access to the server or the timebase. Then, move the selected A-groups to the left list box via **Add** (**Access Groups**). Each user who is a member of one of the selected A-groups, can now access the server or the timebase (provided the user has the control privilege).

When you press the **Remove** button, the members of the corresponding A-group will no longer be able to access to the server or the timebase.

Under **Allow Remote** you will find options for controlling the remote operation, i.e. network access to a server or a timebase from a different PC. These options apply *exclusively* to the access via a network connection!

- Select **Monitoring** to enable other users to monitor the server or timebase.
- Select **Control** to enable other users to perform control access to the entire server or a specific timebase.
- Select **Data Acquisition** to enable other users to start the ➢*Data Acquisition* on a specific timebase.
- Select **Batch Control** to enable other users to start ➢*Batch Processing* on a specific timebase.

Note: Activating an option is possible only on a timebase if the corresponding operation is also permitted on the corresponding server!

Saving the "Server Configuration"

Each modification to the **Server Configuration**, e.g. adding, moving, deleting, or configuring single components, can be saved. There are two possibilities:

- **Save Installation (Name)** saves the current server configuration as a new configuration directly on the server.
- **Save as** saves the current server configuration with a freely selectable name (extension **CFG**) in any directory. The file **CMSERVER.CFG** is not overwritten and is still valid! Configuration files saved with this method are "personal" server configuration files. These enable the user to quickly change from one installation environment to another by simply loading the file.

Loading the Personal Server Configuration to a Server ("Import")

To use a personal server configuration as the valid server configuration CMSERVER.CFG, perform the following steps:

- Start the **Server Configuration**.
- Activate the server, for which the personal server configuration is to be valid.
- Select the **Import...** function from the **File** menu and specify the name and the directory of the personal server configuration. The configuration is loaded to the server.
- Select **Save** to save the personal server configuration under the name CSERVER.CFG. The previous file with this name is overwritten with the contents of the personal configuration. All changes are indicated in the file tree of the **Server Configuration** or when opening the corresponding tab dialog boxes.

Check Configuration

After installing and configuring new components, the current server configuration should be checked.

Choose the **Check Configuration** command from the **Server** menu to start the check.

The Dionex Chromatography Management System shows the result in a separate dialog box. If no errors or conflicts occur, the current server configuration can be saved.

If the system issues one or several warnings, it is up to the user whether to change the current configuration or not.

If the system issues an error message, the cause must be found and remedied. Only then can optimum operation be ensured.

Installation Configuration Report

The configuration report contains information on the server itself (e.g. name, key code, copy protection, access groups) as well as the connected timebases (name, access groups). In addition, the report lists the settings of the instruments assigned to an instrument.

Thus, it is possible to see whether and if so, which channels of a detector are used and the corresponding settings (**Offset**, **Factor**, ..), the **Sharable Devices** the configuration contains, etc.

- Choose the **Create Report** command from the **Server** menu to generate a report.
- Press the **Save** button to store the report in the **CMINST.LOG** file. The old file is then renamed to **CMINST.OLD**. Caution: The report is always saved to the BIN directory of the server!
- Press the **Print** button to copy the report to the **Notepad** text editor and to print it from there. After creating the report, it is also contained in the Windows clipboard and can be inserted in other applications.

The report is also available via the Windows clipboard.

Selecting the Copy Protection Location and Entering the Key Code

Depending on whether you want to enter the software protection location and the ➢*Key Code* for a server PC or for a client PC, perform the following steps:

- In the case of the client PC, select **Preferences** in the **File** menu of the Dionex Chromatography Management System client. The **License** tab of the **Preferences** dialog box allows you to select the copy protection location and to enter the key code as described below.
- In the case of a server PC, open the **Server Configuration** by clicking **Server Configuration**. Double-click the appropriate server name to access the **General** tab. The options described below are only possible if the corresponding ➢*Chromatography Server* was previously started! Generally, this is performed automatically when starting the computer on which the server was installed. If this is not the case, start the Dionex Chromatography Management System via the ➢*Monitor Program*.

Selecting the Software Protection Location

Specify whether your system is protected via ➢*PAL*, ➢*Dongle*, or ➢*License Server*. If applicable, proceed as follows to enter the location of the PAL plug-in board:

- Click the **Hardprotect** option if a separate PAL plug-in board protects your system.

- Click one of the options **Dionex A/D Converter, UVD340S/170S Interface,** or **Pump Control Board**; if the PAL is located on the corresponding Dionex A/D board, the UVD340S/170S interface board or the pump control board.
- Click the **Dongle** option, if your system is protected by a dongle on the parallel PC interface.
- Select **License Server** if your license was generated by a license server. The edit field for the key code will be disabled. Clicking the Browse button "**...**" on the right of the **License Server** opens another dialog for selecting the computer on which the license server of your Dionex Chromatography Management System is running.

Entering the Key Code

The key code is also entered via the **Properties** or **License** dialog box. Enter the 12-digit key code in the corresponding field.

Updating Moduleware

To install new versions of ➢*Moduleware* on modules connected to the ➢*DX-LAN*:

1 Insert the CD containing the new Moduleware version into the CD drive.

2 Start the ➢*Server Configuration* program by selecting **Server Configuration** from the **Start/Programs** menu on the task bar. For example, for PeakNet, choose **Start/ Programs/ PeakNet/ Server Configuration**.

3 Select **Dionex DX-LAN Card** under **Sharable Devices** and select **Properties** from the **Edit** or context menu.

4 Select the **Update Moduleware** tab. The names of the currently connected modules, their DX-LAN ID numbers, and current Moduleware versions are displayed.

5 Click the **Select** button.

6 Select the file containing the new Moduleware version and click **OK**. The selected file appears in the **Moduleware File** box.

7 Select the name of the module to be updated from the list of modules; click the **Update** button. Repeat this step to update additional modules of the same type.

☞ ***Tip***: Make certain the Moduleware matches the module type before updating. Downloading the wrong type of Moduleware can corrupt the module's memory.

The new Moduleware version is downloaded to the selected module. The new version number will appear in the list. For some modules, for example, the AD25 detector, the module's BIOS is also included in the Moduleware file and is updated at the same time as the Moduleware.

Adding Timebases / Instruments

Connection via Serial Interface

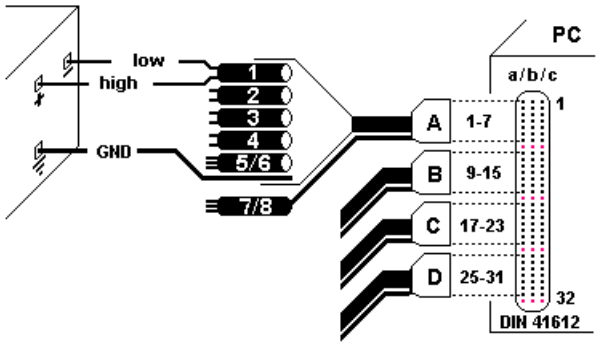
The Dionex Chromatography Management System is capable of integrating a large number of different chromatography instruments into the existing chromatography system. The prerequisite for this is that the instrument and the data system must be connected via an RS232 interface and that the appropriate device ➢*Driver* must be available for the instrument. If this is the case, the new instrument is configured via the ➢*Server Configuration* of the Dionex Chromatography Management System (see **How to ...:Actions in the Server Configuration Changing the Server Configuration**).

Connection via the A/D Converter

Instruments delivering analog ➢*Signals* are connected to the ➢*A/D Converter* via an A/D converter cable. If, for example, you want to record a signal via channel 1, you connect the positive pole (+) of the instrument with the wire "high" of channel 1. Accordingly, connect the negative pole (-) with "low" and the A/D converter ground wire (GND) with the instrument ground.

The connector bar (DIN 41612) of the A/D Converter (3 rows - a/b/c - each for 32 input pins) allows connecting a maximum of four A/D converter cables. Between the connectors, one row of pins is left free.

Via each cable (A/B/C/D), four analog signals (1/2/3/4) and two times two digital signals (5/6/7/8) can be recorded. Two ➢*Remote Inputs* **Dig.Inp1/2** use one ground connection (gnd).



Now, start the **Server Configuration** to install/configure the **Sharable Device Dionex AD Converter**. The channels of the A/D converter are then available for installing instruments with analog signal output.

Connection via a DX-LAN Card

The Dionex Chromatography Management System can control multiple chromatography instruments via a ➢*DX-LAN*. Each instrument and the PC on which the Dionex Chromatography Management System is installed must be equipped with a DX-LAN interface card, connected with DX-LAN cables, and have the appropriate device driver installed. (For details, see **Installing the DX-LAN-Card**.)

After the DX-LAN is connected, start the **Server Configuration** and add the DX-LAN card to the server configuration as a **Sharable Device** (For details, see **Adding the DX LAN Card to the Server Configuration**.) Then, add the DX-LAN devices to one or more timebases.

Connection via the Dionex UCI-100 Universal Chromatography Interface

To control chromatography instruments via the Dionex Chromatography Management System, a **Dionex Universal Chromatography Interface (UCI-100)** can be installed between the Dionex Chromatography Management System and the respective instrument to be controlled. Data transmission is via the USB interface. An Ethernet interface will also be available in future. In addition, the appropriate drivers must be installed and the UCI-100 Universal Interface included in the Server Configuration as a Sharable Device.

For installation information, see **Installing the Dionex Universal Chromatography Interface (UCI-100)**.

Installing a Sharable Device

For PC plug-in boards, switch off the PC, open the cover, and select an appropriate slot. Configure the PC board, as described in the operating instructions and insert it in the PC.

Start the ➢*Server Configuration*, select the required sharable device, and initialize it, as described in the user manual. For detailed installation notes, see the following topics:

Installing the A/D Converter
Installing the 12-Bit-DAC-Board
Installing the 16-Bit-DAC-Board
Installing the Pump Control Board
Installing the Dionex 16-fold Relay Board
Installing the Serial Interface Board
Installing the Dionex DX-LAN Card

Tip: Ensure that the space between the **A/D Converter** and the PC boards is sufficient, as PC boards radiate strong electromagnetic fields due to high-frequency digital currents.

For detailed information on the UCI-100 Universal Chromatography Interface, see **Installing Dionex Universal Chromatography Interface (UCI-100)**.

Enabling and Disabling System Wellness Functions

When a System Wellness supported device is added to a timebase in the Server Configuration, two additional tab pages, Calibration and Diagnostics, are included in the Properties dialog box for the device. These tab pages let you enable or disable individual calibration and/or diagnostic functions. By default, all calibration and diagnostic functions are enabled.

☞ ***Tip***: For a list of System Wellness supported devices, see **System Wellness Overview**.

Follow the steps below to disable calibration and/or diagnostic functions for a device or enable functions that are currently disabled.

1. Start the Server Configuration.
2. Under the ➢*Timebase*, select the device for which you want to disable or enable the calibration and/or diagnostic functions.
3. Select **Properties** from the **Edit** or context menu and select the **Calibration** or **Diagnostics** tab.
4. Enable or disable individual calibration or diagnostics functions by clicking the **Activate** box next to each function in the list. To enable or disable all calibration or diagnostics functions, right-click and select the **Activate All** or **Deactivate All** command from the context menu.

Device Control

Extending a Program

In addition to the standard commands of the ➢*Program*, which are easily created with the **Program Wizard** (**see Control (Programmed)** section), the Dionex Chromatography Management System offers a number of additional ⇒*Control Commands*. The functions and the syntax of these commands are described in the respective control topics below.

Control - Pumps

Control - Autosamplers

Control - Detectors

Control - Fraction Collector

Control - IC, GC, and Temperature

Control - Special Commands, Relays, and Others

- Transfer the structure and syntax of the commands that you want to use to your program file.
- Via **Cut & Paste**, each command can be inserted directly from Online Help at the appropriate position in the standard program.
- Specify the time when to execute each command.
- Save the result of your input as a PGM file.

Control - Pumps

The following commands are available for pump control.

For the "simple" commands, see **Pump Commands**
For further details, see:

Setting the Flow Rate

Determining the Solvent Composition

Determining a Gradient

Determining Pressure and Pressure Limits

Starting/Stopping the Pump Flow

Holding the Pump Flow

In addition, see the following information on

Recording the Pump Pressure

Setting the Automatic Pre-Compression Control

Viewing Leak Sensor and Workload Status.

Pump Commands

A pump can be controlled as follows:

Hold / Continue Gradient

```
0.000   HoldMode                  = On / Off
```

Alternatively, the following short command is valid:

```
0.000   ⇒Hold                     or
0.000   ⇒Continue
```

Stop Pump Flow/Gradient

```
0.000    StopMode                = On  or
0.000    ⇒StopFlow
```

Determining ⇒*Pressure Limits*

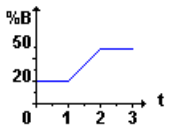
```
0.000    Pressure.LowerLimit     = Value[bar]
0.000    Pressure.UpperLimit     = Value[bar]
```

Generating a Flow or % Gradient

The flow or solvent value determined for the time t is continually adjusted to the following flow or solvent command. If the two values coincide, the flow or solvent value is kept at a specific level (see ramp profile 0 to 1), if they differ from each other, the value is modified. The difference between the two time values corresponds to the length of the ramp (see ramp profile 1 to 2min).

```
0.000    %B.Value    = 20
1.000    %B.Value    = 20
2.000    %B.Value    = 50
3.000    %B.Value    = 50
```

Ramp Profile

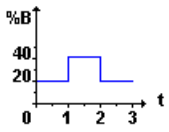


☞ ***Tip***: Dionex GP40/GP50, IP20/IP25, IC20/IC25/IC25A, GS50, and IS25 pumps do not deliver flow gradient ramps. Instead, changing the flow rate between one time value and the next, results in an immediate change in the flow rate (step change).

To determine a sharp increase, two different values must be defined at the same time. The start and end values must be entered at the exact times (see rectangle profile at the time t=1min).

```
0.000    %B.Value    = 20
1.000    %B.Value    = 20
1.000    %B.Value    = 40
2.000    %B.Value    = 40
2.000    %B.Value    = 20
3.000    %B.Value    = 20
```

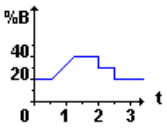
Rectangle Profile



By combining the just mentioned possibilities, any multi-step gradient profile can be realized, e.g.:

```
0.000    %B.Value    = 20
0.500    %B.Value    = 20
1.500    %B.Value    = 40
2.000    %B.Value    = 40
2.000    %B.Value    = 30
2.500    %B.Value    = 30
2.500    %B.Value    = 20
```

Multi-Step Profile



Instead of the arbitrarily selected quantity **%B** used in these examples, any other solvent (see ⇒*%A, %B, %C, %D*) or the flow rate can be changed.

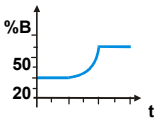
Creating a Non-Linear Gradient Ramp (Dionex GP40/GP50/GS50 pumps only)

A ➢*Curve* command instructs the pump to apply the selected curve number when adjusting the solvent composition between two retention times. In the example below, the Curve = 8 command at 2 min creates a concave ramp between 1 and 2 min.

Consecutive commands with identical solvent compositions generate an isocratic segment, regardless of the curve number selected (see 0 to 1 min and 2 to 3 min below).

```
0.000    %B.Value    = 20
1.000    %B.Value    = 20
2.000    %B.Value    = 50
         Curve       = 8
3.000    %B.Value    = 50
```

Non-Linear Ramp Profile



Setting the Flow Rate

For non-controlled pumps, the ⇒*Flow* rate is set directly on the instrument (also, see the Operating Instructions of the instrument).

For controlled pumps, the flow rate can be set via the corresponding controls on the **Control Panel** (slider, edit field, or button):

- To set a higher or lower flow rate, use the mouse to move the gauge slider in the desired direction.
- Enter the desired flow rate value in the edit field via the keyboard. Confirm your input by pressing Enter (Return).
- Click a button to execute the assigned function.

- Alternatively, choose the **Flow** command from the **Control** menu.

Including the **Flow** command in the ➢*Program* is also possible (see **How to ...: Actions in the PGM Editor** **Creating a Program**). Example:

```
0.000   Pump.Flow          = Value[ml/min%]   ;HPLC/IC pump
0.000   InjectorB.flow     = Value[ml/min%]   ;GC HP5890
```

Several **Flow** commands result in a ➢*Flow Gradient*. For a description on how to enter gradients, see **How to ...: Device Control** **Determining a Gradient**.

Determining the Solvent Composition

Manually

For non-controlled pumps, solvent composition (see ⇒*%A, %B, %C, %D*) is set directly on the instrument (also, see the Operating Instructions of the instrument).

For controlled pumps, the data system features the appropriate controls (sliders, edit fields, switches, etc.). Depending on the control panel layout, the values for %B, %C, and %D can either be set via a slider or via an edit field.

- Use the mouse to move the slider of a gauge in the desired direction.
- Enter a value in an edit field via the keyboard, then press Enter (**Return**).
- Select the ⇒*Flow* command (from the **Control** menu) to determine a **How to ...: Device Control** **Determining a Gradient**.

Programmed

By entering the commands

```
t=....   %B.Value      = Value[%]
t=....   %C.Value      = Value[%]
t=....   %D.Value      = Value[%]
```

in the ➢*Program*, the solvent composition can be changed via the program. If the command is entered several times for at least one component, the result is a ➢*% Gradient*.

For details, see **How to ...: Actions in the PGM Editor Creating a Program**

Determining a Gradient

You can determine the gradient in two ways, either manually from the panel or via a program:

Manual Input

For each installed instrument for which a gradient is determined, the device-specific settings can be changed in tab dialog boxes. Currently, ⇒*Flow* and ➢*%* gradients can be entered for HPLC and IC pumps; and temperature, pressure, and flow gradients can be specified for gas chromatographs. The different gradients can be run either as ramps (in IC, also, see ➢*Gradient Curves*) or as ➢*Step Gradients*.

- Choose the **Flow** command from the Control menu or use the shortcut **Ctrl+F**.
- On the **Gradient** tab (for HPLC/IC or **GC** and **Column1/2** for gas chromatographs), select the desired gradient.

Programmed Input

The easiest way to create a new program is by using the **Program Wizard** (see **Control (Programmed)** section). Open the Wizard via **New** in the File menu and select **Program File**.

HPLC/IC Selecting **Multi-Step Gradient** on the **Pump Options** tab opens the tab dialog box **Flow Gradient Options**, which corresponds to the **Gradient** tab during manual input.

GC On the **GC Options** tab (or the **Front/Back Inlet Options** tabs), select **Ramped Temperature** to program a temperature gradient. In the same way, flow and pressure gradients can be determined on the tabs **Column1** and **Column2** via the options **Ramped Flow** and **Ramped Pressure**.

Entering "Basic points"

HPLC/IC

- In the **Retention** column, enter the time (relative to the injection time) of the desired modification.
- In the **Flow** column, enter the new value for the flow rate.
- In the **%B**, **%C**, and/or **%D** columns, enter the new value for the delivered solvent composition. %A is the difference between the total of the entered values and 100%.
- For Dionex pumps GP40, GP50, and GS50 only: Enter a value in the **Curve** column to determine whether the pump delivers a linear or ➢*Curved Gradient*. Curve 5 (the default) is linear; curves 1 - 4 are convex upward and curves 6 - 9 are concave upward.
- Press the **Insert Line** button to append another line to the table. After appending the first new line, further lines are appended automatically, as necessary. The option can be switched on and off via the **Autom. Append New Lines** command of the context menu.
- Press the **Delete Line** button to remove unnecessary lines from the table.
- Red coloring of the corresponding cell marks each wrong entry. Invalid entries must be corrected immediately.
- Superfluous information can be deleted from a previously selected area by pressing the **Clean Up** button.

- Missing values between two or more time values can be calculated via the **Interpolate** button. The values are automatically added to the table.
- Select the **Fill Column** command in the context menu to fill the cells in the column with the currently selected value. Only the cells below the selected value are filled.

In a graphical representation, each flow and solvent value of the value table is represented as a point. By interpolation between the basic points of a column, an area gradient profile is created. The solvent areas are represented in their caption color; the flow rate is displayed as a narrow line.

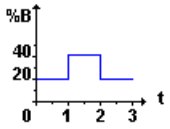
Direct Input into a Program

Knowing the syntax of ➢*Programs*, you can directly determine the gradient in the program. By entering the ⇒*%A, %B, %C, %D*, ⇒*Flow*, and **Temp**. commands in the program, solvent composition, flow rate, and temperature can be modified at a precise time. The gradient profile results from the change in value of a certain quantity at the time t.

☞ ***Tip***: The Dionex GP40/GP50, IP20/IP25, IC20/IC25/IC25A, GS50, and IS25 pumps do not deliver *flow* gradient ramps. Instead, changing the flow rate between one time value and the next, results in an immediate change in the flow rate (step change).

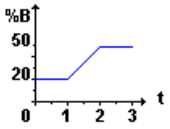
Example: The three different profiles are realized via the respective commands listed below the profiles.

Rectangle Profile



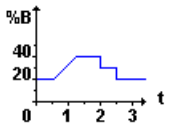

```
0.000 %B.Value = 20
1.000 %B.Value = 20
1.000 %B.Value = 40
2.000 %B.Value = 40
2.000 %B.Value = 20
```

Ramp Profile




```
0.000 %B.Value = 20
1.000 %B.Value = 20
2.000 %B.Value = 50
```

Multi-Step Profile




```
0.000 %B.Value = 20
0.500 %B.Value = 20
1.500 %B.Value = 40
2.000 %B.Value = 40
2.000 %B.Value = 30
2.500 %B.Value = 30
2.500 %B.Value = 20
```

For a rectangle profile, indicate exactly how long the specific solvent composition is valid. If the composition is changed at the same time as another

percent command is defined, the change in solvent composition is executed immediately. The solvent percentage achieved is then maintained until replaced by another command.

To realize an increase over a longer period, the start value and end value must be specified with the precise time. The difference between the two time values corresponds to the duration of the increase (see ramp profile).

By combining the above-mentioned possibilities, any multi-step gradient profile can be realized.

For details on entering basic points in GC, see **Determining a Gradient (GC).**

Determining Pressure and Pressure Limits

Pressure

Determining the operating pressure is only possible for gas chromatographs. The control realizing the setting depends on the layout of the currently used control panel.

- Determine the pressure via the corresponding slider or enter the value in the edit field via the keyboard.

Pressure Limits

Some device drivers offer the possibility to determine the upper and lower pressure limits.

- Enter the corresponding value in the edit field using the keyboard, or
- Position the slider for the upper and lower pressure limits with the mouse cursor. Assign different colors to the controlling sliders (see **How to ...: Actions in the Control Panel Modifying a Control**) so that they indicate whether a pressure limit is exceeded or whether it is within the selected limits.

When defined ⇒*Pressure Limits* (e.g. of an HPLC pump) are exceeded, the Dionex Chromatography Management System automatically switches off the flow, issues an error message and stops the sample batch, as necessary. In addition, all operations are logged in the ➢*Audit Trail*.

Pressure limits can be determined by entering the following commands in the ➢*Program*:

```
0.000    X.Pressure.LowerLimit     =Value[bar]
0.000    X.Pressure.UpperLimit     =Value[bar]
```

where X refers to the name of the instrument defined in the **Server Configuration**.

Starting/Stopping the Pump Flow

- Execute the ⇒*StopFlow* command to stop the pump flow and the ➢*Gradient* formation. During a running batch, ➢*Batch Processing* is stopped.
- Perform the ⇒*Continue* command to continue the pump flow, a running gradient program, or batch processing.

☞ ***Tip***: The ⇒*Hold* command only interrupts gradient formation and automatic batch processing, but not the pump flow.

Holding the Pump Flow

- Use the ⇒*Hold* command to interrupt the ➢*Gradient* formation or a running batch. During a running batch, ➢*Batch Processing* is stopped.

In the **Hold** mode, the pump delivers with constant flow rate and solvent composition, until a stop or a ⇒*Continue* command is entered.

Recording the Pump Pressure

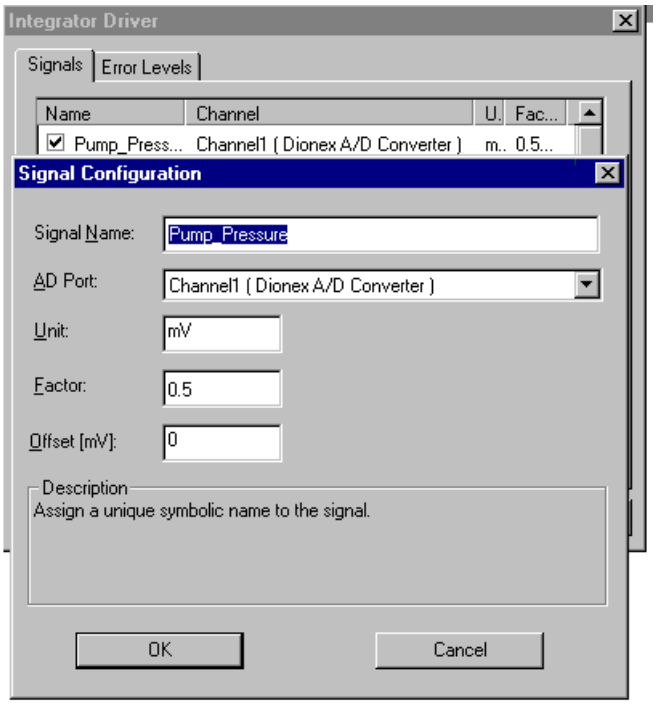
To check whether signal variations are related to pressure variations, i.e., whether the pump causes those variations, we recommend recording the pump pressure as an additional signal.

Hardware Configuration

To be able to display the pump pressure an analog pressure output must be available on your pump. In addition, an ➢*A/D Converter* or an ➢*UCI-100 Universal Chromatography Interface* is required. Connect the pressure output of your pump to one of the free A/D board channels.

Server Configuration

Add an ➢*Integrator Driver* to the devices of the corresponding timebase. Name the unassigned signal e.g. **Pump_Pressure** and press **Change**.



Select the channel to which the pressure output of your pump is connected as **AD Port**. Enter under **Factor** how many bar correspond to an output voltage of 1 mV. For example, enter 0.5 bar/mV for the Dionex P580 pump or 5 bar/mV for the Dionex M480 pump.

Now, data can be recorded for the **Pump_Pressure** channel. Data acquisition can be defined as well in the ➢*PGM File* or by means of the ⇒*AcqOn* **Control** command in the ➢*Control Panel*.

Panel

- Being in the signal plot of your panel select the **Signals** command in the context menu.
- Select the desired signal under **Available Signals** (i.e., for the above example select **Pressure**).
- When starting the data acquisition, select the channel **Pump_Pressure** and define the ⇒*Step* (see **How to ...: Device Control**  **Starting Data Acquisition**).

Setting the Automatic Pre-Compression Control

With the automatic pre-compression control offered by the Dionex pump P 580, it is possible to consider the varying compressibility of different solvents. Automatic pre-compression control can also be used for unknown solvents.

With low-pressure gradients and isocratic pumps, pre-compression control is fully automatic. Choose the **Commands** option from the **Control** menu. Select the solvent and assign the solvent type **Automatic**.

The high-pressure gradient pumps must "learn" the automatic pre-compression control. Choose the **Commands** option from the **Control** menu. Then select the solvent. Assign the solvent type **Custom**. Set the flow to 100% of this solvent. Choose the pump **Learn** command. Wait at least 10 minutes (flow 1ml/min). Choose the corresponding pump **Freeze** command to save the optimum pre-compression setting. For detailed description, see the P580 Operating Instructions.

Change the flow to 100% of the next solvent. To set the pre-compression control, proceed as described above.

Viewing Leak Sensor and Workload Status

The Dionex pump P 580 allows display of the status of the leak sensor. In addition, you can view the ➢*Cumulated Workload*.

To create the corresponding controls, proceed as described in the following sections under **How to ...: Actions in the Control Panel:**

Modifying a Control Panel

Modifying a Control

Linking a Control to a Device

Choose **Commands...** from the **Control** menu. Under **Pump**, select **Leak** to view the status of the leak sensor. Click **Cumulated WorkLoad** to display the total workload [in mega joule, MJ] of the pump.

Control - Autosamplers

Depending on the ➢*Autosampler* type different commands are available. For an overview on the individual commands that are available for the different Dionex autosamplers, see:

Autosampler Commands (GINA 50)

Autosampler Commands (ASI-100 / ASI-100T)

Autosampler Commands (AS50)

The following pages provide details on:

Injecting a Sample

Setting Up Remote Injection

Defining Sample Preparation Steps (AS50)

Opening the AS50 Door during Operation

Monitoring the Status of the AS50

Autosampler Commands (GINA 50)

Suck (see ⇒*Draw*) / ⇒*Dispense* Sample

```
0.000   Suck        Position = Value, Volume = Value [µl],
                    Duration = Value [sec]
0.000   Dispense    Position = Value, Volume = Value [µl],
                    Duration = Value [sec]
```

Note: In the case of the Dionex Autosampler GINA 50, the corresponding operations can be synchronized with the data system via a remote input and the **Suck** and **Dispense** commands. The device automatically reports the completion of each operation to the data system. In the ➢*Program*, the wait command **Sucked** must be inserted. All following commands are executed only after the sampler confirmed the execution of the **Suck** command, i.e., after the sample has been drawn. The program performs this independently of the time required by the sampler for the suck and dispenses processes. This is shown in the following example:

```
0.000   Suck        Position = 20, Volume = 30, Duration = 0
0.000   Wait        Sucked
0.000   Suck        Position = 21, Volume = 30, Duration = 0
0.000   Wait        Sucked
0.000   Dispense    Position = , Volume = 60, Duration = 0
0.000   Wait        Sucked
0.000   ⇒Inject
```

Description of the program part: First, the Autosampler GINA 50 draws 30 µl solution from ⇒*Position* 20 and, upon completion, 30 µl solution from position 21. The entire drawn volume is dispensed in the current vial (current = last position if no other position is specified). Then, the injection volume, which has been specified in the sample list, is drawn and injected from there.

Short command syntax:

```
0.000   Suck        20, 30, 0
0.000   Wait        Sucked
0.000   Suck        21, 30, 0
0.000   Wait        Sucked
0.000   Dispense    Position = , Volume = 60, Duration = 0
0.000   Wait        Sucked
0.000   Inject
```

Relative Sample Location

The Dionex Autosampler GINA 50 is capable of executing the suck and the dispense commands relative to a certain sample position. The **Position+Location** is entered in the field **Position** of the **Suck** or **Dispense** commands. In the program this is expressed as follows:

```
0.000   Suck        Position = 20, Volume = 30, Duration = 0
0.000   Wait        Sucked
0.000   Suck        Position = Position+10, Volume = 30, Duration = 0
0.000   Wait        Sucked
0.000   Dispense    Position = Position+20, Volume = 60, Duration = 0
0.000   Wait        Sucked
```

Description of the program part: The autosampler takes 30 µl solution from position 20, moves 10 positions from the current position in the sample list, and takes 30 µl solution from there. Then, the 60-µl solution is dispensed into a vial that is located 20 positions from the current sample vial.

Air Segment

For the Dionex Autosampler GINA 50, the input position = 100 means an imaginary **Air Vial** from which a certain air volume can be sucked as a separating segment, e.g.

```
0.000   Suck        Position = 20, Volume = 30, Duration = 0
0.000   Wait        Sucked
0.000   Suck        Position = 100, Volume = 30, Duration = 0
0.000   Wait        Sucked
0.000   Suck        Position = 21, Volume = 30, Duration = 0
0.000   Wait        Sucked
```

Description of the program part: After 30 µl solution is sucked from position 20, 30 µl air is sucked before another 30 µl solution is sucked from position 21. Thus, the two solutions encounter each other.

Note: The **Segment** command should only be given in combination with the **Dispense** command, as otherwise the sucked air volume is also injected.

Dispense in Needle Seat

Entering position 101 in a **Dispense** command enables dispensing the volume contained in the needle into the needle seat of the Autosampler and thus into the waste container.

```
0.000   Dispense    Position = 101, Volume = 60, Duration = 0
```

Wash Injection Loop

The ⇒*Wash* command allows rinsing the injection loop of the Autosampler GINA 50 with the solvent. This corresponds to the **normal** solvent flow during the **Inject** command.

```
0.000   DEVICENAME.Wash    or
0.000   Wash
```

Lift/Lower Sample Needle

The ⇒*NeedleUp* command enables the lifting of the sample needle. When lifting the needle, a running Wash process is automatically interrupted, i.e. the solvent no longer flows through the injection loop but directly from the pump to the column.

```
0.000   NeedleUp
```

To lower the needle again the **Wash** command must be executed. Only then will the solvent flow continue through the sample loop (for details see ➢*Autosampler*).

```
0.000   Wash
```

The combination of the two commands prevents crystallization of substances in the sample loop.

For an overview on the individual commands for the GINA 50 or GINA 160 samplers, see: **Dionex Autosamplers GINA 50 and GINA 160.**

Also, see: **Autosampler Commands (ASI-100 / ASI-100 T).**

Autosampler Commands (ASI-100 / ASI-100T)

Many commands of the Dionex ➢*Autosampler* ASI-100/ASI-100T (ASI-100T = with temperature control) are similar to those of the GINA 50 (see **Autosampler Commands (GINA 50)**. However, there are some important differences, which are described below:

Sample Positions

The sample vials are situated in three different segments, which are distinguished by color. Within the segments, the vials are situated in different rows. Thus, the sample ⇒*Positions* are indicated as follows:

Letters according to their color describes the individual segments: R, G, or B (indicating the red, green, and blue segment, respectively). The different rows are described from the outer to the inner row: A, B, C, or D. The individual positions within the respective rows are numbered counterclockwise. The position RA1, for example, is in the outer row of the red segment (also, see the ASI-100/ASI-100T Operating Instructions).

Autosampler Configuration

Specify the device configuration before starting the actual program. It is important to define the sample positions for the reagents and the wash liquid. These positions are valid throughout the entire running time of the program:

```
0.000   Sampler.ReagentAVial   BB1
0.000   Sampler.ReagentBVial   BC1
0.000   Sampler.ReagentCVial   BA1
0.000   Sampler.WashVial       G99
0.000   Sampler.MixVial        R99
```

The following commands define the number of draw and dispense actions (for the **Mix** command):

```
0.000   Sampler.MixRepeat      3
```

⇒*Draw* / ⇒*Dispense* Sample / Mix

Specify which volume shall be drawn or dispensed (or drawn and dispensed for the **Mix** command) from which vial (depending on the selected option, see below) before issuing the respective commands:

```
0.000   MixSubject             option (see below)
0.000   MixVolume              value [µL]
0.000   Draw

0.000   MixSubject             option (see below)
0.000   MixVolume              value [µL]
0.000   Dispense
```

The following options are available for the **MixSubject** command:

Option	Description
MixVial	actual mixing vial position
Sample_Vial	vial for the actual sample in the sample list (actual Sampler.Position value)
WashVial	vial containing the wash liquid (actual Sampler.WashVial value)
Air	air (with the Draw command) and needle port (with the Dispense command), respectively
ReagentA (B, C or D)	Reagents A (B, C, or D) (actual Sampler.ReagentAVial value)

With the Dionex Autosampler ASI-100/ASI-100T, some commands must be synchronized with the data system, i.e., the sampler automatically reports the completion of the respective operation to the data system. In addition, the wait condition **Sampler.Ready** must be included in the ➢*Program*. The following commands are executed only after confirmation by the sampler that the command has been executed. This applies to the **Draw**, **Dispense**, **Mix**, **Test** commands, and ⇒*Wash* and is illustrated below:

```
0.000   MixSubject             Sample_Vial
0.000   MixVolume              30
0.000   Draw
0.000   Wait                   Sampler.Ready
0.000   MixSubject             ReagentA
0.000   MixVolume              30
0.000   Draw
0.000   Wait                   Sampler.Ready
0.000   MixSubject             MixVial
0.000   MixVolume              60
0.000   Dispense
0.000   Wait                   Sampler.Ready
0.000   ⇒Inject                Position = MixVial
```

Description of the program part: First, the Autosampler ASI-100/ASI-100T draws 30 µl solution of the current sample, and, upon completion, 30 µl solution of reagent A. The entire drawn volume is dispensed into the MixVial. Then, the injection volume, which has been specified in the sample list, is drawn and injected from this position.

Air Segment

Define the MixSubject as Air to draw an air segment. Use, for example, the following program part to draw two samples separated by an air segment to prevent early mixing in the needle and to ensure that an exactly defined reaction time is met.

```
0.000   MixSubject            ReagentA
0.000   MixVolume             100
0.000   Draw
0.000   Wait                  Sampler.Ready
0.000   MixSubject            Air
0.000   MixVolume             5
0.000   Draw
0.000   Wait                  Sampler.Ready
0.000   MixSubject            Sample_Vial
0.000   MixVolume             100
0.000   Draw
0.000   Wait                  Sampler.Ready
0.000   MixSubject            MixVial
0.000   MixVolume             205
0.000   Dispense
0.000   Wait                  Sampler.Ready
```

Description of the program part: After drawing 100 µl of reagent A, 5 µl of air is drawn before 100 µl of sample is drawn from the vial. Thus, the two solutions encounter each other in the mixing vial only.

Relative Sample Location

1. Different rings: The Dionex Autosampler ASI-100/ASI-100T can execute commands relative to a certain sample position. The Position + relative entry is entered in the field **Position** of the **Draw** or **Dispense** commands. In the program, this is expressed as follows:

```
0.000   MixSubject            Sample_Vial
0.000   MixVolume             30
0.000   Draw
0.000   Wait                  Sampler.Ready
0.000   Position              Position + RB1 - RA1
0.000   MixSubject            Sample_Vial
0.000   MixVolume             30
0.000   Draw
0.000   Wait                  Sampler.Ready
0.000   Position              Position + RC1 - RB1
0.000   MixSubject            Sample_Vial
0.000   MixVolume             60
0.000   Dispense
0.000   Wait                  Sampler.Ready
0.000   Inject                Volume=30
```

Description of the program part: The autosampler draws 30 µl solution from the actual sample vial, moves to the respective position in the RB ring, and draws 30 µl solution from this position as well. Then, the 60 µl solution is dispensed into the vial at the respective position in the RC ring. If the current sample is situated, e.g., at position RA3, another 30 µl would be drawn from position RB3, and the entire volume of 60 µl would be dispensed at position RC3. After that, 30 µl are injected from position RC3.

Note: To complete things, the **MixSubject** command is repeated with the argument **Sample_Vial** in the above program part. This is not requested as the data system maintains the latest setting. The second command (**= MixVolume**) could be omitted as well as it only repeats the argument "30."

2. Different segments: You can also place the samples to be derivated into the red segment, for example, and execute the mixing process with a reagent in the corresponding sample vial in the green segment using the following commands:

```
0.000   Sampler.MixVial        Position + GA1 - RA1
0.000   MixSubject             MixVial
0.000   Mix
```

The first line specifies that the corresponding vial in the green segment be used as a mixing vial for a sample in the red segment. For example, if you wish to process the sample at RB5, mixing takes place at position GB5.

3. Incrementing the positions: Another way is to increment the positions. Use the following example to define a position 5 after the current position for MixSubject:

```
0.000   Sampler.MixVial        Position + 10
0.000   MixSubject             MixVial
0.000   Mix
```

For example, if you wish to process the sample from position RB3, mixing will take place here in RB8.

Wash Needle

With the **Wash** command, the needle of the Autosampler ASI-100/ASI-100T can be rinsed with the wash liquid. The wash volume is drawn and dispensed into the needle seat.

```
0.000   WashVolume          value [µL]
0.000   Wash
```

For an overview on the individual commands for the ASI-100/ASI-100T sampler, see **Dionex Autosamplers ASI-100/ASI-100T**

Also, see the **Autosampler Commands (AS50)**.

Autosampler Commands (AS50)

Flush the Inject Port

The **Flush** and **Wait** commands must be in the order shown and they must occur before any other ➢*Autosampler* commands, or after all other autosampler commands.

```
Flush       Volume = Value [µl]
Wait        FlushState
```

Autosampler Options

All AS50 autosampler option commands must be grouped together in the ➢*Program*. Place them at the beginning of the program, before t = 0.000.You do not need to specify event times for the AS50 option commands.

```
Devicename.NeedleHeight             = Value [mm]
Devicename.CutSegmentVolume         = Value [µl]
Devicename.SyringeSpeed             = Value
Devicename.ColumnTemperature        = Off / Value [°C]
Devicename.TrayTemperature          = Off / Value [°C]
Devicename.Cycle                    = Value
```

Sample Prep

All AS50 autosampler sample prep commands (Dispense, Dilute, SetNeedleHeight, DelaySP, FlushSP, Mix, and Pipet) must be grouped

together in the program. Place them at the beginning of the program, after the AS50 option commands and before t=0.000. You do not need to specify event times for the sample prep commands. Include a **Wait SamplePrep** command after the sample prep commands to allow them to be completed before injection.

In the example below, 20µl is pipetted from vial 1 and delivered to vial 10. 200µl is dispensed from reservoir A into vial 10. The contents of vial 10 is then mixed by drawing in and then expelling 100µl of the vial contents. The mixing cycle is repeated 5 times.

***Note**:* Due to lack of space, commands are shown on two lines. Normally, one command must be entered on one line.

```
Sampler.Pipet     Volume = 20.0, SourceVial = 1,
                  DestinationVial = 10
Sampler.Dispense  Volume = 200.0, SourceReservoir =
                  Reservoir_A, DestinationVial = 10
Sampler.Mix       SourceVial = 10, NumberOfTimes = 5,
                  Volume = 100.0
Wait              SamplePrep
```

Relative Vial Location

In the sample preparation commands, a vial location can be specified either as an absolute position or as a relative position. In relative positioning, the CurrentVial is the current sample vial position, specified in the sample list in the Sequence. In the example below, 20µl of liquid is pipetted from the current sample vial and then expelled into the vial, 1 position past the current vial.

```
Sampler.Pipet     Volume = 20.0, SourceVial = CurrentVial,
                  DestinationVial = CurrentVial+1
```

Cycle Time

Cycle time controls the time between injections. When a cycle time is specified, the autosampler delays sample injection until the specified time has elapsed since the previous injection. This is accomplished with the **Wait CycleTimeState** command. When running a batch, the **Wait CycleTimeState** command in the first PGM file in the batch is ignored.

The following example sets a cycle time of 30 minutes.

```
       Cycle            =30
0.000  Sampler.Load
```

```
Wait              CycleTimeState
Sampler.Inject
```

Priming the Liquid Lines

The **Prime** command is used to prime the flush reservoir line to the sampling valve and the sample transfer line. In addition, if the sample prep option is installed, the Prime command is used to prime the lines from each installed reagent reservoir. The following example uses the prep syringe to prime the line to reservoir A with 2000µl.

```
0.000   Sampler.Prime     Volume=2000,    PrimeReservoir=Reservoir_A,
                          PrimeSyringe=Prep
```

For an overview on the individual commands for the AS50 sampler, see **Dionex Autosampler AS50.**

Injecting a Sample

Depending on the laboratory equipment, injection is performed

- Manually
- Via ➢*Autosampler* or
- Automatically (the injection is programmed).

How much of a substance is injected (⇒*Volume*) and from which Autosampler ⇒*Position* is determined by the user via the corresponding control on the control panel or via the **Inject** edit box of the **Control** menu.

Then the user executes the ⇒*Inject* command.

Reporting the end of the injection process to the data system completes successful injection. In the case of a hand-operated valve, this is via a contact closure relay. Modern autosamplers automatically send the message via the serial interface or ➢*DX-LAN*. After that, the retention time is started.

Hand-operated valve (manual injection):

The sample is injected via a µl-syringe into the needle seat of the hand-operated valve. In this way, it reaches the sample loop (**Load**). By switching the valve (**Inject**), the solvent flow is directed to the sample loop, and the sample enters the high-pressure circuit of the system. If correctly connected

(via a ➢*Remote Input*), switching the hand-operated valve triggers the **Inject** signal and thus the timer. Very exact operation is possible if the injected volume corresponds to the sample loop size. Then, the sample loop is completely filled. When switching the valve, the exact volume of the sample loop is injected without any loss.

Autosampler (manual injection):

Operation can be via the input panel of the instrument or via the PC. The more convenient method via the PC is only possible if the autosampler is connected with the data system via an RS232 interface or the DX-LAN.

- Choose the ⇒*Inject* command (**Control** menu) and determine the ⇒*Volume* and the ➢*Autosampler* position for the injection.
- If your control panel offers the corresponding controls, the parameters **Volume** and **Position** can be entered directly via an edit box.

The time required by the Autosampler to inject the sample can be indicated optically. For this, a color area or a lamp must be linked with the object property **Inject Wait** (for details, see **How to ...: Actions in the Control Panel Linking a Control to a Device**). In a controlled system, the pump is placed in ⇒*Hold* status during injection.

Automatic injection:

- Enter the **Inject** command at the time t = 0.000 in the ➢*Program*.

If the command is executed by an autosampler that is controlled by the Dionex Chromatography Management System, the sampler sends a signal back to the data system when injection is completed. The timer is then started.

When injecting via a hand-operated valve or an autosampler that is not controlled by the Dionex Chromatography Management System, the data system waits for a signal before it starts the timer. For example, with a hand-operated valve, the signal is given after switching the valve from **Load** to **Inject**, i.e., the execution of a program is delayed until injection is actually performed. This type of automatic injection requires connection of a remote input or remote start device via remote inputs (TTL or relay) and configuration of a remote inject device. See **How to ...: Device Control Setting Up Remote Injection**.

Caution: As an **Inject** signal is not specified, there can only be one injection unit per timebase, i.e., either a hand-operated valve or an autosampler is installed.

Setting Up Remote Injection

If the injection valve is not directly controlled by the Dionex Chromatography Management System, a ➢*Remote Inputs* (remote start) device can be set up to signal the data system when injection has occurred. The setup procedure consists of connecting the remote input device via TTL or relay, configuring a remote inject device in the ➢*Timebase*, and adding an ⇒*Inject* command to the ➢*Program*.

Tip: For the UI20, remote injection can be triggered by the remote input or by pressing the **Run** button on the UI20 front panel. For the DX-120, remote injection can only be triggered by the remote input. The **Load/Inject** button on the DX-120 front panel is disabled during remote control.

Connect the Remote Input Device (TTL or Relay Connections)

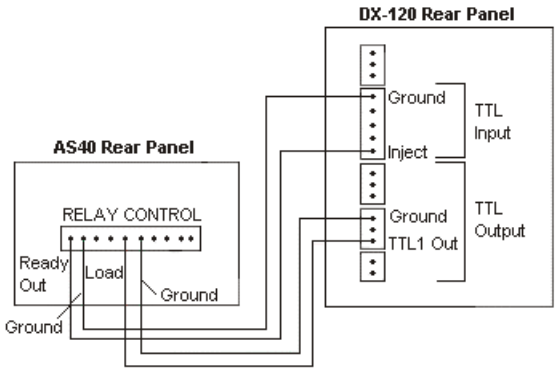
In order for the remote input (remote start) device to signal when injection has occurred, its remote input must be connected via TTL or relay to the injection valve or to another device, for example, an ➢*Autosampler*. When injection occurs, the injection valve or autosampler sends a signal to the remote input device. The remote input device in turn signals the Dionex Chromatography Management System that injection has occurred.

Example Connections: AS40 and DX-120

☞ ***Tip***: For detailed TTL and relay connection instructions, refer to the operator's manual for each device.

The following connections allow completely automated control of the AS40 and DX-120.

1. Connect the **Relay Control Ready Out** pin on the AS40 rear panel to the **Inject TTL Input** pin on the DX-120 rear panel.
2. Connect the **Ready Out Ground** pin on the AS40 to the **TTL Inputs Ground** pin on the DX-120.
3. Connect the **Load** pin on the AS40 to the **TTL 1 Out** pin on the DX-120.
4. Connect the **Load Ground** pin on the AS40 to the **TTL Outputs Ground** pin on the DX-120.



Configure a Remote Inject Device

1. Open the Server Configuration.
2. Select the timebase under which the remote input device is configured.
3. Select **Add Device** from the **Edit** or context menu.
4. Select ➢*Remote Inject* from the list of device drivers and click **OK**. The Properties dialog box for the Remote Inject device appears.

5. The default device name is InjectValve. You can keep the default name or enter a different one.
6. From the **Inject Port** drop-down list, select the remote input device that was connected through TTL or relay. Click **OK**.

Add an Inject Command to the Program

Add the following command to the PGM file. (If you use the  **Program Wizard** (see **Control (Programmed)** section), the command is added automatically.)

```
0.000    Inject
```

When the Dionex Chromatography Management System executes the program, it runs the commands that occur before the Inject command and then waits for the signal from the remote input device. A message in the audit trail is displayed: "Wait for inject response on remote start." When the inject signal occurs, program execution resumes.

Example PGM File: AS40 and DX-120

```
         Data_Collection_Rate  5.00
         Pump =                On
         SRS =                 On
         EluentPressure =      On
         Column =              A
         ECD_TTL_1.State =     5v                Note 1
         Wait                  RinseComplete     Note 2
-0.100   ECD_TTL_1.State =     0v                Note 3

0.000    ECD.Autozero                            Note 4
         Inject                                  Note 5
         ECD_1.AcqOn

10.000   ECD_1.AcqOff

         End
```

Notes:

1. TTL Out 1 turned off.
2. The TTL_1 5v and TTL_1 0 v commands must be separated by one or more commands or they must occur at different times in the program.
3. TTL Out 1 turned on. AS40 Load Cycle starts.
4. Program execution waits until inject signal is received.
5. AS40 Ready Out signals the DX-120 Inject TTL Input. Injection occurs. Program execution resumes.

Defining Sample Preparation Steps (AS50)

AS50 ➢*Autosampler* sample preparation steps are part of a ➢*PGM File* and can be defined using the **Program Wizard** (see below and the **Control (Programmed)** section) or entered manually into the program (see **How to …: Actions in the PGM Editor Manually Creating a Program**).

Perform the following functions from the AS50 Sample Prep Options dialog box in the Program Wizard.

Defining a New Sample Preparation Step

1 Select a ➢*Sample Prep Function* from the **Function** list.

The parameters for the selected function appear.

2 Select the desired parameter values.

3 Click the **Insert** button to add the step to the list.

The new step is added above the currently selected step (if any).

Changing an Existing Step

1 Select the step in the list.

2 Make the required changes, for example, select a new function and enter the function's parameters, or change the parameters for the current function.

3 Click the **Enter** button.

☞ ***Tip***: To delete a step, select it, and click the **Delete** button.

Opening the AS50 Door during Operation

Normally, the AS50 ➢*Autosampler* door must remain closed while the AS50 is running a batch. If the door is opened inadvertently, the sampling arm stops immediately and the batch is aborted. There are certain times during operation, however, when the autosampler is not busy, and it is safe to open the door. The Dionex Chromatography Management System monitors operation and informs you when you can open the door without aborting the batch.

First, press the **Door** button on the AS50 front panel. If the AS50 is busy, a message in the ➢*Audit Trail* window informs you that it is currently not safe to open the door.

When the AS50 is not busy, a message informs you that it is now safe to open the door. A timer then begins counting down the time remaining in which it is safe to have the door open. It continues counting down after the door is opened. The door must be closed again before the timer reaches zero, or the batch will be aborted.

If after pressing the Door button, you decide you do not want to open the door, you can allow the timer to expire or press any button on the AS50's front panel to reset the timer to zero.

Note: To display the timer on the control panel, place a string display, gauge slider, or gauge indicator ➢*Control* on the control panel (see ➢*Layout Toolbar*). Then, link the control to the object property, **DoorSafetyTime.** For details, see **How to ...: Actions in the Control Panel Linking a Control to a Device**.

Monitoring the Status of the AS50

The status of the AS50 ➢*Autosampler* can be displayed on the ➢*Control Panel*. To do this, place a string display ➢*Control* on the control panel (see ➢*Layout Toolbar*). Then, link the control via the **Link** tab dialog box to the sampler object property, **Status.**

The control then displays the action currently being performed by the autosampler, for example, Idle, Preparing to run, Injecting, and so on.

Control - Detectors

Depending on the detector type different commands are available. For an overview on the individual commands that are available for the different Dionex UV and PDA detectors, see

Detector Commands

The following pages provide details on:

Starting Data Acquisition

Defining Signals, Signal Parameters, Axis Decoration, etc.

Modifying Signal Parameters (Overview)

Modifying the Signal Parameters of an UVD Channel

Modifying the Signal Parameters of a 3D-Field

Determining Wavelength Switching

Defining a Waveform

Defining Step and Average

Switching Polarity

In addition, see the following pages for details on:

Viewing or Resetting the Lamp Age

Detector Commands

Modifying Signal Parameters

```
0.000       Channelname.Average             =On / Off
0.000       Channelname.Bandwidth           =Value
0.000       Channelname.Wavelength          =Value
0.000       Channelname.Step                =0.25 / Value [sec]
```

Caution: Select the ⇒*Step* in such a way that 20 to 50 data points are placed on the narrowest relevant peak in your chromatogram. If you acquire more data points, this will use unnecessary disc capacity and the integration might become incorrect, especially with heavier baseline noise. This may also happen when using the Step Auto.

Note: To realize ➢*Wavelength Switching*, a new wavelength is defined for a channel at the switch time.

Switching Detector ⇒*Lamp On/Off*

```
0.000   Devicename.Lamp          =On / Off
```

Switching Detector Lamps On/Off (AD20 Detector)

```
0.000   Devicename.UV_Lamp       =Low / High / Off
0.000   Devicename.Visible_Lamp  =Low / High / Off
```

Switching Detector Lamps On/Off (AD25 and PDA-100 Detector)

```
0.000   Devicename.UV_Lamp        =On / Off
0.000   Devicename.Visible_Lamp   =On / Off
```

Turning the Amperometry Cell On/Off (ED40/ED50/ED50A Detector in Amperometry Mode)

```
0.000   Devicename.Cell          =On / Off
```

Selecting the Electrode (ED40/ED50/ED50A Detector in Amperometry Mode)

```
0.000   Devicename.Electrode     =pH / AgCL
```

Starting Data Acquisition

- Press the ⇒*AcqOn/Off* button on the toolbar and determine the channels to record via the automatically displayed dialog box.
- Press the button again to stop data acquisition.

Alternatively, the command can be performed via the **Control** menu or the corresponding button on the Desktop. Each signal (channel) selected during the start of data acquisition is stored in a separate raw data file.

- Open the context menu within the signal plot to influence the representation of the signals (Autoscale, Autozero, Replot from Beginning, Chromatogram Overlay) or the type of the recorded data (signal parameters) via the context menu.

Defining Signals, Signal Parameters, Axis Decoration etc.

Open the context menu within a signal plot and select:

- **Signals** to determine the signals to be displayed.
- **Axis/Decoration** to display axis decoration, units, timebase names, signal parameters, a grid, the signal value, or the retention time.
- **Chrom. Overlay** to display a comparable chromatogram.

Press F1 for context-sensitive help.

Modifying Signal Parameters (Overview)

Manually / directly:

- Move the mouse cursor to the signal plot of a control panel.
- Open the context menu within a signal plot and select **Signal Parameters**.
- Select the tab of the signal / channel for which you want to change the parameters. Signals of different types have different ➢*Signal Parameters*.
- MS parameters are not available in this dialog box. Define them in a separate METH file.

Programmed / indirectly:

In controlled systems, the parameters can be activated/deactivated during chromatogram run time at exact times.

- Choose **Command ...** in the **Control** menu, select the signal to modify and define its signal parameters - or
- Enter the corresponding command in a ➢*Program* that is executed in automatic ➢*Batch Processing*.

For an example for modifying signal parameters, see

How to ...: Device Control Determining Wavelength Switching.

Modifying the Signal Parameters of an UVD Channel

Modifying one or several signal parameters allows improving the signals provided by the detector. You can change the following signal parameters for your ➢*UV Detector*:

Signal Param.	Description	Comment
⇒*Wavelength*	Changes the recorded wavelength.	Note the possibilities for wavelength switching (see **How to ...: Device Control Determining Wavelength Switching**).
⇒*Bandwidth*	Changes the bandwidth with which the signal is recorded.	If necessary, increase the bandwidth to improve the ➢*Signal to Noise Ratio*.
⇒*RefBandwidth (Reference Bandwidth)*	Changes the reference bandwidth.	If necessary, increase the bandwidth to improve the signal to noise ratio.
Signal	**Value** indicates the current value of a ➢*Signal* **Upper/LowerLimit** allows defining the signal acquisition limits.	If signal acquisition limits are exceeded or fallen below, the running batch is stopped and the emergency program is started.
Delta	Difference between the current signal value and the signal value one second before.	The value cannot be changed.
Retention	Shows the current retention time (no modification possible).	
MaxAutoStep	Input of the maximum step width with the setting **auto**.	The highest possible value is the default: 5.1 s.
⇒*Step*	Changes the step.	Select the step such that the narrowest peak contains approx. 20 datapoints
⇒*Average*	Averaging.	Use this parameter to improve the signal to noise ratio.

Modifying the Signal Parameters of a 3D-Field

By changing various signal parameters of a ➢*Photodiode Array Detector*, the size, and quality of a ➢*3D-Field* can be improved. There are the following possibilities:

Signal Param.	Description	Comment
MaxWavelength **MinWavelength**	Determines the upper/lower limit of the 3D-field.	Use these parameters to limit the size of the 3D-field to the essential section.
⇒*RefWavelength (Reference Wavelength)*	Changes the reference wavelength.	If necessary, increase the bandwidth to improve the ➢*Signal to Noise Ratio*.
⇒*RefBandwidth (Reference Bandwidth)*	Changes the reference bandwidth.	If necessary, increase the bandwidth to improve the signal to noise ratio.
⇒*BunchWidth*	Shows the current value of the bunch width.	Increasing the value improves the signal to noise ratio. However, the resolution decreases.
⇒*Step*	Changes the step.	Select the step such that the narrowest peak contains approx. 20 datapoints
Retention	Shows the current retention time.	The value cannot be modified.

Determining Wavelength Switching

➢*Wavelength Switching* is realized by time-precise modification of the ⇒*Wavelength* (UV detector) or ➢*Emission*, and ➢*Excitation* (fluorescence detector) signal parameters.

- For each wavelength switch, enter the time, the channel and the new parameter value in the ➢*Program*, e.g. for the channel of a fluorescence detector:

```
10.000  UV_VIS1.Wavelength       = 280 nm
10.000  UV_VIS2.Wavelength       = 320 nm
```

or

```
10.000  Emission.ExWavelength    = 240 nm
10.000  Emission.EmWavelength    = 295 nm
```

Displaying the Signal Parameters of a Mass Channel

Different channel types are available for ➢*Mass Spectrometers*:

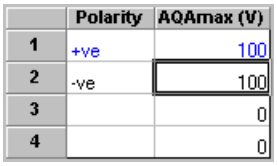
TICF channels (TICF_01 to TICF_4: data acquisition in ➢*Full-Scan* mode)

➢*SIM* channels (SIM_01 to SIM_32: data acquisition in SIM mode)

➢*TIC* channel (total of all TICF or SIM channels)

MS_01 to MS_32 channels (data acquisition in full-scan mode)

Almost no parameters for mass spectrometer channels can be changed from the ➢*Control Panel*. The following parameters for the channels of a mass spectrometer can be displayed:

Signal Param.	Description	Comment
Min/MaxMass	Limits of the mass range that is acquired in this mass channel.	SIM channels cannot be changed. MS channels MS_01 to MS_32: Enter the lower / upper mass range limit.
FilterIndex	Number of the ➢*Filter* of the Finnigan aQa method (METH-File).	With MS_01 to MS_32 channels only: Select the number of the desired filter (1-4): 
Polarity	Ionization polarity of the mass spectrometer.	The value cannot be changed.
Source Voltage	Voltage of the ion source of the mass spectrometer.	The value cannot be changed.
Filter	Filter of the Finnigan aQa method (METH file).	The value cannot be changed.
Delta	Difference between the current signal value and the signal value one second before.	The value cannot be changed.
Retention	Indicates the current retention time.	The value cannot be changed.
Signal	**Value** indicates the current value of a ➢Signal. **Upper/LowerLimit** allows defining the signal acquisition limits.	If signal acquisition limits are exceeded or fallen below, the running batch is stopped and the emergency program is started.

Defining a Waveform

A ➢*Waveform* must be defined when a Dionex electrochemical detector is used in ➢*Integrated Amperometry Mode*. Waveform definitions are part of a ➢*Program* and can be defined using the **Program Wizard** (see below and the **Control (Programmed)** section) or entered manually into the program (see **How to ...: Actions in the PGM Editor Manually Creating a Program**).

Selecting a Standard Waveform from the Program Wizard

1 In the Waveform Options dialog box of the Program Wizard, click the **Waveform** button.

A list of standard waveforms appears.

2 Select a waveform from the list and click **OK**.

The selected waveform's time, potential, and integration settings replace any waveform settings already in the waveform table. After completing the Program Wizard, the waveform can be modified in the resulting program.

Defining a Custom Waveform from the Program Wizard

Perform the following steps from the Waveform Options dialog box in the Program Wizard:

1 In the **Time (Sec)** box, type or select the time to begin the first waveform step.

2 In the **Potential (V)** box, type or select the potential to apply between the reference and working electrode.

3 In the **Integration** box, select an ➢*Integration* option: **Begin** starts integration at this step, **End** stops integration, **No-Change** keeps the setting selected in the previous step.

☞ ***Tip***: Each waveform must have at least one integration period. Integration periods cannot begin or end at Time 0 or at the last step in the waveform, and they cannot overlap.

4 Press the **Enter** button.

The step is added to the waveform table.

5 Repeat the above steps for each subsequent step in the waveform to create the potential vs. time plot.

☞ ***Tips***: To delete a step, select it in the waveform table, and press the **Delete** button.

To edit an existing step, select it in the waveform table, change the time, potential, and/or integration settings and press the **Enter** button.

Defining Step and Average

The time interval between two recorded data points is referred to as ⇒*Step*.

The smaller the selected step, the more data points will be recorded, thus (generally) ensuring a more precise result. As this increases required storage capacity, we recommend a good compromise between the required information and the capacity.

For intelligent minimization of the required storage capacity, the individual instruments (e.g. Dionex detectors) offer the setting Step = Auto. Generally, however, a fixed step should be selected, as an automatic step may result in a faulty integration.

In combination with the ⇒*Average* parameter, the step can optimize the signal to noise ratio. See the following example:

Example: A detector delivers 100 values per channel (A and B) and per second. For channel A, the setting Step = 0.1; Average = ON is selected, and for channel B Step = Auto; Average = ON.

Channel A:

A step of 0.1 corresponds to a sampling rate of 10 values/s. This means that out of the 100 values that are available, only every tenth value is stored. If the **Average** signal parameter is **ON**, the values recorded per step are averaged. From 10 values, one average value is formed and is stored. For channel A, one signal value per second is stored.

Channel B:

Step = Auto means that the Dionex Chromatography Management System decides depending on events, how many values should be recorded per second. As a different number of values is recorded at different times, a varying number of values is averaged in the final value.

☞ ***Tip***: Only use Step = Auto for fast sample chromatograms for which you do not know the peak width to be expected. For a precise and reproducible analysis, a fixed step should be used.

Switching Polarity

In some cases, components appear as negative peaks instead of positive.

In this case, the sign can be changed via the **Polarity (+/-)** switch.

Viewing or Resetting the Lamp Age

The PDA-100 detector allows you to view the number of hours the UV and visible lamps have been on. In addition, the lamp age can be reset to 0, if new lamps are installed.

The lamp age commands are available from the **Command** dialog box. Select **Command...** from the **Control** menu. Under **UV,** select **UVLampAge** or **VisibleLampAge**. The total number of hours the lamp has been on is displayed. The number of hours can also be changed from this dialog box.

The UV and Visible lamp ages can also be displayed on the ➢*Control Panel*. To do this, place a string display ➢*Control* on the control panel (see ➢*Layout Toolbar*). Via the **Link** tab dialog box, then link the control to the UV object property: **UVLampAge** for the UV lamp or **VisibleLampAge** for the visible lamp.

For details, see:

Modifying a Control Panel

Modifying a Control

Linking a Control to a Device

Controlling a Suppressor

The commands used for controlling a ➢*Suppressor* differ, depending on the model of conductivity detector used and the type of suppressor installed:

Detector Model	Supported Suppressor(s)
CD20, CD25, ED40, ED50, IC20, and IC25	SRS
CD25A, ED50A, and IC25A	SRS, AES

Controlling an SRS with a CD20, CD25, ED40, ED50, IC20, or IC25 Detector

Use the following command to set the current applied to the SRS suppressor.

```
SRS_Current              =Off, 50, 100, 300, 500 (mA)
```

Controlling an SRS with a CD25A, ED50A, or IC25A Detector

Use the following commands to select the SRS suppressor and the current applied to it.

```
Suppressor_Type          =SRS
Suppressor_Current       =0...500 (mA)
```

Controlling an AES (CD25A, ED50A, or IC25A Detector Only)

Use the following commands to select the AES suppressor, the eluent concentration, and the current applied to the AES. For details on setting the AES current, see **How to ...: Device Control Setting Atlas Suppressor Currents**.

```
Suppressor_Type          =AAES, CAES
AAES_CO3                 =0.0...12.5 (mM)
AAES_HCO3                =0.0...25 (mM)
AAES_OH                  =0.0...25 (mM)
CAES_H2SO4               =0.0...12.5 (mM)
CAES_MSA                 =0.0...25 (mM)
Suppressor_Current       =0...150 (mA)
```

Setting Atlas Suppressor Currents

Atlas Electrolytic ➢*Suppressors* have a maximum suppression capacity of 25 mN eluent at 1.0 ml/min, which is equivalent to 12.5 mM sodium carbonate for anion separations or 25 mM methanesulfonic acid (MSA) for cation separations at 1.0 mL/min.

For optimal suppressor performance, it is important to use the recommended suppressor currents for the target applications. The Program Wizard of the Dionex Chromatography Management System (see **Control (Programmed) Program Wizard**) guides you in setting the recommended current for the Atlas Electrolytic Suppressor. The Wizard supplies a recommended current based on the eluent concentration and flow rate settings (see the following table). The Dionex Chromatography Management System automatically enters the recommended current into the ➢*Program* and applies that current to the Atlas Electrolytic Suppressor.

Tip: For gradient separations, use the highest eluent concentration in the gradient when you enter the eluent concentration in the Wizard.

Examples of Recommended Operating Currents for Atlas Electrolytic Suppressors:

Column	Eluent	Flow Rate (ml/min)	Current (mA)
4-mm AS4A-SC	1.8 mM Na2CO3/1.7 mM NaHCO3	2.00	36
2-mm AS4A-SC	1.8 mM Na2CO3/1.7 mM NaHCO3	0.50	9
4-mm AS9-HC	9.0 mM Na2CO3	1.00	60
2-mm AS9-HC	9.0 mM Na2CO3	0.25	15
4-mm AS14	3.5 mM Na2CO3/1.0 mM NaHCO3	1.20	32
2-mm AS14	3.5 mM Na2CO3/1.0 mM NaHCO3	0.30	8
3-mm AS14A	8.0 mM Na2CO3/1.0 mM NaHCO3	0.5	28
4-mm CS12A	22 mM MSA	1.00	72
3-mm CS12A-5 µm	20 mM MSA	0.50	32
2-mm CS12A	22 mM MSA	0.25	18

For other column and eluent conditions, the recommended current for the Atlas electrolytic suppressors can be calculated using the following equation:

$$Current\,(mA) = 2 \times 1.67\,(mA * \min / mN * ml) \times [eluent\,(mN)] \times flow\,rate\,(ml / \min)$$

For anion separations:

$$[eluent\,(mN)] = 2\times[CO_3^{2-}\,(mM)]+[HCO_3^{-}\,(mM)]+[OH^{-}\,(mM)]$$

For cation separations:

$$[eluent\,(mN)] = 2\times[H_2SO_4\,(mM)]+[MSA\,(mM)]$$

(Where: [ ] enclosing an ion or eluent indicate concentration.)

***Caution**:* To ensure the optimal performance of the Atlas Electrolytic Suppressors, avoid applying excess current to the suppressors. Excess operation currents lead to excess heat generation, which can reduce the suppressor lifetime and cause higher chromatographic baseline noise. The following table lists the **maximum** operating currents for the Atlas Electrolytic Suppressors under various column diameter and flow rate conditions.

Maximum Operating Currents for the Atlas Electrolytic Suppressors:

Separation Column	Flow Rate (ml/min)	Maximum Current (mA)
2-mm column	0.25 to 0.50	30
3-mm column	0.50 to 1.00	50
4-mm column	1.00 to 2.00	100

Once the recommended suppressor current is determined, turn on the pump flow and apply the current to the suppressor.

Control - Fraction Collection

Depending on the device type, different commands are available for ➢*Fraction Collector* control. We recommend installing the **Fraction Collection Automation** (= FCA) driver in addition to the respective device driver (see **Setting up Fraction Collection**). The FCA driver allows creating a standard ➢*Program* and **Setting the Peak Detection Parameters**. In addition, it provides information on the **Checking the Fraction Collection Status**.

For further information, see:

Recognizing the Peak Start, Peak Maximum, and Peak End

Defining the Reactions to Certain Events

Setting the Fraction Collection Options

Fraction Collection - Program Example

Setting up Fraction Collection

Similar to automating sample injection by means of autosamplers, fraction collectors can be used to automate collecting the fractions after the detector. Controlling ➢*Fraction Collectors* can be exclusively via ⇒*Trigger* commands as well, however, this is rather complex. Below please find some useful hints to facilitate fraction collection:

Server Configuration

Add a **Fraction Collection Automation** (= FCA) driver under the respective timebase (via **Add Device**) and install the ➢*Device Driver* of the respective fraction collector as usual.

Now, the fraction collector can be easily controlled. Define how to collect the fractions in the Program Wizard (see **Control (Programmed) Program Wizard**) or via the control commands under **Fraction Collection** in the ➢*Control Panel*.

Program Wizard

The Program Wizard assists the user in creating a ➢*Program* for fraction collection control. The **Fraction Collection Options** page allows enabling fraction collection according to the individual peaks and specifying the basic parameters needed for fraction collection. On the **Peak Detection Options** page, specify the peak detection algorithm via the fraction collection parameters (see **Setting the Peak Detection Parameters**).

Default Program Example

If you do not have saved a FractionCollectionTemplate.pgm yet, the Program Wizard creates the default program that is given below (for fraction collection control only):

```
DelayVolume =              0
PumpDevice =               "Pump"
TubeMaxVolume =            0
TotalNumberInstalled =     100
CollectOutsidePeaks =      Yes
TubeWrapping =             Yes
BaselineOffset =           0.000
BaselineDrift =            0.000

;*****************************************************************
;*Definition of triggers for fraction collection starts here.
;*****************************************************************
; Definition copied from template PGM::DS\DIR\FractionCollectionTemplate

Trigger PeakStart          PeakStartDetected
EndTrigger
Trigger PeakMax            PeakMaxDetected
EndTrigger
Trigger TubeChange         PeakTubeChange
EndTrigger
Trigger PeakEnd            PeakEndDetected
EndTrigger

;*****************************************************************
;* Definition of triggers for fraction collection ends here.
;*****************************************************************

DetectionChannel =         "UV_VIS_1"
PeakStartSlope =           2.000
PeakStartThreshold =       10000.00
PeakMaxSlope =             -5.000
PeakEndSlope =             -4.000
PeakEndThreshold =         -10000.00
ThresholdNoPeakEnd =       10000.000

0.000                      PeakRecognition =    Yes

10.000                     PeakRecognition =    No
```

Edit the trigger blocks (Trigger PeakStart, PeakMax, TubeChange and/or PeakEnd) according to your type of fraction collector (see ⇒*Trigger*. For a detailed program example, see **Fraction Collection - Program Example**). Save the trigger blocks (given in blue writing) as FractionCollectionTemplate.pgm at the position that is indicated in your default program above the trigger blocks (in the above example: DS\DIR\). Your new trigger blocks will then be used as template for all future fraction collection programs.

For an overview on the available fraction collection topics, see:

Control - Fraction Collection

Setting the Peak Detection Parameters

The Fraction Collection Automation (= FCA) driver provides the following parameters that are available independently of the installed ➢*Fraction Collector*:

Parameter	Min.	Max.	Default	Functionality
DetectionChannel	n/a	n/a	UV_VIS_1	Name of the signal channel used for peak detection (this may be a ➢*Virtual Signal* as well.).
PeakStartSlope	0.000	1e10	2.000	Slope that must be exceeded so that the peak start can be recognized.
PeakStartThreshold	-1e10	1e10	10000.00	Signal threshold value that must be exceeded so that the peak start can be recognized.
PeakMaxSlope	-1e10	1e10	-5.000	Slope that must be fallen below so that the peak maximum can be recognized.
PeakEndSlope	-1e10	0.000	-4.000	Slope that must be exceeded so that the peak end can be recognized.
PeakEndThreshold	-1e10	1e10	-10000.00	Signal threshold value that must be fallen below so that the peak end can be recognized.
ThresholdNoPeakEnd	-1e10	1e10	10000	Signal threshold value that must be fallen below so that the peak end can be recognized.
PeakRecognition	0:No	1:Yes	1	Peak recognition will be performed only if the variable is set to **Yes**. Note: Peaks already detected will trigger related events after the delay time even if PeakRecognition is **No** at that time.

Parameter	Min.	Max.	Default	Functionality
BaselineDrift	-1e10	1e10	0	Slope of the baseline. The Fraction Collection Automation driver subtracts BaselineOffset + Δt*BaselineDrift from the signal value (current signal value - (BaselineOffset + Δt*BaselineDrift)) before comparing with the specified thresholds. Δt is set to 0 whenever BaselineDrift changes. Baseline Offset is then set to the current value of the correction term to match continuously.
BaselineOffset	-1e10	1e10	0	Offset of the baseline. The Fraction Collection Automation driver subtracts BaselineOffset + Δt*BaselineDrift from the signal value before (current signal value - (BaselineOffset + Δt*BaselineDrift)) comparing with the specified thresholds. Δt is set to 0 whenever BaselineDrift changes.

These properties cannot be changed during a peak (i.e., while PeakOn is Yes). Any attempted change will produce a warning (Parameter cannot be changed until the current peak has ended. New value will be assigned at peak end). The change will become effective as soon as the current peak ends.

In addition to these parameters, different variable indicate the

Checking the Peak Detection Status

For an overview on the available fraction collection topics, see:

Control - Fraction Collection

Checking the Fraction Collection Status

The Fraction Collection Automation (= FAC) driver provides the following status variables that are available independently of the installed ➢*Fraction Collector*:

Status Variable	Min.	Max.	Default	Functionality
PeakStartDetected	0:No	1:Yes	0	**Yes** when the peak start is recognized. When the peak end is recognized, the variable is reset to **No**. *Changes are delayed by the Delay Time. The variable is read-only.*
PeakMaxDetected	0:No	1:Yes	0	**Yes** when the peak maximum is recognized. When the peak end is recognized, the variable is reset to **No**. *(Delayed; read-only)*
PeakEndDetected	0:No	1:Yes	0	**Yes** when the peak end is recognized. When a new peak start is recognized, the variable is reset to **No**. *(Delayed; read-only)*
PeakOn	0:No	1:Yes	0	Yes when a peak start or a peak maximum is recognized. *(**Not** delayed!)*
FractionOn	0:No	1:Yes	0	**Yes** while a fraction is collected. *(Similar to PeakOn, but appropriately delayed!)*
PeakTubeChange	0:No	1:Yes	0	Yes when a full tube is recognized. Resets to No automatically. *(Delayed; read-only)*

Except for the **PeakOn** and **FractionOn** variables, these status variables cannot be changed. The PeakOn and FractionOn variables support e.g. creating ➢*Virtual Signals*:

```
Peak_On.Type =          Digital
Peak_On.Formula         Formula = PeakOn*100
Fraction_On.Type =      Digital
Fraction_On.Formula     Formula = FractionOn*80
```

The defined channels can be used to check either online in the ➢*Control Panel* or upon termination of the data acquisition whether the fractions are collected correctly.

In addition to these status variables, different parameters are available for fraction collection:

Setting the Peak Detection Parameters

For an overview on the available fraction collection topics, see:

Control - Fraction Collection

Recognizing the Peak Start, Peak Maximum, and Peak End

To ensure that the ➢*Fraction Collector* fills the desired tube, the peak start, peak maximum, and peak end must be correctly recognized.

Peak Start

The prerequisites for recognizing the peak start (and hence the beginning of a fraction) are as follows:

- No peak start has been recognized so far.
- Peak detection is enabled via the **PeakRecognition** property.
- The signal of the detection channel is greater than the signal that is defined via **PeakStartThreshold**.
- The signal change is greater than the slope that is defined via **PeakStartSlope**.
- Data acquisition on the selected channel is not yet terminated.
- The run itself is not terminated yet
- The condition is fulfilled for at least 1 second.

The **PeakStartThreshold** and **PeakStartSlope** variables influence the peak recognition sensitivity.

The **PeakStartSlope** variable can be changed within broad limits. The higher the value, the later the peak start is recognized. If PeakStartThreshold is exceeded by the detector signal, the peak is recognized only if the slope threshold value is exceeded as well.

The Dionex Chromatography Management System remembers a peak start so that a peak maximum may be recognized next. The peak maximum recognition requires a detected peak start.

Peak Max Recognition

The peak maximum is recognized only if:

- A peak start has been recognized.
- No peak maximum has yet been recognized.
- The signal change, expressed as slope, is less than the signal slope defined by the **PeakMaxSlope**.
- The condition is fulfilled for at least 1 second.

The peak maximum detection depends on whether a peak start is detected. If no peak is recognized, no maximum can be recognized either. The **PeakMaxSlope** variable is defined as negative slope value as it applies to the tailing side of the peak. The closer the value is to zero, the closer to the peak maximum the **PeakMaxRecognition** ⇒*Trigger* will be executed.

The Dionex Chromatography Management System remembers a peak maximum so that a peak end may be recognized next. The peak end recognition requires a detected peak maximum (unless one of the end-run conditions apply).

Peak End Recognition

A peak end (and hence the end of a fraction) is recognized if:

- The signal change, expressed as slope, is greater than the signal slope defined by the **PeakEndSlope** and
- The signal of the detection channel is less than the signal defined by **TresholdNoPeakEnd** and
- A peak maximum has been recognized

OR:

- The signal of the detection channel is less than the signal defined by **PeakEndThreshold** and
- A peak maximum has been recognized

OR:

- A peak start has been recognized and
- The data acquisition on the signal channel is terminated

AND:

- The condition is fulfilled for at least 1 second.

The first group of conditions checks whether the signal is below the signal maximum, which is defined by the **ThresholdNoPeakEnd** variable. With heavily overloaded detector signals, there is a lot of signal noise so that a peak end/start would be recognized several times in the top of the peak that could also be formed like a plateau. To inhibit this set the **ThresholdNoPeakEnd** variable to a value below this level. If the value is set to the maximum for the detector signal, this part of the condition will always be true so that this check will be disabled. The **PeakEndSlope** setting allows delaying the peak end.

The second group of conditions uses the signal height criterion. If the signal value falls below **ThresholdPeakEnd**, the peak is terminated in any case.

The third group of conditions terminates the current peak in case the data acquisition is switched off.

For further information, see:

Defining the Reactions to Certain Events

For an overview on the available fraction collection topics, see:

Control - Fraction Collection

Defining the Reactions to Certain Events

As described above, peak start, peak maximum, and peak end are recognized if certain conditions are fulfilled (see **Recognizing Peak Start, Peak Maximum, and Peak End**). If one of these events occurs, the Dionex Chromatography Management System issues certain commands to the ➢*Fraction Collector*. These commands can be defined in the ➢*Program*. In the respective ⇒*Trigger* block, you can define device-specific actions for your fraction collector.

Event	Condition	Action
PeakStartDetected	A peak start "arrives" at the switching valve/ tube.	Switch to next fraction.* Switch to **collect**.
PeakMaxDetected	A peak maximum "arrives at the switching valve/ tube.	Usually no action.
PeakEndDetected	A peak end "arrives" at the switching valve/ tube.	Switch to **waste**. Switch to next fraction.*
PeakTubeChange	The tube is filled to the limit.	Switch to next fraction.

* Switching to the next fraction is needed only once. It might depend on the type of hardware whether this is better at the peak start or at the peak end.

The events are generated with a delay that takes the volume between the detector and the switching valve or tube into account. The following parameters are available:

Parameter	Min.	Max.	Default	Function
DelayVolume	0 µl	5000 µl	0	Volume between the detector and the switching valve or tube. Also useful with flow gradient.
PumpDevice			Pump	Pump used to convert between flow and time.

Note: The **Fraction Collection Automation** (= FCA) driver calculates the delay time between the detector and the switching valve or tube by integrating the flow of the respective pump device.

The driver is capable of tracking several peaks in the capillary between the detector and the fraction collector as it internally maintains a queue of peak recognition events.

Tip: Do not change **DelayVolume** and/or **PumpDevice** while collecting fractions. Usually this does not make sense either. Performing such a change in the program, e.g. when a part of the peak is in the capillary between the detector and the fraction collector, will lead to unexpected results.

For further information, see:

Recognizing the Peak Start, Peak Maximum, and Peak End

For an overview on the available fraction collection topics, see:

Control - Fraction Collection

Setting the Fraction Collection Parameters

The following variables allow specifying the tube of the ➢*Fraction Collector* that is currently used for collection:

Variable	Min.	Max.	Default	Function
TubePosition	0	9999 ➢*Rack* dependent	1	Tube position used for the current fraction. May be set as start value (only at negative retention times), otherwise updated by the driver. Ready Check will issue a warning if the value is not 1 at batch start.
TubeStartPosition	0	9999 Rack dependent	1	Tube position where the current fraction has been collected at peak start (read only).
TubeMaxPosition	0	9999 Rack dependent	1	Tube position where the current fraction has been collected at the time of the peak maximum (read only). May be different from TubeStartPosition if e.g. the tube volume is smaller than the fraction volume.
TubeEndPosition	0	9999 Rack dependent	1	Tube position where the current fraction has been collected at the time of the peak end (read only). May be different from TubeStartPosition and TubeMaxPosition if e.g. the tube volume is smaller than the fraction volume.
TubeMaxVolume	0 ml	1000 ml	0 (Disabled)	The maximum volume to be filled in one tube. When this volume is collected, the next tube will be used. ***Tip***: Set the TubeMaxVolume to 0 to disable automatic switching to the next tube.
TubeFilling	0 ml	1000 ml	0	Volume collected so far in the current tube (read only - not delayed).

Variable	Min.	Max.	Default	Function
TotalNumberInstalled	0	9999	100	Number of tubes available in the rack. Exceeding the set number resets it to 1 if the TubeWrapping option is enabled. Otherwise, the batch is aborted. ***Tip***: The wrap around is logged in the audit trail as warning.
TubeWrapping	0 (No)	1 (Yes)	No	Resets TubePosition to 1 when TubePosition exceeds TotalNumberInstalled.
CollectOutside	0 (No)	1 (Yes)	No	Specifies whether to collect fractions outside peaks as well. The device will switch to a new tube at each peak start or peak end or when the current tube is filled. When CollectOutside is set to No the eluent outside the peak is directed to the waste after the detector.

For an overview on the available fraction collection topics, see:

Control - Fraction Collection

Fraction Collection - Program Example

A ➢*Program* for a timebase including ➢*Fraction Collector* might look as follows:

```
-0.300   Flow =   1.000
   %B =  10
   UV_VIS_1.Step =   0.50
   UV_VIS_1.Average =   On
   UV_VIS_1.MaxAutoStep =  1.0

; delay volume between detector output and switching valve or tube:
   DelayVolume =  1000
   PumpDevice =   "Pump"

; maximum filling volume of a tube in uL:
   TubeMaxVolume =   8000

; maximum number of installed fraction tubes:
   TotalNumberInstalled =  240
   CollectOutsidePeaks =   No
   TubeWrapping = No
```

```
   BaselineOffset =  0.000
   BaselineDrift =   0.000

;*********************************************************************
;* Definition of triggers for fraction collection starts here
;*********************************************************************
; Definition copied from template PGM::DS\FractionCollectionTemplate
Trigger PeakStart PeakStartDetected
   Z.Nominal = Z.Nominal
   ; moves the needle to the upper zero position
   Collect.On
   ; switches the collection valve to "Collect" (= on)
EndTrigger

Trigger TubeChange PeakTubeChange
   Collect.Off
   ; switches off the fraction collector valve
   Tube =   TubePosition
   ; selects the next tube
   Z.Nominal = Z.Nominal
   ; moves the needle to the upper zero position
   Collect.On
   ; switches the collection valve to "Collect" (= on)
EndTrigger

Trigger PeakEnd PeakEndDetcted
   Collect.Off
   ; switches off the collection valve
EndTrigger
;*********************************************************************
;* Definition of triggers for fraction collection ends here
;*********************************************************************

; conditions for online peak recognition at peak start
   DetectionChannel =   "UV_VIS_1"
   PeakStartSlope =  2.000
   ;slope at the start of a peak
   PeakStartThreshold = 80.00
   ;minimum signal height at the start of a peak
   PeakMaxSlope = -4.000
   ;slope after the maximum of a peak
   PeakEndSlope = -4.000
   ;slope at at the end of a peak
   PeakEndThreshold =   50.00
   ;maximum signal height at the end of a peak
   ThresholdNoPeakEnd = 2000
   ;signal mst be less than this threshold value
   ;before a new peak start is recognized in a peak group

; separation start with injection
-0.100   Autozero.On Duration=1.00
0.000 Wait  Ready
   Sampler.Inject
   1_UV_VIS.AcqOn
```

```
; start of the separation gradient program
   Flow =   30.000
   %B =  10.0
10.000   %B =  90
13.000   %B =  90

13.000   1_UV_VIS.AcqOff

; regeneration and equilibration phase of the gradient program
15.000   Flow =   30.0
   %B =  90

16.000   %B =  10
   End
```

For an overview on the available fraction collection topics, see:

Control - Fraction Collection

Control - IC, GC, and Temperature

For the control commands for the DX-120 see:

Controlling a DX-120 Ion Chromatograph

The following pages provide details on:

Controlling the Eluent Generator Concentration

Monitoring the Eluent Generator Cartridge Lifetime

Monitoring the DX-120 Operating Status.

For information on the flow and pressure control, which is an important aspect of gas chromatographs, see **Flow/Pressure Control for Gas Chromatographs** as well as **Determining a Gradient (GC)**.

In addition, some instruments allow temperature control. For general information, see:

Temperature Control (On/off)

Controlling the Temperature

For information on controlling the column thermostat ST585, see

Controlling the Column Temperature

Controlling a DX-120 Ion Chromatograph

The following commands are available for controlling DX-120 operating functions:

Controlled AC	Switches the AC power outlet on the DX-120 rear panel on and off. This provides on off control of an external accessory connected to the outlet. See the DX-120 operator's manual for cabling instructions.
Column/Eluent	If the DX-120 is in ➢*Column Mode*, the **Column** command sets the flow path to column A or column B. If the DX-120 is in ➢*Eluent Mode*, the **Eluent** command selects the eluent reservoir (A or B). Note: These commands are active only if the DX-120 is equipped with the dual-column option.
Data Collection Rate	Sets the ➢*Data Collection Rate* of the detector.
Eluent Pressure	Turns the pressure to the eluent reservoir(s) on and off.
Pressure Unit	Selects the units of pressure to use (psi or MPa).
Pump	Turns the pump on and off.
SRS	Turns the current supplied to the ➢*Self-Regenerating Suppressor (SRS)* on and off.

These commands can be included in a ➢*Program*, executed directly from the Commands dialog box (select **Command** from the **Control** menu), or linked to a ➢*Control* on the control panel.

To link a command to a control, place an edit box or switch control on the control panel (see ➢*Layout Toolbar*). Then, link the control to the desired object property. For example, to turn the DX-120 pump on and off from the control panel, link the **Pump** object property to a switch control.

For details, see **How to ...: Actions in the Control Panel Linking a Control to a Device**.

The corresponding commands in the program are as follows:

```
0.000     ControlledAC              =On/Off
0.000     Column                    =A/B
;         Only for a DX-120 equipped with
          the dual-column option.
0.000     Data_Collection_Rate      =Value [Hz]
0.000     Eluent                    =A/B
;         Only for a DX-120 equipped with
          the dual-column option.
0.000     EluentPressure            =On/Off
0.000     PressureUnit              =psi/MPa
0.000     Pump                      =On/Off
0.000     SRS                       =On/Off
```

Controlling the Eluent Generator Concentration

The EG40 ➢*Eluent Generator* can generate eluent concentrations from 0.0 to 100 mM, in 0.1 mM increments. The maximum concentration (X) depends on the pump flow rate and is calculated as:

0.1 to X mM at 1.0 to 3.0 ml/min

Where X mM = 100/Flow Rate in ml/min

The concentration can be set manually or controlled via a ➢*Program*.

Manually Setting the Eluent Generator Concentration

1. Open the control panel for the ➢*Timebase*. For example, if the timebase is configured with a GP50 pump, EG40 eluent generator, and CD25 detector, open the Dionex_Pump_EG40_Conductivity_Detector panel.
2. Move the **Concentration** slider to select the desired value or enter the value into the edit field.

-or-

Enter the concentration from the **Command** dialog box. To do this, select **Command...** from the **Control** menu. Under **Pump** and **EluentGenerator**, select the **Concentration** command.

Programming the Eluent Generator Concentration

Commands for setting the eluent concentration can be added to a program (see **Control (Programmed)**).

You can use the **Program Wizard** to enter the concentration command(s). With the Wizard, you can enter a single concentration value for the entire analysis or program a ramp or multi-step gradient, in which the generated concentration of eluent changes over time. When completing the Wizard, click the **Help** button to see details about the eluent generator and gradient options.

Monitoring the Eluent Generator Cartridge Lifetime

The Dionex Chromatography Management System monitors the lifetime status of the EluGen cartridge currently being used by the EG40 eluent generator and displays the information in the **Server Configuration** of the Dionex Chromatography Management System.

To view the cartridge lifetime status information:

1 In the **Server Configuration**, select the pump to which the eluent generator is connected.

2 Select **Properties** from the **Edit** menu and then select the **Eluent Generator** tab.

The **Remaining Lifetime** is the percentage of ions remaining in the cartridge. The ion percentage is counted down in 1% increments. At 10%, the Dionex Chromatography Management System logs a warning each time the cartridge is used. At 0%, the Dionex Chromatography Management System displays a message that the ion count is depleted and the cartridge must be replaced before continuing operation.

The **Expiration Date** is 2 years from the date of manufacture. One month before expiration, the Dionex Chromatography Management System logs a warning each time the cartridge is used. Although you can continue operation with the cartridge after the expiration date, performance will be impaired until a new cartridge is installed.

Note: The EluGen cartridge status information can be displayed on the control panel. To do this, place a string display ➢*Control* on the control panel (see ➢*Layout Toolbar*). Then, link the control via the **Link** tab dialog box to the object property, **CartridgeExpirationDate**. Use the same procedure for the object property, **CartridgeRemainingLifeTime**. For details, see **How to ...: Actions in the Control Panel Linking a Control to a Device**.

The **Cartridge Number** and **Cartridge Type** properties can also be displayed on the control panel.

Monitoring the DX-120 Operating Status

You can monitor the status of many DX-120 operating functions from the control panel. For example, the control panel can include ➢*Controls* that display the current DS4 temperature set point and status, the current flow rate, and the ➢*SRS* status.

To add the corresponding controls to the control panel and link the desired status functions, proceed as described in the following sections under **How to ...: Actions in the Control Panel**

Modifying a Control Panel

Modifying a Control

Linking a Control to a Device

The following DX-120 functions can be monitored from the front panel.

DX-120 Function	Description
Column Configuration	Indicates whether the DX-120 is configured with a single- or dual-column set.
DS4 Status	Indicates whether the current DS4 temperature is under, at (ready), or over the temperature set point.
DS4 Temperature	Displays the current DS4 temperature set point.
Flow Rate	Displays the pump flow rate.
Full Scale	Indicates the microSiemens output (100 or 1000) of a full-scale detector response.

DX-120 Function	Description
Pressure	Displays the current pump pressure transducer reading.
SRS Status	Indicates the status of the ➢*SRS*, not installed, off, or the selected operating current (if on).
System Mode	Indicates whether the DX-120 is in ➢*Column Mode* or ➢*Eluent Mode*.

Tip: The Dionex Chromatography Management System reports the status of the above DX-120 functions only. Except for the system mode, values for these functions are selected with DIP-switches on the DX-120. Refer to the DX-120 operator's manual for details. The system mode is selected in the DX-120 Properties dialog box (Mode tab page) in the **Server Configuration**.

For functions that can be controlled by the Dionex Chromatography Management System, see **Controlling a DX-120 Ion Chromatograph**.

Determining a Gradient (GC)

For basic information on determining a gradient, see **How to ...: Device Control Determining a Gradient**.

To enter basic points proceed as follows:

- First, select the initial temperature in the Init line.
- Then, in the **Iso Time** column, enter for how long this temperature is maintained.
- In the next line, select the ramp (**Rate** in °C/min) to be used to change the temperature, as well as, in the **Temperature** column, select the temperature that the GC should reach with this first ramp. Then, in the **ISO Time** column, enter for how long this temperature is maintained.

Program up to six temperature ramps in this way.

In the same way, temperature gradients for inlets are defined on the tabs **FrontInlet** or **BackInlet**. Currently this is possible for **PTV** and **Cool on Column** inlets.

In the same way, flow, and pressure gradients can be determined on the tabs **Column1** and **Column2**. Select in the checkbox **Type: Ramped ...** whether a flow gradient (**Flow**) or a pressure gradient (**Pressure**) shall be programmed. The gradient will then be displayed in the color indicated at the top right.

Flow/Pressure Control for Gas Chromatographs

Gas chromatographs offer the possibility to operate at a constant gas flow or at a constant pressure. It is possible to switch from one mode to the other.

Two mutual switches are assigned the property **FlowMode**. Setting the flow and the pressure is in the corresponding mode via a separate control (gauge or edit field).

Temperature Control (On/Off)

If a ➢*Control* (e.g. a switch) in a control panel is assigned the property **TempCtrl** (see **How to ...: Actions in the Control Panel Linking a Control to a Device**), temperature control for the corresponding instrument can be switched on and off. The actual temperature setting is performed via an additional control (see **How to ...: Device Control Controlling the Temperature**).

Instruments providing temperature control are e.g. column ovens, coolable autosamplers (Dionex GINA 50T), specific detectors, or gas chromatographs (HP5890).

Switching on the temperature control is also possible via a ➢*Program*. The corresponding command syntax is:

```
0.000     X.TempCtrl=On            or
0.000     X.TempCtrl=Off
```

Where X is the name under which the corresponding instrument was created in the ➢*Server Configuration* program, e.g.

```
0.000     GC.TempCtrl=On           or
0.000     sampler.TempCtrl=On
```

Controlling the Temperature

Instruments offering temperature control, e.g. column ovens, coolable autosamplers (Dionex GINA 50T), electrochemical detectors (Antec DECADE)

or gas chromatographs (HP5890), can be operated directly from the Dionex Chromatography Management System if the corresponding device driver supports this function. The prerequisite is that the **Temperature Control (On/Off) (How to ...: Device Control)** option of the instrument has been activated via the switch.

Then the temperature of the instrument can be controlled via a corresponding ➢*Control* (gauge or edit field) of the ➢*Control Panel*.

***Note**:* For this purpose, the control is assigned the property **Temperature**. For details, see **How to ...: Actions in the Control Panel Linking a Control to a Device**

Manual Cooling

- Move the slider with the mouse to the desired temperature value.
- Enter the nominal temperature in an edit field.
- A slider can have an additional gauge for the upper and lower temperature limits. The Dionex Chromatography Management System monitors the set temperature range.
- Move the mouse cursor over the gauge to view the exact value of the set temperature.

If an instrument reports that the set temperature value was actually reached (**Ready**), this can be indicated via an LED integrated in the control panel (see **How to: ...: Ready Signal**).

Programmed Cooling

In the ➢*Program*, the temperature of an instrument can be adjusted as follows:

```
0.000   TempCtrl                          = On/Off
;       This command activates and
        deactivates the temperature
        control.
0.000   X.Temperature                     = Value[°C]
;       This command sets the nominal
        temperature. X corresponds to
        name of the instrument as defined
        in the "Server Configuration"
        program.
0.000   X.Temperature.UpperLimit          = Value[°C]
0.000   X.Temperature.LowerLimit          = Value[°C]
;       These commands define the upper
        and lower limit. The limits are
        monitored by the data system.
0.000   Wait                              SampleTempOK (or
                                          similar)
;       The Wait command delays all
        further operations on the
        instrument until there is a
        feedback as soon as the nominal
        temperature is actually reached.
```

Controlling the Column Temperature

The Dionex Column Oven STH-585 allows controlling the column temperature in the range between 5°C and 85°C.

Depending on the type of ➢*Control* (see ➢*Layout Toolbar*), the current temperature can be given (alphanumeric display), a new temperature value can be set (edit field), or an upper and/or a lower temperature limit can be determined (gauge slider). For details on changing controls, see **How to ...: Actions in the Control Panel**.

Controlling the column temperature is also possible within the ➢*Program*. The corresponding commands are:

```
0.000   ColumnOven.Temperature                = Value[°C]
;       This command determines the
        nominal temperature.
0.000   ColumnOven.Temperature.UpperLimit     = Value[°C]
0.000   ColumnOven.Temperature.LowerLimit     = Value[°C]
;       These commands determine the
        upper and lower limits. The
        limits are monitored by the data
        system.
```

Control - Special Commands, Relays, and Others

In addition, the Dionex Chromatography Management System makes some special commands available (see the following pages):

Virtual Channel Commands

Trigger Commands

Mixed Commands

For information on relays, see

Relay and Remote Input Commands

Switching a Relay

For additional general hints on controlling instruments, see

Device Successfully Connected

Ready Signal

Virtual Channel Commands

Changing the Sampling Step for Data Acquisition

```
0.000   VirtualChannel_01.SamplingStep   = Value [sec]
```

Default setting: SamplingStep = 0.1 sec. The input must be between 0.01 and 10 seconds.

Note: The **SamplingStep** defines the time step after which the virtual channel driver (= VCD) re-evaluates the expressions assigned to the channels. Only after re-evaluation will changes to the terms in the expression take effect on the virtual channel signal. Choosing a small sampling step allows recording changes more precisely. However, this will increase the workload of the processor and will slow down your computer.

Changing the Time Lag Threshold

```
0.000   VirtualChannel_01.LagThreshold   = Value [sec]
```

Default setting: LagThreshold = 0.01 s. The value should be between 0.001 and 100 seconds.

Note: The ➢*Virtual Channel Driver (VCD)* keeps the channel time deviation (number of generated data points multiplied by the SamplingStep) from the actually passed time as small as possible. Comparing the two values performs this task. If the difference exceeds or falls below the time interval defined by **LagThreshold**, an additional data point is interpolated or a data point is omitted to approximate the channel time to the real time. With a larger interval, less data is falsified, but the time deviation increases (especially in the case of very long data acquisition periods!).

All channels of a Virtual Channel Driver have the same sampling and monitoring rate. Differing sampling and monitoring rates can only be defined if two or more **Virtual Channel Drivers** are installed.

Changing the Channel Type

To optimize signal recording, the VCD offers the possibility to assign each virtual channel a type. Three types are currently defined (see **Installing the Virtual Channel Driver: Channel Types**:

```
0.000   VirtualChannel_01.Type   = Analog, Digital or Fixed
```

Analog	Suitable for expressions that are composed of other analog signals.	`e.g.: UV_VIS_1/UV_VIS_2`
Digital	Suitable for digital expressions.	`P580Relay_1.State AND P580Relay_2.State`
Fixed	Suitable for expressions that change slowly.	`Pump.%A`

The type selection affects the settings of **Step**, **MaxAutoStep**, and **Average** of the corresponding signal as well as the selection of appropriate raw data compression. In the case of the standard compressor, these three parameters have the same significance as with normal signal channels. For the step compressor, the values have no significance as this compressor always uses a fixed step of 0.01s. The default values are as follows:

	Step	**MaxAutoStep**	**Average**	**Compression**
Analog	Auto	5.1s	On	Standard compressor
Digital	Fixed, 0.01s			Special compressor for step signals
Fixed	Fixed, 0.01s	5.1s	Off	Standard compressor

In the case of analog or fixed channels, the values for **Step**, **MaxAutoStep**, and **Average** can be changed after selecting the type. In the case of a fixed channel, it makes sense to set the step rate identical to the **SamplingStep**. This ensures that the compressor will only record the originally sampled data points.

Use the **Formula** command to specify the expression to record. The same expressions as for ⇒*Trigger* conditions are possible, i.e., arithmetic and logical links. The expression must be numeric. During the program execution, the last calculated value of the expression is stated in the property **FormulaCur** (changes after each **SamplingStep**). **FormulaMin** and **FormulaMax** define the minimum and maximum values resulting from the expression.

Similar to other signal channels, the current (or interpolated) signal value can be viewed via the property **Value** (changes every 0.01s)

The property **Equate** allows to enter a user-defined name for the virtual channel during the analysis. This name can be included in the Audit Trail via the system command **Log**.

During data acquisition, it is not possible to change the properties **Step**, **MaxAutoStep**, **Average**, **Formula**, and **Type**. The **FormulaMin**, **FormulaMax**, and **FormulaCur** properties indicate the status.

Program Examples for Virtual Channels

Sum of two channels (Analog Signals)

The sum of two UV channels should be recorded as a virtual channel. As this steady signal is likely to change frequently, the virtual channel should have the type analog. Using the default settings, this channel is recorded as precisely as the two UV channels:

```
0.000      Pressure.LowerLimit =         0
           Pressure.UpperLimit =         400
           Inject
           VirtualChannel_01.Formula     UV_VIS_1+UV_VIS_2
           VirtualChannel_01.Type =      Analog
           UV_VIS_1.AcqOn
           UV_VIS_2.AcqOn
           VirtualChannel_01.AcqOn
2.000      UV_VIS_1.AcqOff
           UV_VIS_2.AcqOff
           VirtualChannel_01.AcqOff
```

Relay Status (Digital Signals)

The status of a relay should be recorded as a virtual channel. For this rectangle signal, using the virtual channel of the type digital is recommended:

```
0.000      Pressure.LowerLimit =         0
           Pressure.UpperLimit =         400
           Inject
           VirtualChannel_01.Formula     P580_Relay1.State
           VirtualChannel_01.Type =      Digital
           VirtualChannel_01.AcqOn
0.000      P580_Relay1.On
0.100      P580_Relay1.Off
0.200      P580_Relay1.On
0.300      P580_Relay1.Off
0.400      P580_Relay1.On
0.500      P580_Relay1.Off
0.600      P580_Relay1.On
0.700      P580_Relay1.Off
0.800      P580_Relay1.On
0.900      P580_Relay1.Off
1.000      P580_Relay1.Off
1.000      VirtualChannel_01.AcqOff
```

Recording a Gradient (Slow Signals)

The currently set gradient should be recorded as a virtual channel. As this steady signal is unlikely to change frequently, a virtual channel of the type Fixed is recommended. It is sufficient to record the current value once per second:

```
0.000      Pressure.LowerLimit =         0
           Pressure.UpperLimit =         400
           Inject
           Flow = 10
           %B = 100
           VirtualChannel_01.Formula     Pump.%B
           VirtualChannel_01.Type =      Fixed
           VirtualChannel_01.Step =      1
           VirtualChannel_01.AcqOn
0.500      %B = 100
1.000      %B = 50
1.500      %B = 50
2.000      %B = 0
2.000      VirtualChannel_01.AcqOff
```

Correcting a signal from a radioactive substance:

To determine the concentration of a radioactive substance, the decay of the substance must be taken into account and the signal corrected accordingly. The VCD allows you to solve this problem as follows:

In the example below

- The half-life is t½ min
- The run time of the chromatogram is **t**l min
- The uncorrected signal (UV_VIS_1) is between - 10.000 and 10.000 mAU,

```
0.000   Pressure.LowerLimit = 0
        Pressure.UpperLimit = 400
        Inject

        VirtualChannel_01.Formula   UV_VIS_1 / 2.718**
        (-0.69314718* System.Retention /t½)
        VirtualChannel_01.FormulaMin = -10000 / 2.718**
             (-0.69314718* tl /t½)
         VirtualChannel_01.FormulaMax = 10000 / 2.718**
             (-0.69314718* tl /t½)
        VirtualChannel_01.Type = Analog

        UV_VIS_1.AcqOn
        VirtualChannel_01.AcqOn

tl      UV_VIS_1.AcqOff
        VirtualChannel_01.AcqOff
```

In each case, enter into the program the actual half-life instead of **t½**. In addition, enter the actual run time of your program with three decimal points for **tl**.

When the program is modified accordingly, the virtual channel records the signal that would be measured by the detector if the radioactive decay were stopped with the injection into the chromatography system. The decay that occurred before the injection will not be corrected.

***Note**:* If you know the signal area to be expected for your chromatogram (in the example for the channel UV_VIS_1) you may enter this value instead of **-10,000** and **10,000** for calculating FormulaMin/Max to map your chromatogram more precisely.

Trigger Commands

Note: The trigger name must be unique, i.e. no triggers by the same name can be used, nor device, relay or signal names that were already assigned. The same trigger can initiate any number of reactions. The reactions of the trigger list are not supplied with time information. The trigger must always be completed by an EndTrigger command, e.g.:

```
0.000   Trigger <NAME>  Condition=      [Value](Operator)[Value]
                                        ,OperatorValue,True=Value[sec]
                                        ,Delay=Value[sec],Limit=Number
        Reaction 1      =Value/Status
        ...                             ...
        Reaction n      =Value/Status
        EndTrigger
```

If a trigger condition consists of several values, operators can combine them. Available operators are **+**, **-**, *****, **/**, **AND**, **OR**, **NOT**. The Trigger condition is fulfilled if the corresponding value is reached, not reached, or exceeded. This is indicated by the operators **<**, **>**, **<=**, **>=**, **=** and **<>**. Any dependence on various values can be realized via parentheses.

If the value is preceded by the name DELTA, the slope, i.e. the first derivation, is processed as the trigger condition. Remote input signals or relay states can also be processed.

Note: Due to lack of space, line breaks are inserted here. Normally, one command must be entered in one line. For a detailed description of the **Trigger** command, see ⇒*Trigger* in the Reference Manual section.

Example 1: Peak Recognition via Absolute Value

```
0.000   Trigger EXAMPLE1        UV_VIS_1>100,True=1,Delay=5,Limit=4
        Sound                   File="TEST.WAV"
        ...                     ...
        RELAYNAME               =On
        EndTrigger
```

Description: The trigger with the Trigger Name **EXAMPLE1** monitors the channel UV_VIS_1. If the signal exceeds the value 100 for more than 1 second ((Trigger-) True), the Audio file TEST.WAV is played after a (Trigger-) Delay of 5 seconds (if no sound card is installed in the PC, there is a short **Beep** instead). At the same time, the relay RELAYNAME is switched on.

The entire process, i.e., exceeding the signal value 100 of channel UV_VIS_1 with a subsequent reaction, is limited to 4 times (**Limit=4**). If the condition (Trigger-) Limit is not entered, the process is always repeated, as soon as...

Example 2: Peak Recognition via Slope

```
0.000   Trigger EXAMPLE2       UV_VIS_1.DELTA>1
        Sound                  File="TEST.WAV"
        EndTrigger
```

Description: The trigger **EXAMPLE2** monitors the channel UV_VIS_1. At a slope value (DELTA) above 1, the Audio file TEST.WAV is played. If no sound card is installed in the PC, there is a short beep instead.

Example 3: AND, OR, NOT

```
0.000   Trigger EXAMPLE3       ((UV_VIS_1>100) AND (UV_VIS_2>100) OR
                               (UV_VIS_3>200)) AND NOT REMOTE1
        Sound                  File="TEST.WAV"
        EndTrigger
```

Description: The **EXAMPLE3** trigger monitors the UV_VIS_1, UV_VIS_2, and UV_VIS_3 channels as well as the REMOTE1 remote input. If the channels 1 and 2 simultaneously (**AND**) exceed the value 100, or (**OR**) if the channel UV_VIS_3 exceeds the value 200 and if the remote input REMOTE1 delivers no signal (**AND NOT**) at the same time, the TEST.WAV Audio file is played (without a sound card, there is a short beep instead).

Example 4: Further parameters that can be triggered

```
0.000   Trigger EXAMPLE4       Pressure.LowerLimit<20 OR
                               Pressure.UpperLimit>300 OR
                               Temperature>60
        AbortBatch
        EndTrigger
```

Description: The trigger **EXAMPLE4** monitors the pump pressure and the temperature of the column oven. If the pressure falls below 20 bar or exceeds

300 bar, or if temperature exceeds 60°C, the running sample batch is aborted (**Abort Batch**).

Example 5: Fraction Collector FoxiJr.

```
       FoxiJr.Valve = Off              ; switches the valve of the
                                       ➢Fraction Collector  to the "Waste"
                                       position

0.000  Trigger PEAKSTART               FoxiJr.Valve = 0 AND
                                       UV_VIS_1.Delta >1, True = 2
       FoxiJr.Valve = On               ; switches the valve to the
                                       "Collect" position
       EndTrigger

       Trigger TUBEFULL                FoxiJr.Valve = 1,True = 60
       Protocol "Tube full"
       FoxiJr.Valve = Off
       EndTrigger

       Trigger PEAKEND                 FoxiJr.Valve = 1 AND
                                       UV_VIS_1.Delta > -1,
                                       True = 2, Delay = 5
       FoxiJr.Valve = Off              ; switches the valve to the "waste"
                                       position
       FoxiJr.Tube = FoxiJr.Tube +1
       EndTrigger
```

Description: The **PEAKSTART** trigger causes the valve to switch to the **Collect** position if the valve is previously in the **Waste** position and if the slope of the UV_VIS_1 channel exceeds the value 1 for more than 2 seconds (True). After 60 seconds, the trigger TUBEFULL ensures that the collection container does not overflow. The valve is switched again (back to the **Waste** position). For larger collection containers, the time can be adjusted as needed. If the signal is below the slope value -1 for more than 2 seconds, and if the valve is still in the **Collect** position, this is interpreted as the end of the peak. After a delay of 5 seconds, the valve is switched to the **Waste** position. Simultaneously, the x/y-arm of the fraction collector is moved by one position (FoxiJr.Tube = FoxiJr.Tube +1).

Also, see

Controlling Fraction Collection

Fraction Collection - Program Example

Mixed Commands

Produce Sound

```
0.000   Sound             File="TEST.WAV"
```

For details, see ⇒*Sound* command.

Temperature Regulation for Column Oven

```
0.000   Temperature.Nominal  =Value [°C] (nominal value)
```

In combination with a ⇒*Trigger* condition, the actual value can also be inquired:

```
0.000   Trigger OVENTEST     Condition=Temperature>50[°C]
        Sound                File="TEST.WAV"
        EndTrigger
```

Description: The trigger OVENTEST monitors the current oven temperature. Each time, the temperature exceeds 50 °C, the Audio file TEST.WAV is played. If the PC has no sound card, there is a short beep.

Comments, Protocol and Message Texts

```
;       Comment Text...
0.000   Protocol             "Text ..."
0.000   Message              "Text ..."
```

Note: Comments can be added to any program instruction via " ; ". They can easily be recognized by their green color. Protocol and message texts must be indicated by quotation marks ("Text...")! Both are included in the Audit Trail. While the ⇒*Protocol* command serves for documentation purposes only, the ⇒*Message* text appears on the screen. Continuation of the program is only possible after confirming with the Enter key.

Example 6: Delayed Execution of the Inject Command ("Wait")

```
0.000   Acquisition          =On
0.000   Wait                 UV_VIS_1 < 10
0.000   Inject
```

Description: Program execution is delayed until the absorption on channel UV_VIS_1 is below 10 mAU. As soon as this is the case, injection is started.

The **Wait** command is also required for Suck and Dispense operations of the Dionex Autosamplers GINA 50 and GINA160 (see **How to ...: Device Control**  **Control - Autosamplers**).

Relay and Remote Input Commands

Activate / Deactivate Relays

```
0.000   RELAYNAME.State          =On / Off
```

Alternatively, the following short command is valid:

```
0.000   RELAYNAME.On
0.000   RELAYNAME.Off
```

Activate / Deactivate Relay for a specific duration

```
0.000   RELAYNAME.On             =Value[sec]
0.000   RELAYNAME.Duration       =Value[sec]
```

Alternatively, the following short command is valid:

```
0.000   RELAYNAME.On             Duration= Value[sec]   or
0.000   RELAYNAME.Off            Duration= Value[sec]
```

Switching a Relay

Every ➢*Relay* can be integrated as a simple switch in the control panel interface. The two switch settings correspond to the relay states **On** and **Off**. In addition, ➢*Controls* in the ➢*Control Panel* are linked to **State**. Each relay can be executed with a time relay, using the **Duration** parameter.

If a 3-way-valve is integrated in the fluidics at the detector output, two switch states can be controlled via an internal device relay (e.g. the Dionex Pump M480).

- In the **Server Configuration**, double-click the respective instrument to open its **Property** dialog box and choose **Relays**.
- Activate a currently free device relay and choose OK.
- Save the new ➢*Server Configuration*.
- In the control panel, any switch can be linked to the new relay function (**Object=Relayname**, **Object Property=State**). See **How to ...: Actions in the Control Panel**  **Linking a Control to a Device**.
- If necessary, create an additional control, e.g. an edit field (see ➢*Layout Toolbar*), to set the on/off duration of the valve.

In the ➢*Program* the switch procedure of a relay can be realized via the following commands:

```
0.000   RELAYNAME.State          =On/Off
0.000   RELAYNAME.Duration       =Value[sec]
```

Device Successfully Connected

Many devices automatically inform the Dionex Chromatography Management System of their current status, i.e. they communicate whether they were successfully integrated in a system or not.

This signal can be made visible on the ➢*Control Panel*, e.g. via an LED or color area integrated in the control panel (see ➢*Layout Toolbar*).

- Link the corresponding ➢*Control* via the **Link** tab dialog box to the object property **Connected** (for details, see **How to ...: Actions in the Control Panel** **Linking a Control to a Device**).

If the LED or the color area is active, the device was successfully integrated into the system. In this state, it can be operated from the PC via the data system.

Ready Signal

If an instrument supplies a feedback (**Ready** signal) when reaching a nominal (set) value, this can be indicated via the corresponding ➢*Control* on the control panel (LED or color box).

Ready signals are sent by column ovens, coolable autosamplers, electrochemical detectors (Antec DECADE), or gas chromatographs (HP5890; FISONS 8000).

With the coolable Dionex Autosampler GINA 50T, the **SampleTempOK** signal is sent instead of the **Ready** signal.

Using Keyboard Shortcuts

Many operations, especially in Online Control, can be performed via shortcuts.

	Action	Where	Reaction
General	Esc or right mouse button		Aborts Drag/Move
	F1		Opens the context-sensitive help;
	F2		activates the Edit mode
	Alt+Enter	➢*Browser* + ➢*Control Panels*	Opens the respective **Properties**
	Ctrl + Tab		Toggles between open windows
	Ctrl	Signal plot in the ➢*Report* and in the ➢*QNT Editor*	For zooming (changes the cursors to the zoom cursor)
Edit	Ctrl. + X		Cut
	Ctrl. + C		Copy
	Ctrl. + V		Paste
	F9		Fills the column / selected cell(s) with the first value of the selection

	Action	Where	Reaction
Control	Ctrl. + F		Flow Command
	Ctrl. + I		Inject
	Ctrl. + Break		Pump Stop
	Pause		Hold Mode
	Ctrl. + A		Data Acquisition On
	Ctrl. + B		Edit Batch
Signal plot	Double-click...	- Overview window	Unzoom
		- Time axis	Auto Plot Speed
		- Signal axis	Autoscale
		- Plot range	Signals...
		(- otherwise:...)	Axis/Decoration
	Shift	- when Zooming	Retains scale ratio between signal and value axis (i.e., the shape of chromatograms is maintained)
Gauge/Slider	Ctrl.-key	Press when dragging	Toggles the **Snap To Scale** option
Command Button	Click	Pressed button	Indicates running program. Stops program upon confirmation.
Edit Field	Tab/Enter		Sends the new value
	Esc		Aborts entry
Layout Mode	Alt+Click	In selected panel	Draws selection frame within the panel
	Alt+Drag:		Temporarily toggles the **Snap To Grid** option
	ESC		Deselect all
	Arrow keys		Drag selection pixel by pixel
	Shift + Arrow keys		Increase/reduce selection pixel by pixel
	Shift + Select		Extend Selection
	Ctrl+Select		Highlight selected control (the highlighted control is used in Align...)
	Ctrl+Drag		Copies controls
	Double click	In the Online Signal Plot of the panel	Opens **Properties...**

Installation Instructions

Introduction

The Dionex Chromatography Management System allows connecting the most diverse HPLC instruments and gas chromatographs.

Upgrading the server PC by installing additional PC plug-in boards may be necessary, e.g. when the number of serial PC ports is not sufficient. However, you can also use the ➢*UCI-100* Universal Chromatography Interface. For a detailed description on the installation and configuration procedures for the additional plug-in boards that are available from Dionex and for the UCI-100, see **Installing PC Plug-in Boards / Interfaces**.

In addition to Dionex instruments, the Dionex Chromatography Management System supports controlling a number of instruments from other manufacturers (= third-party instruments). For a list of the supported instruments and information on their installation, see **Installing and Controlling Third-Party Instruments**. Nevertheless, knowing the corresponding device manual is required!

☞ ***Tip:*** As not all instruments provide optimum suitability for direct control, it is possible that not all functions offered by the instrument can be supported!

Enabling third-party instrument control is via three steps:

- **Establishing a Serial Connection between the Server PC and the Third-Party Instrument**
- **Switching the Third-Party Instrument to Remote Operation**
- **Installing the Appropriate Device Driver in the Dionex Server Configuration**

The last topic also applies to some of the ➢*Sharable Devices* (e.g. **A/D Converter**, **Pump Control Board**, and **Dionex Universal Chromatography Interface (UCI-100)**!

Establishing a Serial Connection Between the Server PC and the Third-Party Instrument

For direct control, the third-party instrument must have a serial port. This port is then connected to the serial PC port (COM port) via a serial interface cable.

If the cable for a specific instrument has a special pin assignment, this will be described in detail under **Cable and Pin Assignments**.

Switching the Third-Party Instrument to Remote Operation

The **Installing and Controlling Third-Party Instruments** section usually provides information on the required steps for setting DIP-switches and jumpers, command input via the instrument keypad, or setting the communication parameters on the instrument. If you do not find specific information in the section on your instrument, you can use the default settings.

Installing the Appropriate Device Driver in the Dionex Server Configuration

Proceed as follows to load a third-party device driver:

- Start the server that should control the third-party instrument.
- Start the ➢*Server Configuration* program of the Dionex Chromatography Management System.
- Click the required server in the **Server Configuration** and expand the installation tree structure by clicking the **+** sign.

***Note**:* If this is not possible and the server is labeled with a red Stop sign, there is no connection between the server and the **Server Configuration**. In this case, choose the **Connect to Remote Computer** command in the **Server** menu.

- Click the timebase to which to assign the third-party instrument.
- Choose **Add Device...** via the **Edit** menu or the context menu.
- Choose the required instrument from the list of supported instruments.

***Note**:* If the desired third-party instrument is not included in the list, the required device driver cannot be found in the BIN directory of your Dionex Chromatography Management System installation. Please ask the Dionex Service for the appropriate device driver.

- Click **OK**.
- A dialog box with several tabs for configuring the selected instrument appears.
- Via the **General** tab, define the instrument name to appear in the Dionex Chromatography Management System (**Device name**), and also the port and the communications parameters (baud rate, data bits, stop bits, parity) to be used. These parameter settings must correspond to the settings on the instrument itself!
- All other configuration options depend on the functionality offered by the third-party instrument. Detectors have a **Signal** tab for selecting various channels, pumps, and autosamplers usually offer the possibility to choose from several pump or rack types.

Press the F1 key or the **Help** button to view instrument and type-specific information on the available settings.

Installing PC Plug-In Boards / Interfaces

The Dionex Chromatography Management System supports several PC plug-in boards and interfaces, which are mainly operated as ➢*Sharable Devices*. For information on how to install the different PC plug-in boards and interfaces, see the following pages:

1. PC plug-in boards and interfaces with separate drivers that can be installed as **Sharable Devices**:

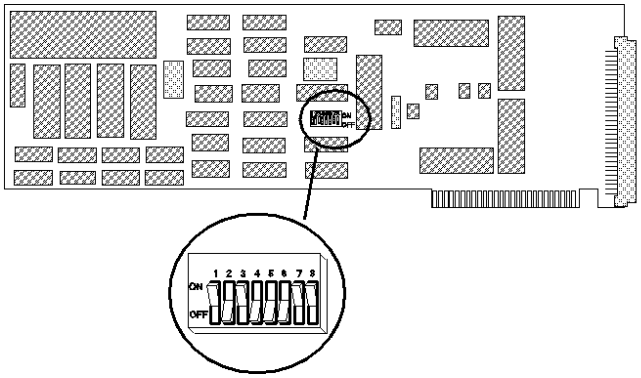
- **A/D Converter (*"16 Chl. A/D Converter"*)**
- **Universal Chromatography Interface (*"UCI-100 Interface*")**
- **Pump Control Board**
- **16-Relays Boards ME63 (ISA) and ME630 (PCI)**
- **Digital I/O-Boards ME14 (ISA) and ME1400 (PCI)**
- **16-Bit DAC Board "DAC340" (*"PDA DA Converter (16 Bit)"*)**
- **12-Bit DAC Board (*"Pump DA Converter"*)**
- **DX-LAN (*"LAN Card"*)**

2. PC plug-in boards without separate drivers that cannot be installed as **Sharable Devices**:

- **M68 - PC Interface Board for the UVD 340**
- **Serial ISA Interface Board**
- **Serial PCI Interface Board (Vscom)**
- **Serial PCI Interface Board (Equinox)**

Installing the A/D Converter (*"16 Chl. A/D Converter"*)

In the following, we assume that you already have removed the A/D Converter from your computer. Place the new ➢*A/D Converter* on a clean and dry surface, with the modules pointing upward. See the figure below for a schematic representation.



Position the board as indicated in the figure, using the block with the eight switches for setting the I/O-address as a guideline. Proper installation is in three steps:

- **Selecting an I/O-Address**
- **Setting the Base Address**
- **Selecting an Appropriate Slot**

Caution: Use a ballpoint pen to set the switch. Do not use a pencil, as graphite particles could cause a short circuit in the switch.

The board is then ready for recording and processing analog or digital signals.

Also, see:

- **Pin Assignment on the A/D Board Connector and Cable Connection**
- **Shielded Cables**
- **Analog Inputs**
- **Remote Inputs**

In the Edit menu of the **Server Configuration**, select the driver **Dionex A/D Converter** via **Add** ➢***Sharable Devices*** (➢*Server Configuration*). Establish

and assign the port address and the channels on the *General* page (link available in the Online Help only).

Selecting the I/O-Address

The ➢*A/D Converter* is fitted with a 8-fold DIP-switch. Setting the switch determines which I/O-address (port address) in the PC's address space is used for controlling the A/D board. The default setting can be used in most cases.

Should the default address collide with that of an additional board (e.g. a network interface board), you must set a new address. This procedure is described in the following. If an address modification is not necessary, skip this section and continue with the section: **Selecting an appropriate slot**.

Also, see: **Setting the Base Address**

Setting the Base Address

On MS-DOS computers, up to 1024 I/O-addresses are available (represented by 10 binary digits (Bits)). Among these 1024 addresses, sufficient I/O-addresses are available for the ➢*A/D Converter*, even if your computer contains other boards. The board requires four consecutive I/O-addresses. From 10 bits, only the higher eight bits must be coded via the switches. With the switch block, the first (=base address) of the four required addresses is set. The following table shows the allocation of the eight switches to the binary digits.

Digit	Switch	Default	Meaning
1	-	-	Not coded
2	-	-	Not coded
3	1	OFF	4-digit
4	2	ON	8-digit
5	3	OFF	16-digit
6	4	ON	32-digit
7	5	ON	64-digit
8	6	ON	128-digit
9	7	OFF	256-digit
10	8	OFF	512-digit

An open switch (OFF) corresponds to a binary 1; a closed switch (ON) corresponds to a binary 0. The default setting on the A/D board corresponds to the following base address:

4 + 16 + 256 + 512 = **788 (decimal) = 314H (hexadecimal)**.

If you use the default settings, the A/D board uses the I/O-addresses 788, 789, 790, and 791 (decimal) or 314H, 315H, 316H, and 317H (hexadecimal) of the I/O-address range of your PC. Any other board in the PC may not use these addresses. If another board (e.g. a network interface board) already uses one of the addresses, a different address must be set. Try one of the following settings:

Base Address	**Switch**							
hex: 300H (dec: 768)	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
	ON	ON	ON	ON	ON	ON	OFF	OFF
hex: 310H (dec: 784)	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
	ON	ON	OFF	ON	ON	ON	OFF	OFF
hex: 320H (dec: 800)	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
	ON	ON	ON	OFF	ON	ON	OFF	OFF
hex: 330H (dec: 816)	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
	ON	ON	OFF	OFF	ON	ON	OFF	OFF
hex: 340H (dec: 832)	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
	ON	ON	ON	ON	OFF	ON	OFF	OFF
hex: 360H (dec: 864)	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
	ON	ON	ON	OFF	OFF	ON	OFF	OFF

If your technical documents do not specify whether another board already uses the address on the A/D board, it is within your responsibility to use the presetting and to proceed with the following steps:

Caution: An I/O-address conflict usually has no serious consequences. Nevertheless, a short circuit on the bus resulting from an address conflict may destroy components on one of the two boards. This is especially true for very cheap or old boards.

After setting the switches, you can install the board in your computer.

Tip: Make a note of the current base I/O-address setting of the A/D board, as it is required for configuring the A/D board driver in the **Server Configuration**.

Selecting an Appropriate Slot

The ➢*A/D Converter* is a highly sensitive board that allows measuring voltages in the microvolt range. However, some of the available PC boards may interfere with the A/D board, as they radiate highly electromagnetic fields due to digital currents with high frequency. When starting the device driver for the A/D board, a message appears stating that the self-test was not successful. It is therefore recommended to select a **slot** that is as far away as possible from these strongly radiating boards. When you have selected a convenient slot, proceed as follows:

Remove the power and other cables, and open the computer! Refer to the Installation manual for your computer.

Select a free 8-bit- (short) or 16-bit-slot (long) in your computer.

Remove the cover plate on the back end of the slot. Keep the screw for later use. Now remove the protective cover.

⚠ ***Caution***: By static charging, modules on the A/D board may be destroyed. The risk of suffering static charging is especially high when the floor is of a well insulating material (e.g. most carpets). The risk is even higher when the air is very dry (e.g. in the winter when the heating is on) and when wearing well insulating shoes (e.g. shoes with rubber or plastic soles). In these cases, persons can be charged with high electric voltages when walking around. Electronic components could be damaged if touched. Divert static charging by touching the grounded computer housing with your hand before touching electronic components or the A/D Converter. Before standing up and walking around, discharge yourself in the same way before touching electronic components.

Align the A/D board exactly above the selected slot. Ensure that the board slides into the guide rails with the end opposite to the connector. Insert the board until it catches. If it touches the bottom, ensure that the gilded board connector points directly to the PC slot connector (slightly tilt the board to the sides, as necessary). Then, carefully insert the board.

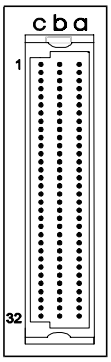
Now, fasten the metal plate of the A/D board as tight as the cover plate was before.

After you have replaced the computer housing, you can connect the analog and remote (digital) inputs of the board to your system.

Pin Assignment on the A/D Converter Connector / Cable

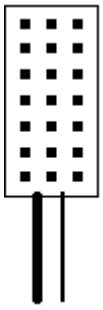
Connection

The ➢*A/D Converter* is fitted with a commonly used DIN 41612 connector (DIN = German Industry Standard). It has three vertical columns each comprising 32 contacts. The distance between the contacts is 0.1 inch. Viewing the contact pins of the connector from the rear of the computer, the right column is column a, the middle one column b, and the left column is c. The upper contact corresponds to contact 1, the lower to contact 32.



c1 Channel 1 High	b1 Channel 1 Dig. Inp.	a1 Channel 1 Low
c2 GND	b2 GND	a2 GND
...	...	...
…	…	…
c15 Channel 8 High	b15 Channel 8 Dig.Inp.	a15 Channel 8 Low
c16 GND	b16 GND	a16 GND
c17 Channel 16 High	b17 Channel 16 Dig.Inp.	a17 Channel 16 Low
c18 GND	b18 GND	a18 GND
...	...	...
…	…	…
c31 Channel 9 High	b31 Channel 9 Dig.Inp.	a31 Channel 9 Low
c32 GND	b32 GND	a32 GND

Connect the connector with the cables pointing downwards to the corresponding position:



As the positions are not defined, connect a single cable to the top position (i.e. from channel 1 to 4). If required, additional cables can be connected below.

Analog Inputs

The analog inputs of the ➢*A/D Converter* are designed for an input voltage of -10 up to +10V. Most chromatographic detectors yield a maximum voltage at their **integrator outputs**, of 1V or 2V nominally. The input range of the A/D board, therefore, is not utilized fully. Due to its automatic signal amplification, however, it yields highly resolved measuring values.

Since the inputs of the A/D board are designed as **differential inputs**, ripple voltage, as caused by the fields of the electric power supply, is inhibited, i.e., input signals are not connected between Ground (GND) and High at the A/D board connector, but between High and Low. However, the potential at the high input as well as at the low input must remain between -10V and +10V at any time with relation to ground. In order to ensure that the ground of the signal source (HPLC detector) and the ground of the A/D board have a continuous level of good quality, it is necessary to have a separate ground line between the **ground connection** at the signal source and the GND connection at the A/D converter. In case a detector has several channels that are to be connected to the A/D board, it is not necessary to have a separate ground line for each of these channels. The correct connection of the high and low line is sufficient for further channels. However, if a further detector is to be connected to the A/D board, the ground of this detector must be connected to the ground of the A/D board via a separate ground line.

Shielded Cables

When using shielded cables, the shield may only be connected to one end of the cable. If the signal source output is grounded, as is the case with most HPLC instruments, the shield ought to be connected to the ground of the HPLC instrument. The cables delivered by Dionex are screened. We recommend using only these.

Remote Inputs

In order to enable a reaction to external events (such as sample injection), the ➢*A/D Converter* is supplied with remote (digital) inputs. These remote inputs are designed for an input voltage between 0 and +5V (TTL level). If a higher voltage is applied, this may cause a malfunction of the microprocessor on the A/D board, damage to the input elements for the digital signals, or more serious damage.

Without an externally connected voltage source, internal board resistors keep the remote input level at +5V (pull-up resistance). Therefore, it is possible to

use a **contact closure relay**, without an additional voltage source. This closure has to be between GND and the respective remote input. Once the relay is shut, the digital voltage is grounded. The relay itself is under a low current of about 1mA. In case the signal source itself is active, i.e. emitting voltage, the polarization of the remote input must be correct: The ground of the signal source must be connected to the ground of the A/D board and the digital output of the signal source must be connected to the remote input of the A/D board.

Installing the Universal Chromatography Interface (*"UCI-100 Interface")*

The instrument is connected to the power supply via a primary clocked standard power unit offering a "wide range" input (auto-sensing) so no adjustment is required to select the voltage according to country-specific requirements.

The UCI 100 Universal Chromatography Interface is equipped with eight analog inputs, 8 (digital) ➢*Remote Inputs*, eight digital outputs (relay outputs), plus BCD inputs for the sample position. Additionally, four RS232 ports are available.

☞ ***Tip***: Use the RS232 interfaces (COM ports) via USB only (**no** TCP/IP)! WINDOWS NT4 computers do not support USB. Thus, if LAN connections are required, additional Equinox boards must be used for instrument control via RS232. We recommend using a peer-to-peer connection for analog data acquisition via LAN (= installation of a second network interface card (= NIC; in the operating system = adapter) in the server PC - see **Connecting the UCI-100 via a Peer-to-Peer Connection under WINDOWS NT4**).

☞ ***Tip***: Controlling GILSON instrumentation via the RS232 ports of the **Dionex Universal Chromatography Interface (UCI-100)** is **not** supported. Connect the GSIOC adapter to the multi-serial PCI interface board (Equinox) instead.

In addition to their analog inputs, the eight analog connectors provide one digital output (potential-free relay contact) and one digital input each.

Via the eight digital inputs, the data system is informed on external events such as the injection of a sample. They are distributed to the individual analog connectors but are also available all together in one separate socket.

The relay outputs allow potential-free switching of external signals. The sample position is available in the commonly used BCD format. Control of external devices such as pumps, detectors, and autosamplers is via the RS232 ports. Data transmission between the ➢*UCI-100* Universal Chromatography Interface and the Dionex Chromatography Management System is via either the inbuilt USB interface or LAN interface (Ethernet).

For detailed information on the pin assignments of the analog, digital, and BCD inputs as well as the RS232 ports, see **Pin Assignments**. The USB and Ethernet interfaces correspond to their respective standards.

Caution: Wrong polarity (remote inputs) and input voltages outside the valid range can cause damage to the unit.

See the following sections for information on hardware installation and installation under Windows:

Hardware Installation

Installation under Windows

To use the UCI-100 under the Dionex Chromatography Management System, the **Dionex UCI-100 Universal Chromatography Interface** must be installed via **Add** ➢***Sharable Devices*** in the ➢*Server Configuration* program. For details, see **Adding the UCI-100 to the Server Configuration**.

For operating the UCI-100 Universal Chromatography Interface in the network, you have to configure an IP address as well as the corresponding subnet mask. For further details, see

Configuring the UCI-100 for Network Operation (CMIPUTIL)

Pin Assignments

For information on the pin assignment of the individual connectors, see the tables below:

RS232 Ports

The pin assignment for the 9-pin D-SUB connector (male) is indicated in the table below. The pin numbers correspond to the numbers given on the connector.

Pin	Signal Name	Signal Level	Remark
1	DTR		
2	RX	RS232	
3	TX	RS232	
4	DCD		
5	GND	GND	
6			Not used
7	CTS	RS232	
8	RTS	RS232	
9			Not used

Tip: Use the RS232 interfaces (COM ports) via USB only (**no** TCP/IP)! WINDOWS NT4 computers do not support USB. Thus, if LAN connections are required, additional Equinox boards must be used for instrument control via RS232. We recommend using a peer-to-peer connection for analog data acquisition via LAN (= installation of a second network interface card (= NIC; in the operating system = adapter) in the server PC - see **Connecting the UCI-100 via a Peer-to-Peer Connection under WINDOWS NT4**).

Digital Inputs

The pin assignment for the 9-pin D-SUB connector (female) is indicated in the table below. The pin numbers correspond to the numbers given on the socket.

Pin	Signal Name	Signal Level
1	Digital Input 1	TTL
2	Digital Input 2	TTL
3	Digital Input 3	TTL
4	Digital Input 4	TTL

Pin	Signal Name	Signal Level
5	Digital Input 5	TTL
6	Digital Input 6	TTL
7	Digital Input 7	TTL
8	Digital Input 8	TTL
9	Digital Ground	GND

BCD Input

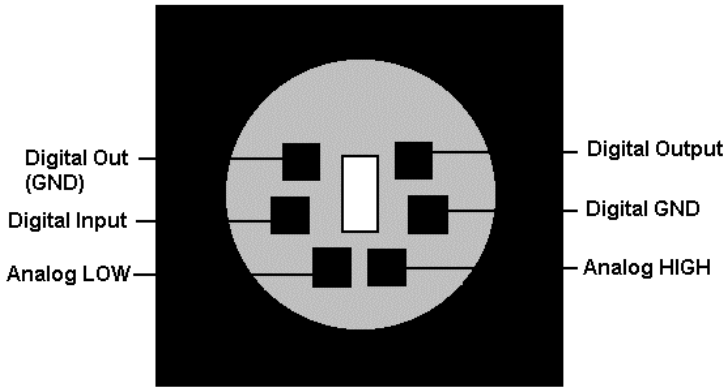
The pin assignment for the 25-pin D-SUB connector (female) is indicated in the table below. The pin numbers correspond to the numbers given on the socket. If the marked wire of a flat ribbon is connected to pin no. 1 of the female connector, the numbering within the flat ribbon will be as follows:

Pin	Wire	Signal Name	Signal Level
1	1	BCD-1A	TTL
2	3	BCD-1B	TTL
3	5	BCD-1C	TTL
4	7	BCD-1D	TTL
5	9	GND	GND
6	11	BCD-2A	TTL
7	13	BCD-2B	TTL
8	15	BCD-2C	TTL
9	17	BCD-2D	TTL
10	19	GND	GND
11	21	GND	GND
12	23	GND	GND
13	25	GND	GND
14	2	BCD-3A	TTL
15	4	BCD-3B	TTL
16	6	BCD-3C	TTL
17	8	BCD-3D	TTL
18	10	GND	GND
19	12	BCD-4A	TTL
20	14	BCD-4B	TTL
21	16	BCD-4C	TTL
22	18	BCD-4D	TTL
23	20	GND	GND
24	22	GND	GND
25	24	GND	GND

☞ ***Tip***: Internal device resistors keep the levels of the digital and the BCD inputs at + 5 V (pull-up resistance). Therefore, it is possible to use a **contact closure** relay, without an additional voltage source. This closure has to be between GND and the respective digital or BCD input. Once the relay is shut, the digital voltage is grounded.

The relay itself is under a low current of about 50 µA. In case the signal source itself is active, i.e. emitting voltage, ensure the correct polarization of the digital input (BCD input, respectively). The ground of the signal source must be connected to the ground of the ➢*UCI-100* Universal Chromatography Interface and the digital output (BCD output, respectively) of the signal source must be connected to the digital inputs (BCD output, respectively), of the UCI-100 Universal Chromatography Interface.

Analog Inputs



The range of the 6-pin analog input is as follows:

	Range
Analog LOW ↔ Analog HIGH	± 10 V
Digital Input ↔ Digital GND	0 or +5 V
Digital Out (GND) ↔ Digital Output	Turn-on voltage: 100V switching current: 0,5 A limiting value of mean on-state current: 1,0 A rupturing capacity: 10 W/10 VA forward resistance: max. 150 mOhm

☞ ***Tip***: If the UCI-100 Universal Chromatography Interface is connected to the server of the Dionex Chromatography Management System via LAN, the equipment grounding of the UCI-100 is potential free (contrary to a USB connection). With some detectors, this may affect the analog signal quality. To connect the equipment grounding of the UCI-100 to the detector grounding, use the (green) **Digital GND** wire of the signal cable and connect it to the corresponding connection to ground of the detector.

Hardware Installation

First, connect the instrument to the mains using the power unit, which is included in the shipment.

Via the two supplied signal cables one analog and one digital signal each can be sent to the ➢*UCI-100* Universal Chromatography Interface. In addition, one of the eight relay contacts can be connected to an external device. Plug the 6-pin signal cable connector into one of the inputs on the instrument' rear panel. Note the wire labels when connecting the individual wires to the desired components. The ground wire can be connected to the corresponding detector connector in order to avoid errors in measuring. Additional signal cables (part no. 8911.0001) are available from Dionex on request. Use the cable labeling set, which is included in the shipment of the UCI-100 Universal Chromatography Interface to label the connected signal cables as required.

☞ ***Tip***: The serial interface of the UCI-100 corresponds to the serial interface of commercially available PCs. Thus, the same cables that are used for the connection to the PC can be used for instrument connection as well. (For details see the operating instructions for the respective instruments; in case of third-party instruments, see **Installing and Controlling Third-Party Instruments**). Note that the UCI-100 provides a 9-pin interface so that a respective adapter might be required.

When using the **Digital Input** and **BCD Input** connections see the respective tables for information on the required pin **Pin Assignments**.

☞ ***Tip***: The USB connection to the PC or USB hub must not exceed 5 m. Longer connections are possible via a special USB extension cable (Dionex part no. 8911.0004). Up to five of these extension cables may be connected in series. Due to system reasons, the total connection length must not exceed 30 m.

Installation under Windows

USB Installation

The ➢*UCI-100* Universal Chromatography Interface offers the possibility to exchange data with the server of the Dionex Chromatography Management System via USB (Universal Serial Bus - that is available on almost all PCs). This kind of data exchange requires the corresponding USB installation under Windows. The installation procedure described below refers to Windows 98. Installing the instrument under Windows 2000 may be slightly different.

Connect the device to the mains and establish the USB connection between your PC and the UCI-100 Universal Chromatography Interface. As soon as the USB cable is plugged in, a message appears on the screen saying that the driver information is loaded. Afterwards, the Hardware Wizard guides you through installation process. Press **Next** to confirm the message that the wizard is searches for new drivers for the UCI-100. On the next page, click the recommended procedure **Search for the best driver for your device** and press **Next** to proceed to the next page.

If the Dionex Chromatography Management System is already installed on your PC, the driver will be located in the \Chromel\bin directory by default (starting with version 6.10). Specify this directory and proceed to the next wizard page by pressing **Next**. On this page, the previously selected driver position is displayed once again. Confirm with **Next** to continue the installation.

☞ ***Tip***: In case an error message appears stating that the file **UCI100**.**SYS** could not be found, confirm with **OK** to repeat the copy run. The driver will be installed correctly nevertheless.

Upon termination of the installation procedure, the last wizard page states that the software has been installed correctly. Press **Finish** to terminate the installation. The USB LED on the instrument's front panel illuminates as soon as the installation is finished correctly.

☞ ***Tip***: If the USB connection to the UCI-100 Universal Chromatography Interface is established again, you do not have to repeat the above installation procedure as your computer will already know the UCI-100 and the corresponding driver.

LAN Installation

We generally recommend connecting the UCI-100 via USB (Universal Serial Bus) to the server PC of the Dionex Chromatography Management System. If this should not be possible (e.g. Windows NT4 does not support USB), a network connection (LAN) can be used for the communication between the UCI-100 and the server of the Dionex Chromatography Management System instead.

To ensure robust communication between the UCI-100 and the server of the Dionex Chromatography Management System with a LAN connection we recommend a private network between the UCI-100 and the server PC of the Dionex Chromatography Management System (a so-called "Peer-to-peer connection). This type of connection requires a second network card to be installed in the server PC of the Dionex Chromatography Management System. For details on how to connect the UCI-100 Universal Chromatography Interface using a Peer-to-Peer connection under Window NT4, see **Connecting the UCI-100 via a Peer-to-Peer Connection under WINDOWS NT4**).

Dionex will not be able give warranty as to the operation of the UCI-100 in the Office LAN as the load of the Office LAN is a decisive factor. Overload of the Office LAN may result in timeouts and data losses and thus disturb the automatic operation of the Dionex Chromatography Management System. Therefore, we advise against operating the UCI-100 in the Office LAN.

☞ ***Tip***: For an Ethernet connection to be established to the UCI-100 Universal Chromatography Interface, assignment of an IP address and the corresponding subnet mask to the instrument is required in the CMIPUTIL configuration tool (see: **Configuring the UCI-100 for Network Operation (CMIPUTIL)**).

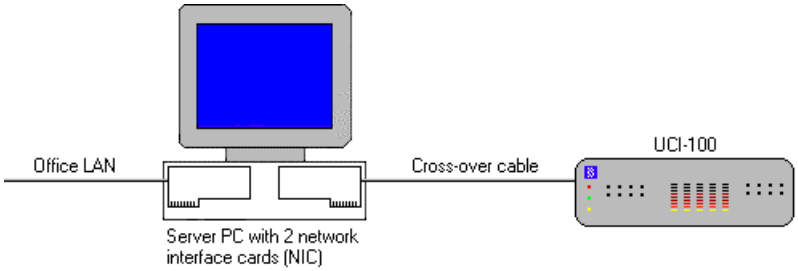
Connecting the UCI-100 via a Peer-to-Peer Connection

under WINDOWS NT4

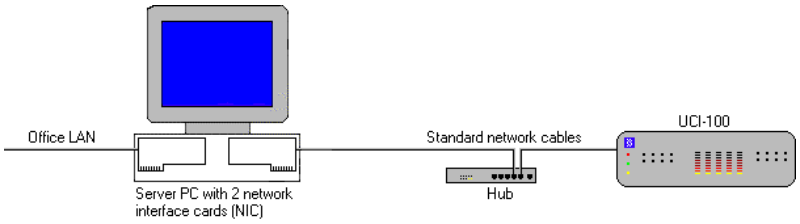
Connection of the ➢*UCI-100* Universal Chromatography Interface under WINDOWS NT4 can be via LAN only. Using a Peer-to-Peer connection between the UCI-100 and the server of the Dionex Chromatography Management System allows building up an independent network. This ensures trouble-free operation even if all analog channels and RS232 channels are used.

☞ ***Tip***: Use the RS232 interfaces (COM ports) via USB only (**no** TCP/IP)! WINDOWS NT4 computers do not support USB. Thus, if LAN connections are required, additional Equinox boards must be used for instrument control via RS232. We recommend using a peer-to-peer connection for analog data acquisition via LAN (= installation of a second network interface card (= NIC; in the operating system = adapter) in the server PC.)

The connection between the server PC and the UCI-100 is via a so-called "cross-over" cable, i.e., a special network cable with crossed over data lines. Usually, these lines are marked by colors (red, yellow) to distinguish the cable from standard network cables. Thus, the structure of the peer-to-peer connection is as follows:

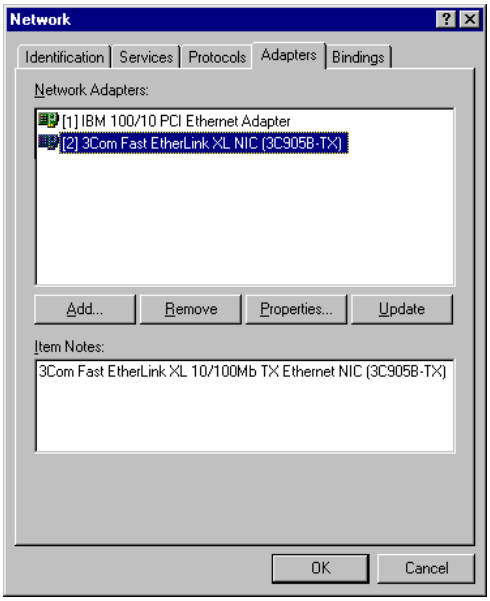


Alternatively, a hub (10Mbit) can be used with standard network cables:

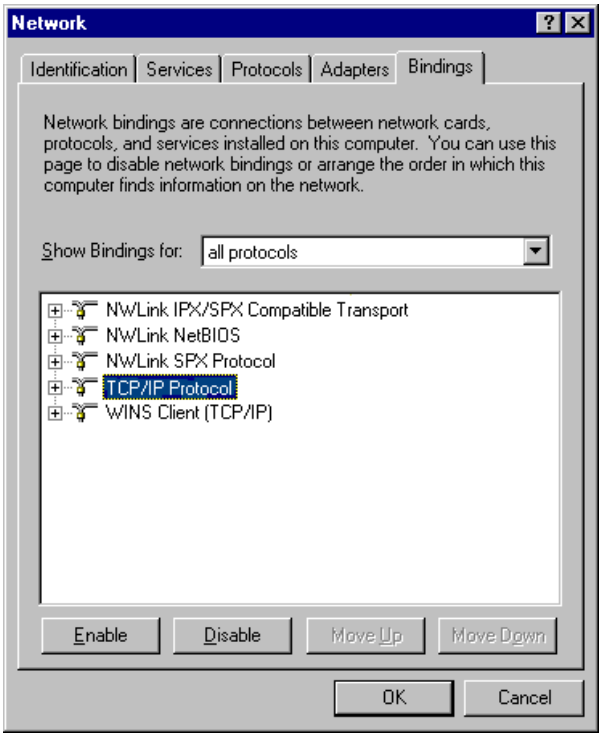


Network Interface Card (NIC)

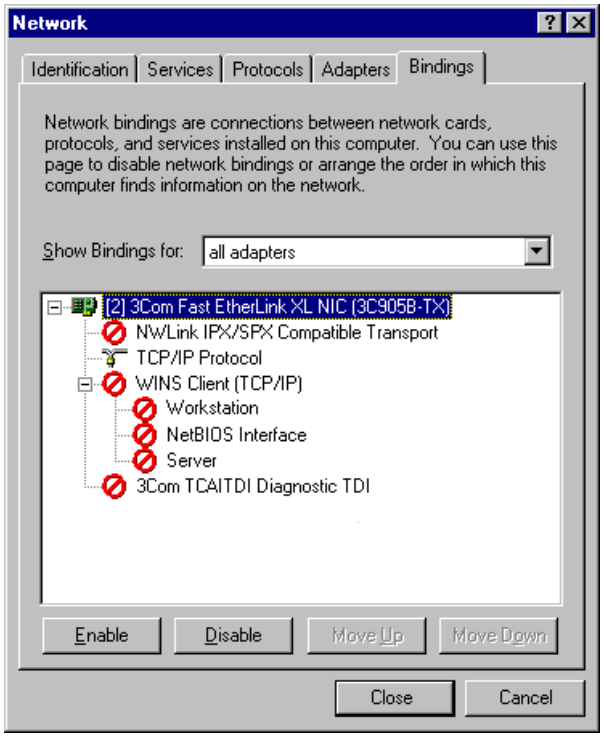
A LAN connection between the UCI-100 and the server of the Dionex Chromatography Management System, which is independent from the office LAN, requires the installation of a second network interface card (NIC, in the operating system = adapter) in the server PC of the Dionex Chromatography Management System. Install the card according to the manufacturer's instruction via Start => Settings => Control Panel => Network => Adapters => Add).



Configuring the network adapter (here [2] 3Com EtherLink XL NIC (3C905B-TX)) is on the **Bindings** tab. First, check via **all protocols** under **Show Bindings for** whether the TCP/IP protocol is installed. Install the TCP/IP protocol, if necessary:



Then, select **all adapters** under **Show Bindings for** and deactivate all protocols for the peer-to-peer connection except the TCP/IP protocol:



As the TCP/IP protocol is used for the peer-to-peer card, an IP address and a subnet mask are required for the second network adapter. Adjust the properties of the TCP/IP protocol via Start => Settings => Control Panel => Network => Protocols. Select TCP/IP protocol, right-click and select Properties... .

Caution: In the **Adapter** field, select the network interface card for the peer-to-peer connection. The settings for the office LAN network interface card must not be changed.

Caution: For the peer-to-peer adapter, deactivate all other network protocols and services (see above).

The network adapter for the peer-to-peer connection must have a fixed IP address assigned (i.e., the address must **not** be assigned by a DHCP server). Select the address in a range which is not considered for Internet routing and can be freely used for local networks.

IP Range1: 192.168.yyy.xxx
Subnet mask: 255.255.255.0

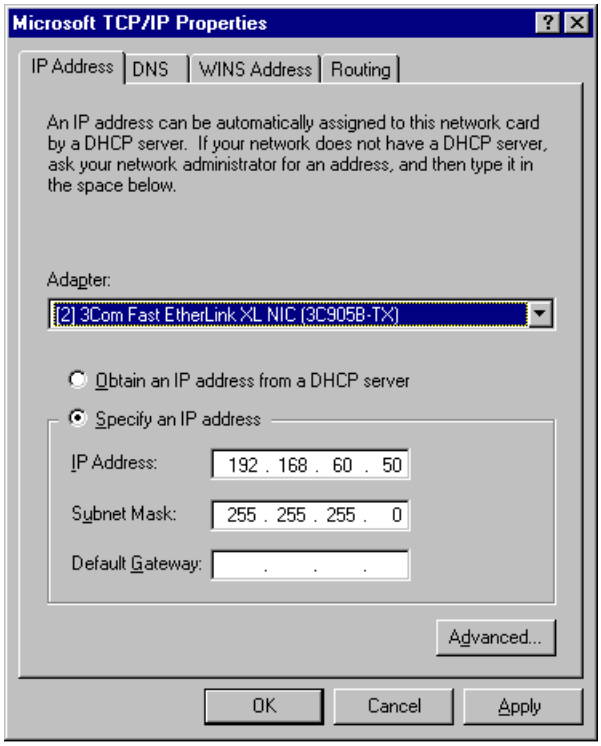
xxx and yyy are freely selectable between 1 and 254

IP Range2: 172.zzz.yyy.xxx
Subnet mask: 255.255.255.0

zzz is freely selectable between 16 and 31
xxx and yyy are freely selectable between 1 and 254

(Also, see RFC1918)

Do not enter a gateway address as no gateway is available within a peer-to-peer network and the above addresses cannot be routed. Communication between the UCI-100 and the server of the Dionex Chromatography Management System is always direct.



When selecting the IP address of the network adapter of the server PC ensure as well that, with the above subnet mask (255.255.255.0), only its last digit differs from the IP address of the UCI-100. Otherwise, the UCI-100 cannot be addressed.

☞ ***Tip***: Do not use identical IP address within a network. Example:

UCI-100: IP address 192.168.60.51

Subnet mask 255

Server: IP address 192.168.60.50

Subnet mask 255.255.255.0

☞ ***Tip***: Use neither 0 nor 255 as last numbers in IP addresses.

Checking the selected settings is via three commands, which are entered on DOS level:

```
Ipconfig /all
```

to list the configuration of all network interface cards,

```
route print
```

to check whether you can address the UCI-100 with the network interface card used for the peer-to-peer connection, and

```
ping 192.168.60.51
```

to check the connection to the UCI-100 with the IP address 192.168.60.51.

Configuring the UCI-100

Assign the UCI-100 Universal Chromatography Interface an IP address, gateway address, and subnet mask via the CMIPUTIL program (see: **Configuring the UCI-100 for Network Operation (CMIPUTIL)**). The address to be set depends on the address assigned to the network adapter in the server PC that is used for the peer-to-peer connection.

	Network Interface Card	UCI-100
IP address	192.168.yyy.xxx	192.168.yyy.aaa
Subnet mask	255.255.255.0	255.255.255.0
Gateway		192.168.yyy.aaa

☞ ***Tip***: See the information above for selecting xxx and yyy. For the UCI-100, select the same number for yyy as for the network adapter. aaa is freely selectable between 1 and 254. However, it must be different from the address set for the network adapter. For a peer-to-peer connection, the gateway address of the UCI-100 must be identical to its IP address.

Configuring the UCI-100 for Network Operation (CMIPUTIL)

In order to be able to operate the ➢*UCI-100* Universal Chromatography Interface within a network, an IP address plus the corresponding subnet mask must be configured. The responsible network administrator determines and programs these parameters by means of the CMIPUTIL configuration tool. Valid and reserved IP addresses are to be used only.

☞ ***Tip***: Only the responsible network administrator is able to ensure that an IP address is assigned only once and that IP address, subnet mask, and gateway address match correctly. Otherwise, the network connection to the UCI-100 might not be established or the communication between other participants in the network might be disturbed.

Programming and changing the parameters is possible only while no data are transferred between the UCI-100 and the server of the Dionex Chromatography Management System. Stop the server via Start/Programs/Chromeleon (or PeakNet)/Server Monitor.

In addition, the PC on which the CMIPUTIL configuration program is running must be connected to the same subnet as the UCI-100 to be programmed.

Via the CMIPUTIL tool, UCI-100 modules with firmware version 2.0 or higher (LAN support) can be programmed. Besides, the TCP/IP protocol must be available on your computer.

☞ ***Tip***: To take advantage of the network capabilities of the UCI-100 Universal Chromatography Interface if you are using a module with a firmware version < 2.0, first download the latest firmware via USB to the module (see *General* in the Online Help), and then configure the module as described below.

- Copy the **CMIPUTIL.exe** program from the supplied driver disk or the CD to a separate directory on your computer.
- Double click the program to start the configuration tool

The **Module Information** window lists all modules, which are active within the network together with their IP address, serial number (S/N), server name (the name or IP address of that server is given with which data are currently exchanged), gateway address, subnet mask, and Ethernet address. The IP address for modules, which are not yet configured, is 0.0.0.0 or 255.255.255.255.

- Select the module to be configured by its serial number.
- In the **Available IP Addresses** window, select the IP address to be assigned to the UCI-100. If it is not listed, click **Add/Remove** to enter the desired address.
- Enter the required subnet mask and the gateway address in the respective fields.
- Having made the necessary entries, assign them to the module by clicking Assign.
- Exit the program. After about 1 second, the instrument will be displayed with the new parameters.
- Checking the settings is via the **Query** button.

Based on the assigned IP address the module can then communicate with the server of the Dionex Chromatography Management System in the LAN.

☞ ***Tip***: The TCP/IP protocol, which is known from the Internet, is used for the Ethernet communication between the UCI-100 Universal Chromatography Interface and the Dionex Chromatography Management System. The network traffic depends on the amount of raw data to be transported (number of active analog channels).

☞ ***Tip***: As operating the UCI-100 Universal Chromatography Interface via an Ethernet connection in case of high network traffic may lead to transmission failures the raw data are temporarily stored in the UCI-100. However, the available memory capacity is limited as it depends on the amount of raw data to be transported.

If the network failure exceeds the buffer time, analog data may be lost.

If you notice these effects, we recommend you to establish an USB connection between the UCI-100 and the server of the Dionex Chromatography Management System. As the USB bus

is capable of performing real-time operations, overloading effects will not occur. If a USB connection cannot be established, act appropriately to avoid interruptions of the network communication between the server of the Dionex Chromatography Management System and the UCI-100.

Recommendations for Network Operation

Due to the system and contrary to USB connections, Ethernet-LAN connections have limited real-time capabilities, only. Data transmission can be performed only when any other connected user does not use the network. In order to take full advantage of the real-time capabilities of the UCI-100 Universal Chromatography Interface ensure to select a peer-to-peer connection (see **Connecting the UCI-100 via a Peer-to-Peer Connection under WINDOWS NT4**). This ensures that other participants in the network do not delay the server communication.

Furthermore, make sure that the injection signal of the autosampler and the corresponding analog detector signals are connected to the same UCI-100. The result is that possible delays in the server communication do not influence the chronological relation of these signals.

Operating the UCI-100 via a router (gateway) is possible in principle, but does not make sense.

Tip: Dionex will not be able to give warranty as to the operation of the UCI-100 in the Office LAN as the load of the Office LAN is a decisive factor. Overload of the Office LAN may result in timeouts and data losses and thus disturb the automatic operation of the Dionex Chromatography Management System. Therefore, we advise against operating the UCI-100 in the Office LAN.

Adding the UCI-100 to the Server Configuration

Before adding the ➢*UCI-100* Universal Chromatography Interface to the **Server Configuration**, connect the interface to the data system computer or an Ethernet-LAN via the USB or LAN connection on the instrument's rear panel.

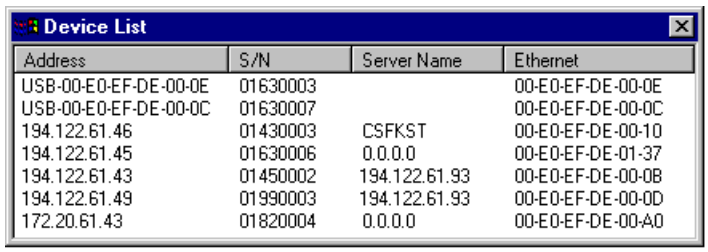
☞ ***Tip***: Use the RS232 interfaces (COM ports) via USB only (**no** TCP/IP)! WINDOWS NT4 computers do not support USB. Thus, if LAN connections are required, additional Equinox boards must be used for instrument control via RS232. We recommend using a peer-to-peer connection for analog data acquisition via LAN (= installation of a second network interface card (= NIC; in the operating system = adapter) in the server PC - see **Connecting the UCI-100 via a Peer-to-Peer Connection under WINDOWS NT4**).

1. Start the Server Monitor program by selecting **Server Monitor** from the Start/Programs menu on the task bar. For example, for Chromeleon, select **Start/ Programs/ Chromeleon/ Server Monitor**.
2 Click the **Start** button to start the server.
3. Click the **Close** button to close the Server Monitor program window. The Server Monitor icon appears on the task bar.

☞ ***Tip***: Clicking the **Quit Monitor** button, quits (exits) the Server Monitor program, but it does not stop the server. To stop the server, click the **Stop** button.

4. Start the **Server Configuration** by selecting **Server Configuration** from the Start/Programs menu on the task bar. For example, for Chromeleon, select **Start/ Programs/Chromeleon/ Server Configuration**.
5. If necessary, click the **+** character beside the server name to show the items under the server.
6. Select ➢*Sharable Devices* in the left window section. Then choose **Add Sharable Device** from the **Edit** menu (or right-click).
7. Select **Dionex UCI-100 Interface** from the list and click **OK**. The UCI-100 will be installed and shown under Sharable Devices in the left window section.
8. The Dionex UCI-100 Interface properties dialog box appears. Pressing **Browse** provides information on all UCI-100 interfaces which are available

via Ethernet (TCP/IP) or USB - with their respective serial number (= S/N). All UCI-100 modules, which are available via USB, appear with a USB prefix and their respective Ethernet addresses. If a listed UCI-100 is already connected to a server of the Dionex Chromatography Management System, the server name is displayed in the **Server Name** column. If an UCI-100 is available for connection to your server, the column shows 0.0.0.0 or is empty (for further details, see *General* in the Online Help).



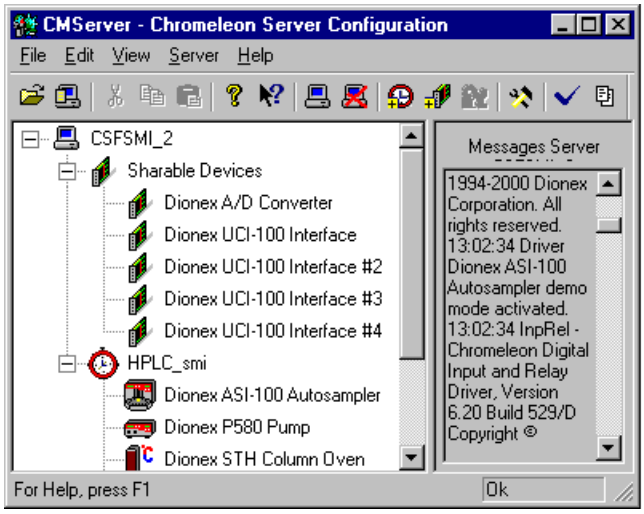
9. Select the desired UCI-100 Universal Chromatography Interface and confirm your selection by pressing Enter (or double-click). Clicking **OK** establishes the connection to the instrument and the corresponding **Connect** message including the firmware version is displayed in the Audit Trail.

To use the UCI-100 analog inputs with the Dionex Chromatography Management System, the ➢*Integrator Driver* (or the respective device driver for a third-party analog detector) must be added to the timebase and configured correspondingly (in the Server Configuration via **Add Devices** in the context menu of the respective timebase). Installing and accessing the remote inputs, BCD inputs, and relay outputs is via installing the ➢*Shared Relays and Inputs Driver* (INPREL.CDD) (as well in the Server Configuration under **Add Devices** in the context menu of the respective timebase). For controlling a device via an RS232 port, ensure that the corresponding serial communication port is assigned in the device's configuration (select the **Properties** of the respective device in the **Server Configuration**).

Adding more than one UCI-100 Interfaces to the Server Configuration

If you already have a UCI-100 Universal Chromatography Interface installed and wish to add another one to your server configuration as described above, a message appears informing you that a driver of this type has already been installed:

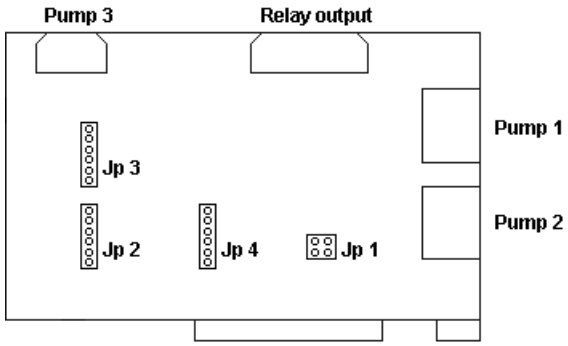
Answer the question whether to load an instance with **Yes** and proceed as described under items 8 and 9 above. Upon completion of the installation the newly installed UCI-100 Interface is shown in the server configuration together with its respective instance number.



One Dionex Chromatography Management System server can control up to four UCI-100s.

Installing the Pump Control Board

Before installing the **Pump Control Board**, connect the second slot sheet (attached) to the board. The board can be operated with an 8-bit or 16-bit slot. Ensure protection against electrostatic charge. Install the board only while the computer is switched off.



The figure illustrates the elements of the pump control board that are relevant for installation. Installation requires the following steps:

- **Selecting an I/O-Address**
- **Pulse Width and Frequency Modulation**
- **Pump Connection and Pin Assignment**

Caution: Use a ballpoint pen to set the switch. Do not use a pencil, as graphite particles could cause a short circuit in the switch.

Operation of the pump control board under the Dionex Chromatography Management System requires its installation in the ➢*Server Configuration* program. Select the **Dionex Pump Control Board** driver under ➢*Sharable Devices* and assign the port address on the *General* page (link available in the Online Help only).

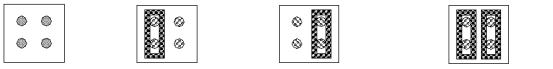
Via the pump control board, three frequency-controlled pumps can be controlled. Install the **Pump Control Board Pump(s)** device driver via **Add Device** under the corresponding timebase.

In addition, four relays and four inputs can be established. Install the **Shared Relays and Inputs** (INPREL.CDD) driver under **Add Device** to establish and assign relays and remote inputs.

Selecting the I/O-Address on the Pump Control Board

On the pump control board, there is a pin field containing four pins named JP1. By setting the jumpers, the pump control I/O-address can be configured.

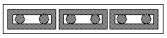
The pump control board requires 13 consecutive I/O-addresses. 350H is the default address. The following figure illustrates the I/O-addresses corresponding to the jumpers.



300H 310H 340H 350H (Default)

Pulse Width and Frequency Modulation

For each of the two pump types, the pump control board can be appropriately configured. Use the pin field marked JP3 for pump 1, the pin field marked JP2 for pump 2 and the pin field marked JP4 for pump 3. Configure the pin field as follows:



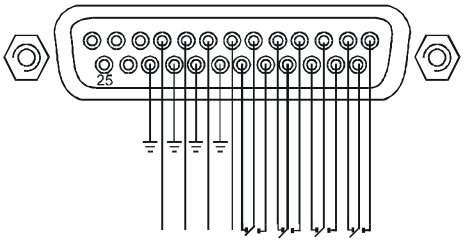
Pulse width modulation

Frequency modulation (default)

Caution: Pump control via pulse width modulation is rare nowadays. The Dionex Chromatography Management System therefore does not support this mode.

Pump Connection and Pin Assignment

The relay output of the pump control board can be connected to the outside via a 25-pin SUB-D connector. Four remote inputs (I1 - I4) and four additional relays (R1 - R4) are available. The pin assignment is shown in the illustration below:



The maximum switching potential of the relays is 100 V with a contact rating of 10 W. Ensure not to exceed a max. current of 0.5 A. To enable a reaction to external events (e.g. inject signal), the relay board offers four remote inputs, which are released when a relay closing contact (e.g. of the autosampler) grounds the corresponding input signal.

The relay connections are situated on the 25 Sub-D socket of the separate slot sheet. A connecting cable with ribbon cable is part of the accessories.

Description	Connector Pin	Ribbon Cable No.
Relay 1, normal open	1	1
Relay 1, common	14	2
Relay 1, normal closed	2	3
Relay 2, normal open	15	4
Relay 2, common	3	5
Relay 2, normal closed	16	6
Relay 3, normal open	4	7
Relay 3, common	17	8
Relay 3, normal closed	5	9
Relay 4, normal open	18	10
Relay 4, common	6	11
Relay 4, normal closed	19	12
Remote Input 1	7	13
GND	20	14
Remote Input 2	8	15
GND	21	16
Remote Input 3	9	17
GND	22	18
Remote Input 4	10	19
GND	23	20

Installing the 16-Relays Boards ME63 (ISA) and ME630 (PCI)

The M63 and M630 relay boards supply 16 relays plus 4 remote inputs (ME63) or 8 remote inputs (ME630). These are ➢*Sharable Devices*, i.e. all relays and remote inputs can be used independently of timebases.

Before you install the PCI board under the Dionex Chromatography Management System, install the respective Meilhaus hardware drivers first. The current drivers as well as a setup program for installing the drivers are available on the supplied Meilhaus CD-ROM. This is not required for the ME63 ISA board.

Install the ISA board in an 8- or 16-bit ISA slot (for the PCI board use the PCI slot instead) while the computer is switched off. Ensure protection against electrostatic discharge!

The relay contacts of the board are located on a 37-pin (ISA board) or 78-pin (PCI board) Sub-D connector (included in the delivery) on the PC. (The pre-configured cables are included in the delivery.)

Selecting an I/O-Address (ME63/ISA)

Pin Assignment on the 37-pin Sub-D Connector (ME63/ISA)

To use the board under the Dionex Chromatography Management System, the **Dionex 16 Relays ISA Board (ME63)** must be installed under **Sharable Devices** in the **Server Configuration**. To install the respective PCI board, install the **Dionex 16 Relays PCI Board (ME630)** driver instead.

Installing and assigning relays and remote inputs are via installing the device driver **Shared Relays and Inputs** (INPREL.CDD) under **Add Devices**.

Selecting the I/O-Address (ME63/ISA)

The DIP-switch block (Dual Inline Package) on the pump control board allows configuring the I/O-address of the relay board.

Starting from the base address, the relay board requires four addresses, but no interrupts. The I/O-base address is set to 300H (default) and should only be modified if there are address conflicts with other ➢*Sharable Devices*, e.g. with the pump control board.

The following table shows the assignment of the eight switches to the binary digits.

Switch	Default	Function
1	ON	8-digit
2	ON	16-digit
3	ON	32-digit
4	ON	64-digit
5	ON	128-digit
6	OFF	256-digit
7	OFF	512-digit
8	ON	1024-digit

An open switch (OFF) corresponds to a binary 1 and a closed switch (ON) corresponds to a binary 0. According to the table, the presetting on the relay board corresponds to the following base address:

256 + 512 = **768 (decimal) = 300H (hexadecimal)**.

Also, see:

Installing the 16 Relays Boards ME63 (ISA) and ME630 (PCI)

Pin Assignment on the 37-pin Sub-D Connector (ME63/ISA)

Pin Assignment on the 37-Pin Sub-D Connector (ME63/ISA)

The following connector assignment is used:

Pin	Function	Pin	Function
1	Reserved	20	Relay 9 A
2	Relay 1 A	21	Relay 9 B
3	Relay 1 B	22	Relay 10 A
4	Relay 2 A	23	Relay 10 B
5	Relay 2 B	24	Relay 11 A
6	Relay 3 A	25	Relay 11 B
7	Relay 3 B	26	Relay 12 A
8	Relay 4 A	27	Relay 12 B
9	Relay 4 B	28	Relay 13 A
10	Relay 5 A	29	Relay 13 B
11	Relay 5 B	30	Relay 14 A

Pin	Function	Pin	Function
12	Relay 6 A	31	Relay 14 B
13	Relay 6 B	32	Relay 15 A
14	Relay 7 A	33	Relay 15 B
15	Relay 7 B	34	Relay 16 A
16	Relay 8 A	35	Relay 16 B
17	Relay 8 B	36	Reserved
18	Reserved	37	Ground
19	Reserved		

For further details, see the Meilhaus manual.

Also, see:

Installing the 16-Relays Boards ME63 (ISA) and ME630 (PCI)

Selecting the I/O-Address (ME63/ISA)

Installing the Digital I/O-Boards ME14 (ISA) and ME1400 (PCI)

The digital I/O-boards support 24 digital inputs and outputs, respectively, on TTL level. In the Dionex Chromatography Management System, these 24 channels of the board are alternatively configured as digital inputs or outputs. On the PC bus, 16 successive I/O-addresses are required.

With the ME14 ISA board, set the board's base address via the DIP-switches. This procedure is not required for the ME1400 PCI board. For operating the PCI board, install the Meilhaus hardware drivers first. The current drivers as well as the Setup Program for installing the drivers are available on the attached Meilhaus CD-ROM. This step is not required for the ME14 ISA board.

Install the ISA board in an 8 or 16 bit ISA (for the PCI board use the PCI slot instead) while the computer is switched off. Ensure sufficient protection against electrostatic discharge!

The digital inputs of the board are located on a 37-pin (ME14) or 78-pin (ME1400) sub-D connector (included in the delivery) on the PC. For information on the pin assignment, see the Meilhaus manuals.

Note: The connectors on the ME14 and ME1400 filler brackets are different. Therefore, cables, which are suitable for the ME14, cannot be used with the ME1400.

Also, see: **Selecting an I/O-Address (ME14/ISA)**

To use the board with the Dionex Chromatography Management System, the **Dionex Digital I/O-ISA Board (ME14)** or **Dionex Digital I/O-PIC Board (ME1400)** driver must be installed in the **Server Configuration** under ➢*Sharable Devices*. The ME14IO24.CDD or ME1400.CDD driver is required.

With the ISA board, the I/O-basic address must be entered into the driver configuration. With the PCI board, the PCI board number must be indicated. For information on the numbering of the PCI slots of your PC, please see your PC Mainboard manual. If you know the slot number, install the board using this number. If you do not know the slot number, enter any number and install the board. In the Audit Trail, a message informs you that no PCI board has been found in the indicated slot and it states the number of the slot where a PCI board is available. Re-install the board using this number.

On the **Port Configuration** page, define whether to use the ports as outputs or as inputs. The port type can be changed only if any other device in your configuration does currently not use it.

Installing and accessing the remote inputs or outputs is via installing the **Shared Relays and Inputs driver** (INPREL.CDD) under **Add Devices**.

Selecting the I/O-Address (ME14/ISA)

On the digital I/O-board ME14, there is a DIP-switch block (dual inline package) for configuring the I/O-address of the board. The default setting is 300H (standard). To avoid conflicts with other Dionex boards, we recommend changing the setting to 340H.

The following table shows the assignment of the six switches to the binary digits.

Switch	Setting	Function
1	OFF	512
2	OFF	256
3	ON	128
4	OFF	64
5	ON	32
6	ON	16

An open switch (OFF) corresponds to a binary 1, a closed switch (ON) to a binary 0. According to the table, the setting on the board corresponds to the following base address:

64 + 256 + 512 = **832 (decimal) = 340H (hexadecimal)**.

Also, see: **Installing the Digital I/O-Board ME14 (ISA) or ME1400 (PCI)**

Installing the 16-Bit DAC-Board "DAC340" (*"PDA DA Converter (16 Bit)"*)

The Dionex 16-bit DAC-board converts digital signals from the Dionex detectors UVD 340S, UVD 170S, UVD 320S, and UVD 160S into analog signals.

The board has four independent 16-bit analog outputs, i.e. up to four detector channels can be output in analog form. The output voltage range (-10V to +10V) is constant and has a resolution of approx. 0.3mV.

For the installation of the board, a 16-Bit ISA-slot, and 40 free hex I/O-addresses are required. The following steps must be performed:

Selecting the I/O-Address

Setting Interrupts, Wait States, Jumpers

Connecting the Analog Outputs

To operate the board under the Dionex Chromatography Management System, it must be installed in the ➢*Server Configuration* program. Select the driver **Dionex PDA DA Converter (16 Bit)** under ➢*Sharable Devices*. Assign the port address on the *General* page (link available in the Online Help only).

Caution: Use a ballpoint pen to set the switches. Do not use a pencil, as graphite particles could cause a short circuit in the switch.

To avoid conflicts, use the default settings whenever possible.

Selecting the I/O-Address

The default value for the I/O-base address of the board is 280hex. The board thus uses the range from 280hex to 2Bfhex, which is available in most PCs. This does not affect the default settings of other Dionex boards (A/D Converter, UVD340 board, and pump control board).

If the base address must be changed, do this in steps of 40hex via the DIP-Switch SW1. Other possible I/O-addresses are 240hex and 380hex. The addresses are coded as follows:

Switch	Addressbit2	240hex	280hex	380hex
8	6	OFF	OFF	OFF
7	7	ON	ON	OFF
6	8	ON	OFF	OFF
5	9	OFF	ON	ON
4	10	ON	ON	ON
3	11	ON	ON	ON
2	12	ON	ON	ON
1	13	ON	ON	ON

Setting Interrupts, Wait States, and Jumpers

Setting the PC-IRQ is via the jumper block (JP3). It is located on the lower rim of the board below the red DIP-switch element. As the board is operated **without interrupt** in the Dionex Chromatography Management System, no additional alterations are required.

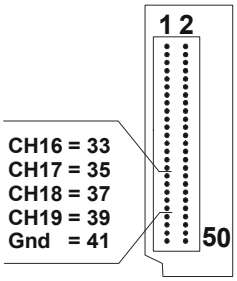
The jumper JP2 (on the left rim of the board) serves to set additional **wait states**. The default setting (1 wait state) is usually sufficient. Should there be problems with the board (e.g. spikes, no signal), a larger number of wait states can be set. The function of the jumpers is indicated directly on the board.

Do not change the settings of **any other jumpers** (JP1, 6-13) on the board.

Connecting the Analog Outputs

After inserting and configuring the 16-Bit DAC board, four analog outputs can be used on the PC, via the two-row 50-pin board output. Use the ribbon cable supplied with the board.

The 16-bit analog outputs are the pins with the names Chan 16, 17, 18, and 19 on the component side of the board. If the pins on the board output are counted from left to right and from top to bottom, these are the pins 33, 35, 37, and 39 located directly below each other on the left row. The corresponding analog ground is also located directly below (pin 41).



Caution: Always use the analog ground (Pin 41), **not** the digital ground (pin 44)!

Installing the 12-Bit DAC-Board (*"Pump DA Converter"*)

In addition to the **Pump Control Board** (frequency/pulse width control), the Dionex 12-Bit DAC board enables the voltage-controlled operation of two HPLC pumps. The board can be operated in an 8-bit slot or a 16-bit slot. The computer must be switched off before installing or removing the board.

The pumps are connected with the 25-pin Sub-D output of the board via the supplied 2 x 3pin connecting cable. Each line (**Pump1** and **Pump2**) has three wires (gnd/signal bipolar/signal unipolar). The wires correspond to pins 1, 17, and 23, or 1, 18, and 24 of the Sub-D connector. (The numbering is from top to bottom and from left to right, i.e. pin 1 is on the top left, pin 2 is directly below, etc.)

If the connectors **GND** and **bipolar** (pin 1 and 17, or 23) are used for controlling a pump, the output voltage varies depending on the jumper settings D/A or D/A1 between -5/-10 and +5/+10V.

If the connections **GND** and **unipolar** are used for controlling a pump (pin 1 and 18, or 24), the output voltage varies depending on the jumper setting D/A0 or D/A1 between 0 and +5/+10V.

Caution: We recommend using the unipolar output for controlling a pump, as only this guarantees 0V at the output when switching on the computer. Otherwise, the active -5 or -10V can trigger an immediate reaction of the pump (e.g. maximum delivery).

After inserting the board, the following settings must be performed or verified:

Selecting the I/O-Address

Jumper Settings, Wait States

Caution: Use a ballpoint pen to set the switches. Do not use a pencil, as graphite particles could cause a short circuit in the switch.

To avoid conflicts, use the default settings whenever possible.

To operate the board under the Dionex Chromatography Management System, it must be installed in the ➢*Server Configuration* program. Select the driver **Dionex Pump DA Converter (12 Bit)** under ➢*Sharable Devices*. Assign the port address on the *General* page (link available in the Online Help only).

The device driver supplies the channels **Pump_DAC_CHL1** and **Pump_DAC_CHL2** for a pump controlled via DA-channel. If the device driver for a voltage-controlled pump (**DAC pump(s)**) is installed below a specific timebase (**DAC-pump**), an assignment and control of the individual flow components (%A, %B) can be performed via the DA-channels. The Online Help provides support on the special DAC page in the **Server Configuration**: *DAC Flow A/B* (link available in the Online Help only).

Tip: If attempting to install the **DAC Pump** device driver first, the Dionex Chromatography Management System will automatically install the required driver **Dionex Pump DA Converter (12 Bit)** first so that only the board must be installed then.

Selecting the I/O-Address

The I/O-address is set via the DIP-switch element on the lower left corner of the board. The default value for the I/O-base address of the board is 300hex and usually it is not necessary to change it.

If the board is used in addition to a Dionex pump control board, it is recommended to change the address (e.g. 350hex). To avoid conflicts, check the address setting if a network card is used.

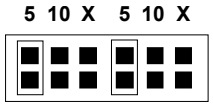
The addresses are coded as follows:

Digit	Switch	Default setting (300hex)	Function
1			Not coded
2			Not coded
3	2	ON	4-digit
4	3	ON	8-digit
5	4	ON	16-digit
6	5	ON	32-digit
7	6	ON	64-digit
8	7	ON	128-digit
9	8	OFF	256-digit
10	9	OFF	512-digit

An open switch (OFF or DOWN) corresponds to a binary 1, and a closed switch (ON or UP) corresponds to a binary 0. At the base address 300hex, the switches 8 and 9 are open. The resulting decimal value is 512 + 256 = 768. To set the base address 350hex (=848 decimal), the switches 6 and 4 must be opened in addition (512 + 256 + 64 + 16 = 848), etc.

Jumper Settings, Wait States

On the upper right corner of the board, there is a jumper block labeled D/A0 and D/A1. It serves to select the required output voltage on the bipolar and unipolar outputs. If a jumper connects both pins of the setting 5, the voltage range is limited to 5V. If the corresponding jumper is set to 10, the maximum output voltage is 10V or -10V. The settings of the block labeled D/A0 are valid for the first; the settings of the block D/A1 are valid for the second channel.



D/A0 D/A1

In the above example, the 5V setting was chosen twice, i.e. channel 1 and channel 2 supply voltage in the -5 to +5V range via the bipolar output (pins 17 and 23) and voltage in the 0 to +5V range via the unipolar outputs (pins 18 and 24).

The setting X serves to adjust the dynamic range. The voltage applied at the pin 16 or 22 of the Sub-D connector defines the maximum voltage range of both channels. The smaller the selected voltage, the smaller the steps between neighboring values, enabling a more exact pump flow setting.

On the lower right corner of the board, there is the wait state jumper. Set the jumper to ON, if no wait state is required. Usually the selected presetting (ON) must not be changed.

Installing the DX-LAN Card

In order to support instruments via ➢*DX-LAN*, the PC on which the Dionex Chromatography Management System is installed must have a DX-LAN Computer Interface Card installed.

☞ ***Tip***: Windows 95, Windows 98, Windows 2000, or Windows NT must be installed before the DX-LAN card is installed in order for the card to be set up correctly.

Complete the following steps to install the card:

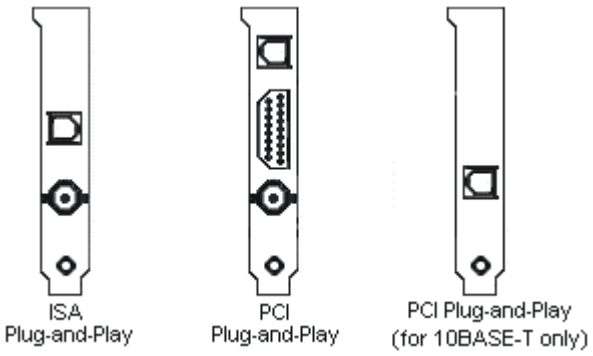
- **Install the DX-LAN Card in the Computer**
- **Connect the DX-LAN Network**
- **Install the DX-LAN Card Driver**
- **Adding the DX-LAN Card to the Server Configuration**

Identifying the DX-LAN Card Type

The following types of ➢*DX-LAN* cards are supported:

- ISA Plug-and-Play card (P/N 052351)
- PCI Plug-and-Play card (P/N 052350)
- PCI Plug-and-Play card for 10BASE-T only (P/N 056908)

To determine the type of card you have, check the card's part number and the figure below.



Installing the DX-LAN Card in the Computer

Important: **To prevent electrostatic discharge from damaging the card's electronic components, use an electrostatic grounding strap during the installation. If one is not available, do the following: before removing the card from its anti-static bag, touch the computer's metal frame to discharge any static electricity from your body.**

☞ ***Tip***: If you are not sure which model of card you have, see **Identifying the DX-LAN Card Type**.

1. Turn off the computer and disconnect its power cord.
2. Remove the computer cover.
3. Locate an empty expansion slot into which the ➢*DX-LAN* card will fit. Use the type of slot appropriate for the card (either PCI or ISA). If several slots are empty, leave as much space as possible around each installed card to ensure adequate air circulation.
4. A metal filler bracket covers the rear panel opening for the selected expansion slot. Unscrew and remove the bracket; save the screw.
5. Carefully slide the DX-LAN card into the slot, aligning the card's metal mounting bracket with the expansion slot opening on the rear panel.
6. Align the card's bottom edge connectors with the connectors on the motherboard. Firmly push the card into the motherboard connectors until the card is fully seated.
7. Replace the computer cover and any cables you removed.

Connecting the DX-LAN Network

The ➢*DX-LAN* network consists of a PC and at least one additional DX-LAN-equipped device; for example, a DX-600 module, UI20 Universal Interface, or DX-120 Ion Chromatograph. Each device to be connected must have a DX-LAN interface card installed. When the card is installed, a BNC or RJ45 (telephone style) connector extends from the opening in the rear panel of the device.

DX-LAN network connections vary depending on the type of network being installed: 10BASE-T or BNC.

10BASE-T DX-LAN Network Connections

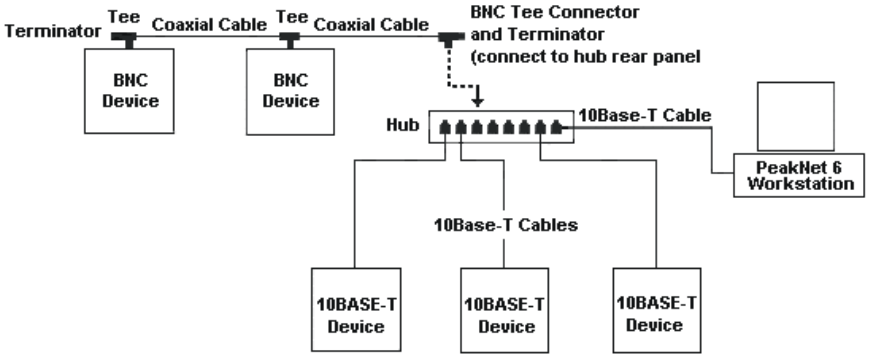
Follow these instructions when at least one of the devices on the network is equipped with a 10BASE-T (RJ-45) DX-LAN connector.

1. Plug a 10BASE-T DX-LAN cable (P/N 960279) into a 10BASE-T port on the front panel of the "combo" 10BASE-T Ethernet hub (P/N 056910). If connecting to port 8, set the Normal/Uplink push button to Normal.
2. Connect the other end of the 10BASE-T cable into the 10BASE-T DX-LAN connector on the rear panel of a 10BASE-T-equipped device, for example, the PeakNet 6 workstation.
3. Repeat Steps 1 and 2 for the remaining 10BASE-T-equipped devices.

4. If the network includes any BNC devices, follow the directions below to connect the BNC DX-LAN network.

***Important*:** **The 10BASE-T DX-LAN cable is a Category 5 unshielded twisted-pair cable. Do not substitute a cable of an inferior grade. Failure to use the correct cable will cause a device to lose communication with the host computer.**

***Important*:** **When using 10BASE-T cabling, you must install a hub. If you simply plug the 10BASE-T cable from a device into the connector on the computer's DX-LAN card, the connection will not work.**



☞ ***Tips*:** Select normal, not uplink for port 8.

The PeakNet6 Workstation can be connected to any port.

A terminator plug must be installed at each end of a BNC device network.

BNC DX-LAN Network Connections

1. Attach a BNC tee connector (P/N 921914) to the BNC connector on each device and on the BNC port on the rear panel of the "combo" 10BASE-T Ethernet hub (P/N 056910) if used.

   Note the two small locking pins protruding from either side of the BNC connector; twist the tee onto the BNC connector until the locking pins are fully engaged in the slots on the tee connector. Pull firmly on the tee connector to verify that it cannot move.

2 Connect a coaxial DX-LAN cable (3 ft, P/N 960406; 6 ft, P/N 960404; 12 ft, P/N 960405) to the first device.

   a. Slide the metal sleeve on the end of the DX-LAN cable over the BNC tee connector.

   b. Twist the metal sleeve onto the tee connector until the locking pins on the tee are fully engaged.

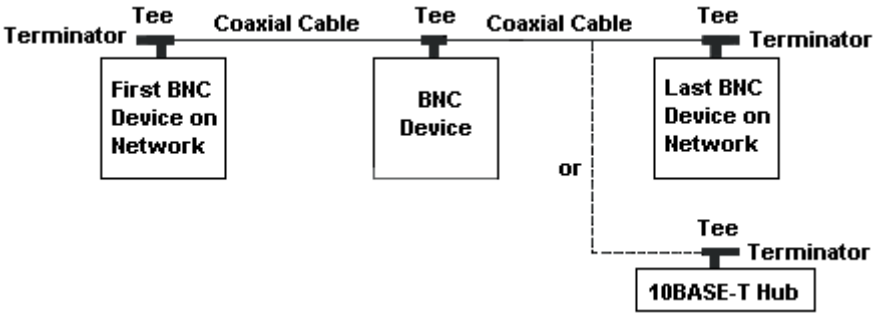
   c. Pull on the end of the cable to verify that it cannot move.

   ***Important*:** **The coaxial DX-LAN cable is a 50-ohm coaxial impedance cable. (Fifty-ohm cables are imprinted with "RG-58U.") Do not substitute an inferior cable, such as a 75-ohm television coaxial cable. Failure to use the correct cable or to lock it into place on the BNC tee connector will cause the device(s) to lose communication with the Dionex Chromatography Management System.**

3. Plug the free end of the coaxial DX-LAN cable into one of the following:
   - The BNC connector on another device, or
   - The BNC connector on the rear panel of the "combo" 10BASE-T Ethernet hub (P/N 056910).

4. Repeat Steps 2 and 3 for each device to be connected.

5. Install 50-ohm terminator resistor plugs (P/N 921034) in the BNC tee connectors at each end of the DX-LAN network.



☞ ***Tips***: Link the devices in a single line in any order.
The PeakNet6 Workstation can be anywhere in the network.
A terminator plug must be installed at each end of the network.

Installing the DX-LAN Card Driver

The ➢*DX-LAN* card driver installation depends on the version of Windows installed on your computer.

- **Windows 95B**
- **Windows 98**
- **Windows 2000**
- **Windows NT**

Windows 95B

1. After installing the ➢*DX-LAN* Plug-and-Play card in the computer and cabling the DX-LAN network, turn on the computer.

   When Windows starts, it will detect the new card and the Update Device Driver Wizard will appear.

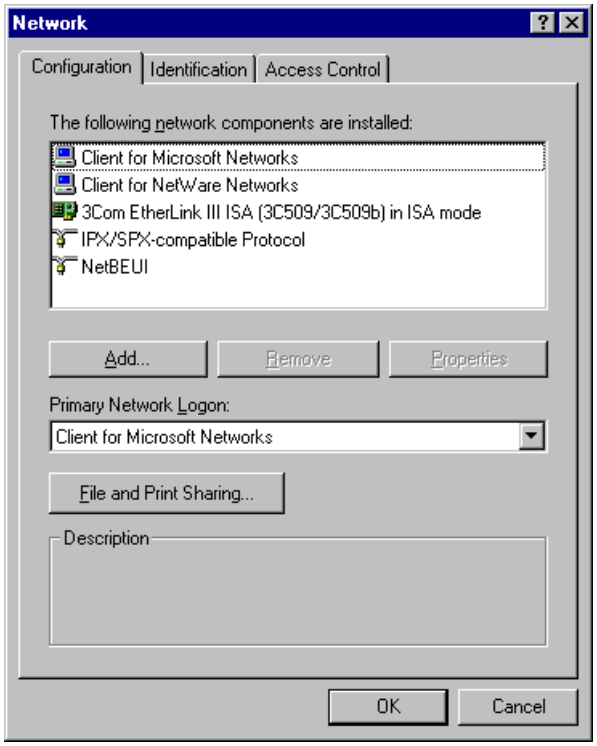
2. If Windows asks for a driver disk, insert the disk provided in the card's installation kit into an available disk drive (A or B).

3. Click **Next**.

   Windows will find the driver for the card you installed.

4. Click **Finish**.
5. A Network information box informs you that you must provide computer and workgroup names. Click **OK**.
6. Enter names for the computer and the workgroup. The computer description is optional. Click **Close**.
7. When prompted, insert the Windows 95B CD-ROM and click **OK**.
8. If prompted to insert the driver disk, click **OK** and then enter the diskette drive letter.
9. After restarting the computer, open the Control Panel and double-click the **Network** icon.

   The Network dialog box appears.

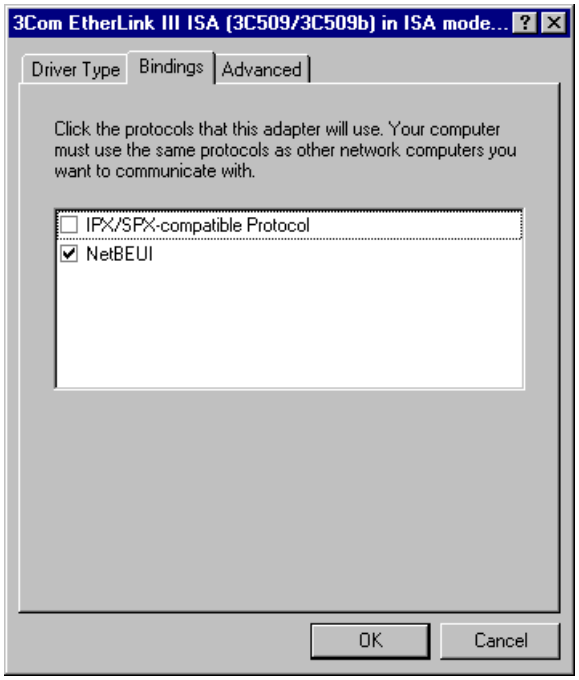


10. Double-click the entry for the card you installed.

    The Properties dialog box for the adapter appears.

11. Select the **Bindings** tab.

    As an example, the Bindings tab for the 3Com EtherLink III ISA adapter is shown below:



12. Deselect all protocols except NetBEUI.
13. Click **OK** to close the dialog box, and click **OK** again to close the Network dialog box.
14. Restart the computer.

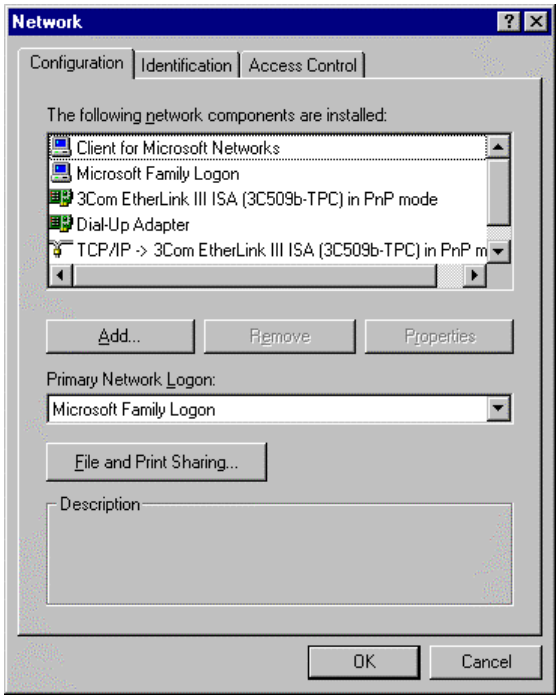
Windows 98

1. After installing the ➢*DX-LAN* Plug-and-Play card in the computer and cabling the DX-LAN network, turn on the computer.

   When Windows 98 starts, it will detect the new card and begins installing the driver.

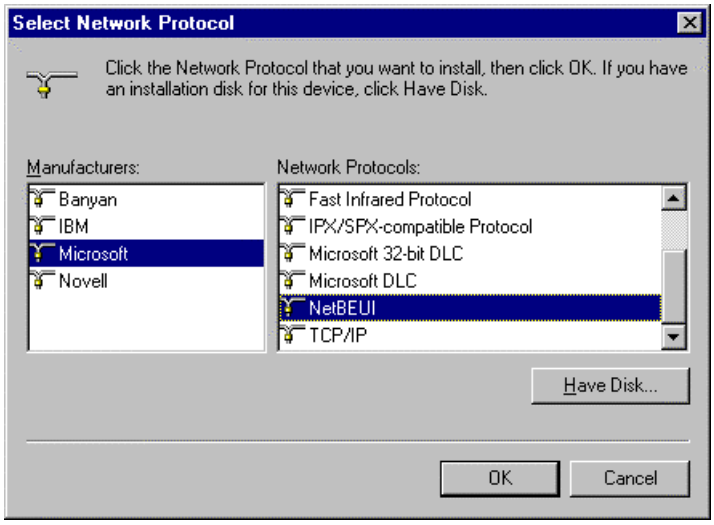
2. When prompted, insert the Windows 98 CD-ROM and click **OK**.
3. When the installation is complete, restart the computer.
4. Open the Control Panel and double-click the **Network** icon.

   The Network dialog box appears.



5. Select the entry for the card you installed and click **Add**.
6. Select **Protocol** and click **Add**.

   The Select Network Protocol dialog box appears.

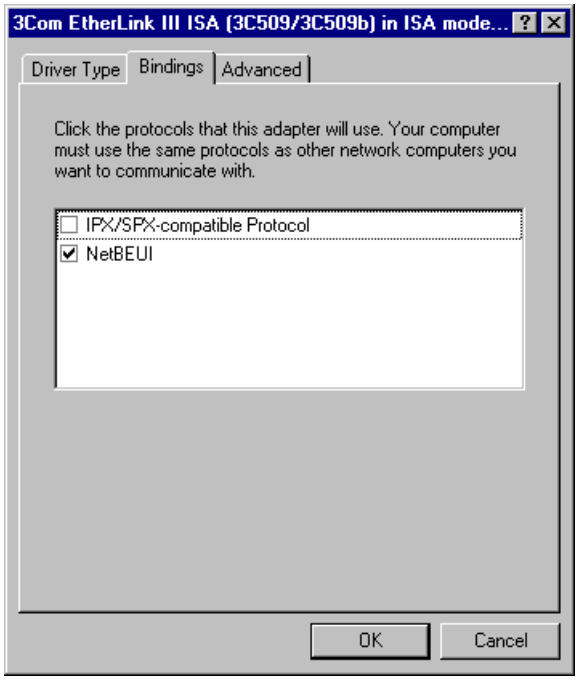


7. Select **Microsoft**.
8. Under Network Protocols, select **NetBEUI**.
9. Click **OK**.

   You will be returned to the Network dialog box.
10. Double-click the entry for the card you installed.

    The Properties dialog box for the adapter appears.
11. Select the **Bindings** tab.

    As an example, the Bindings tab for the 3Com EtherLink III ISA adapter is shown below.



12. Clear all protocols except NetBEUI.
13. Click **OK** to close the dialog box, and click **OK** again to close the Network dialog box.
14. Restart the computer.

Installing the DX-LAN Card Driver: Windows 2000

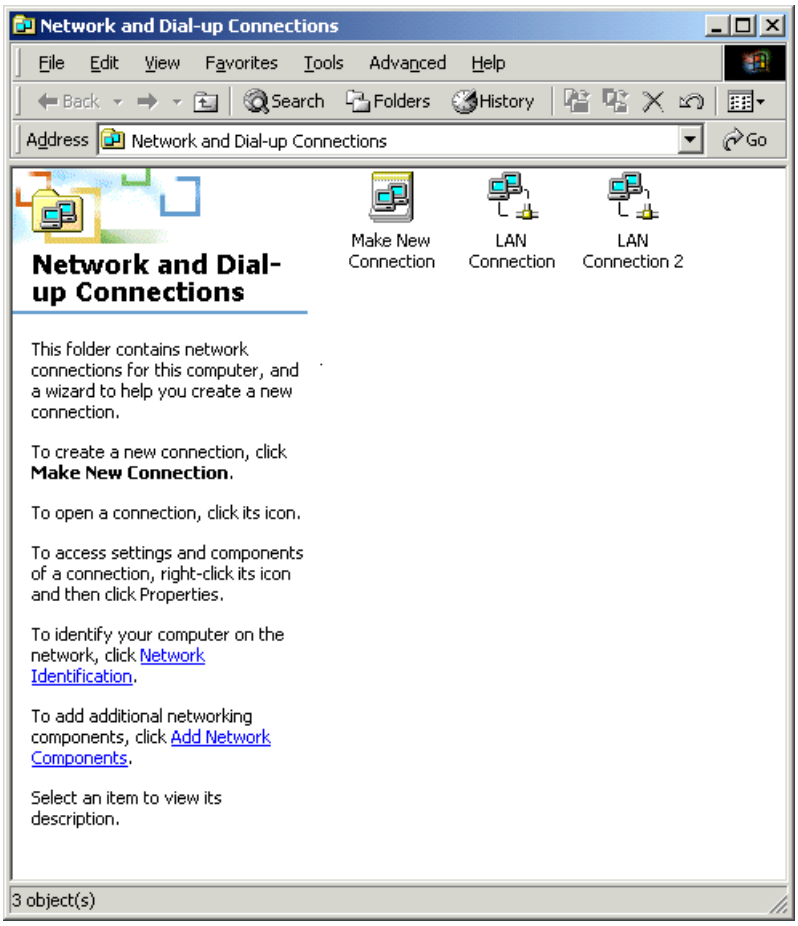
1. After installing the ➢*DX-LAN* Plug-and-Play card in the computer and cabling the DX-LAN network, turn on the computer.

   When Windows 2000 starts, it detects the new card and automatically installs the driver.

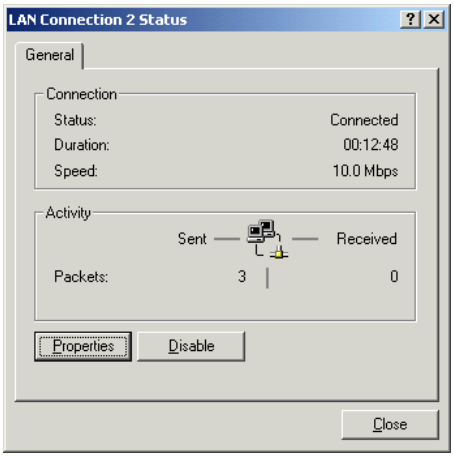
2 When Windows 2000 has completed starting, click the **Start** button and select **Settings>Network and Dial-up Connections**.

   The Network and Dial-up Connections dialog box appears. The contents of the dialog box vary depending on what network cards were previously installed on the computer. In the following example, two LAN cards are

installed. The first LAN connection is for the company's network. The second connection is for the DX-LAN.

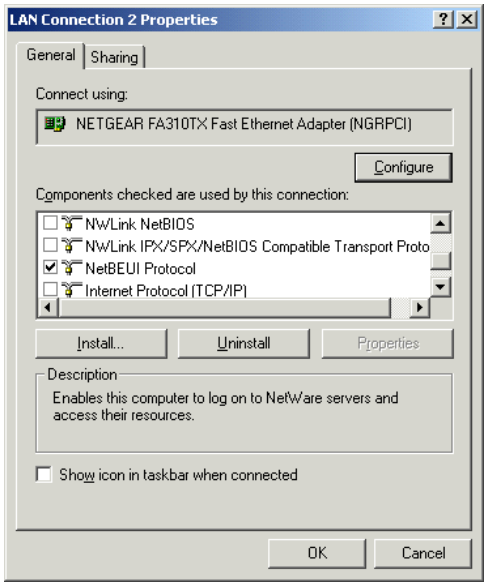


3 Double-click the icon for the DX-LAN connection (LAN Connection 2 in the example above). The following dialog box appears:



4 Click the **Properties** button. The DX-LAN card Properties dialog box appears.

5 In the **Components checked...** list, clear all check boxes, ***except*** for the **NetBEUI Protocol** box.



6 Click **OK** to close the dialog box.

Windows NT

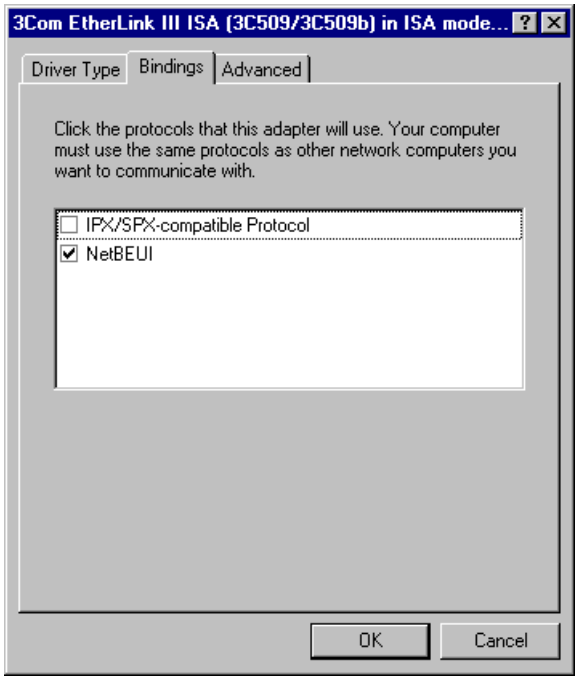
Important: **In order to install the DX-LAN card driver, you must be logged onto NT with administrator privileges. If necessary, ask the Windows NT administrator to grant you administrator privileges temporarily.**

1. After installing the ➢*DX-LAN* Plug-and-Play card in the computer and cabling the DX-LAN network, turn on the computer.
2. Open the Control Panel and double-click the **Network** icon.

   If the Network dialog box appears, go on to Step 3.

   If the Network Configuration message box appears, go to **Installing Windows NT Networking and the Plug-and-Play Driver**.
3. In the Network dialog box, select the **Adapters** tab.
4. Click the **Add** button.

   The Select Network Adapter dialog box appears and displays a list of network adapters.
5. Click the **Have Disk** button.
6. The Insert Disk dialog box appears. The default disk drive is A. If your disk drive is B, select the B drive.
7. Dionex provides a disk with drivers in the Dionex Chromatography Management System installation kit. Insert the disk into the drive and click **OK**.
8. In the list of network adapters, select the entry for the adapter you installed and click **OK**.
9. When Windows NT has finished copying the required files, select the **Bindings** tab.



10. In the Show Bindings for box, select **All Adapters**.
11. In the list of adapters, double-click the entry for the adapter you installed, to display a list of protocols for the adapter.
12. Disable all protocol entries except NetBEUI. To do so, select each entry and click the **Disable** button.
13. Click **OK** to close the dialog box.
14. When the system asks to restart Windows now, click **Yes**.

Installing Windows NT Networking and the Plug-and-Play Driver

☞ ***Tip***: Complete the steps below if the Network Configuration message box appears after you double-click the Network icon in the Control Panel. This indicates that Windows NT Networking has not been installed on your computer.

1. Click **Yes** to install Windows NT Networking now.

   The Network Setup Wizard appears.

2. Accept the default setting, Wired to the network, and click **Next**.
3. Click the **Select from list** button.

   The Select Network Adapter dialog box appears.

4. Click the **Have Disk** button.
5. The Insert Disk dialog box appears. The default disk drive is A. If your disk drive is B, select the B drive.
6. Dionex provides a disk with drivers. Insert the disk into the drive and click **OK**.
7. The Select OEM Option dialog box appears. Select the entry for the adapter you installed and click **OK**.

   The selected adapter will appear in the Networks Adapter list in the Network Setup Wizard.

8. Click **Next**.
9. The Network Protocols list appears. Select the NetBEUI protocol and deselect all others.
10. Continue following the Network Setup Wizard. Accept default settings for all the remaining steps.
11. When prompted, insert the Windows NT CD-ROM, enter the CD-ROM drive letter, and click **OK**.
12. When the dialog box appears informing you there is more than one hardware bus, accept the default settings and click **OK**.
13. Continue following the Network Setup Wizard; when finished, click **Yes** to restart the computer.

Adding the DX-LAN Card to the Server Configuration

Before adding the card to the **Server Configuration**, connect the ➢*DX-LAN* card and devices via DX-LAN cables (see **Connecting the DX-LAN Network**), and install the card driver (see **Installing the DX-LAN Card Driver**).

1. Turn on the power to all devices (detector, pump, etc.) connected to the DX-LAN network.
2. Start the Server Monitor program by selecting **Server Monitor** from the Start/Programs menu on the task bar. For example, for PeakNet, select **Start/ Programs/ PeakNet/ Server Monitor**.
3 Click the **Start** button to start the server.
4. Click the **Close** button to close the Server Monitor program window. The Server Monitor icon appears on the taskbar.

☞ ***Tip***: Clicking the **Quit Monitor** button, quits (exits) the Server Monitor program, but it does not stop the server. To stop the server, click the Stop button.

5. Start the **Server Configuration** by selecting **Server Configuration** from the Start/Programs menu on the task bar. For example, for PeakNet, choose **Start/ Programs/ PeakNet/ Server Configuration**.
6. If necessary, click the **+** character beside the server name to show the items under the server.
7. Select ➢*Sharable Devices* and then select **Add Sharable Device** from the Edit menu (or right-click).
8. Select **Dionex LAN Card** from the list and click **OK**.
9. The Dionex LAN card properties dialog box appears, displaying the name of the DX-LAN card and all other network cards installed in the computer. There are two methods for binding to the DX-LAN card: automatic and manual.

   Automatic Binding

   Click the **Automatic Binding** button (do not first select an adapter in the Network Adapters list) to have the Dionex Chromatography Management System search for the DX-LAN card. When the DX-LAN card is found, the Dionex Chromatography Management System binds to it and then establishes communication with the DX-LAN devices(s) installed on the network.

   During automatic binding, the Dionex Chromatography Management System sends commands to all installed network adapters until it finds the DX-LAN card. It is possible for this process to affect communication with the network(s) associated with the other network adapter(s). A message warning you of this appears when you click the Automatic Binding button.

For most adapters, the commands sent from the Dionex Chromatography Management System do not cause a problem and you can click **Yes** to continue. If however, you do not want the Dionex Chromatography Management System to communicate with other adapters, click the **No** button and use the manual binding procedure instead.

Manual Binding

Select the DX-LAN card in the Network Adapters list and click the **Bind to DX-LAN** button. The Dionex Chromatography Management System binds to the DX-LAN card and then establishes communication with the DX-LAN device(s) installed on the network.

☞ ***Tips***: During manual binding, the Dionex Chromatography Management System only sends commands to the adapter selected in the list.

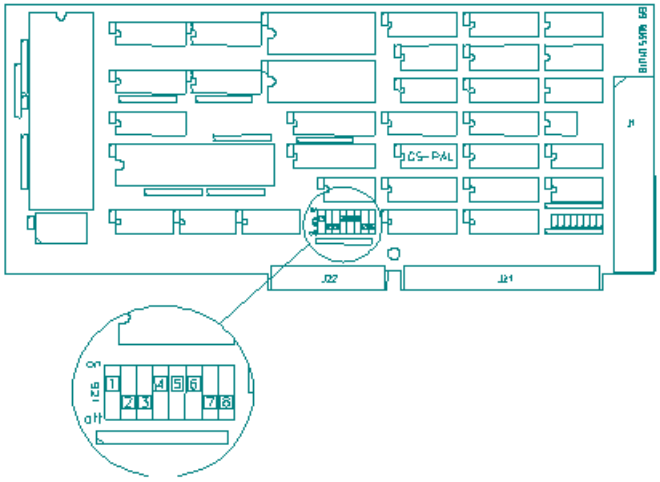
Once the DX-LAN card is successfully bound (either automatically or manually), the Dionex Chromatography Management System never sends commands to another network adapter.

10. When binding is complete, the Active DX-LAN box displays the name of the DX-LAN card. Click **OK** to close the Dionex LAN Card dialog box.

The devices connected to the DX-LAN network can now be added to a timebase (see **How to ...: Actions in the Server Configuration Changing the Server Configuration**).

Installing the M68 PC Interface Board for the PDA

The M68 PC interface board serves to receive the digital signals of the Dionex UVD 340S and UVD 170S detectors.



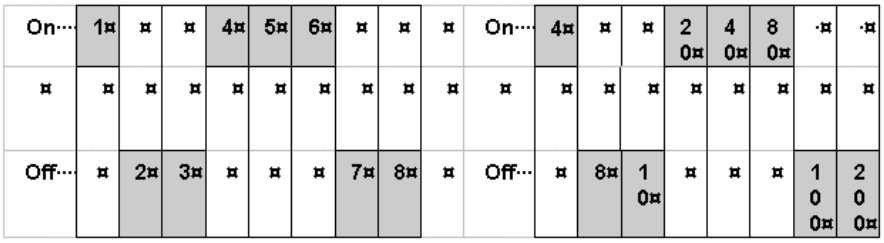
Address Settings on the M68 Board

For the selection of the I/O-base address, the board is fitted with a DIP-switch (dual inline package). The board occupies four addresses, starting at the selected base value that is factory set to 318H. Normally, this value needs not to be changed, unless operating in combination with network and/or other interface boards. Then, the address settings of all PC boards should be checked before installation.

Caution: Ensure that the PC is switched off and the power cord disconnected before installing the board.

Caution The interface board must be protected against electrostatic charge at all times. Should you encounter mechanical problems when installing the M68 board into your computer, contact your **Dionex** representative.

Tip: The board can be inserted in an 8-bit or 16-bit slot.



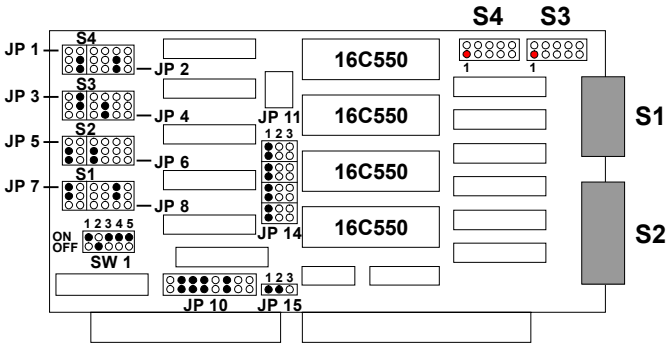
An open switch (OFF) indicates a binary **1**, a closed switch (ON) a binary **0**. On the right, the binary values are converted into hexadecimal values. The selected value can be determined by adding the value. Therefore, the default setting of the UVD 170S/340S interface board has the following base address:

$8 + 10 + 100 + 200 =$ **318H (hexadecimal)**.

Installing the Serial ISA Interface Board

Note: In addition to the ISA interface boards described here, Dionex also offers a PCI bus board. One 4-fold and one 8-fold version is available. As PCI-boards are currently more expensive than conventional boards and since they do not offer decisive advantages, they are recommended only if there are no free ISA slots or interrupt addresses in the PC. For detailed information, please contact the Dionex Service.

The ISA serial interface board available from Dionex offers four serial 16-byte FIFO interfaces. The interfaces **S1** and **S2** are directly accessible after inserting the board; **S3** and **S4** must be connected with the outside via the supplied cable. Please ensure the correct pin assignment (the red line must be connected to pin 1).



Each physical interface corresponds to a logical interface that is configured via different address combinations (I/O-address). Each logical interface can be assigned to one of a maximum of eight available interrupts.

- I/O-addresses are selected on the board via the DIP-switch **SW 1**.
- The interrupt assignment is via the interrupt jumper fields **JP 2**, **JP 4**, **JP 6**, and **JP8**.
- Interrupt through switching to the ISA-bus of the PC is via the interrupt enable jumper field **JP 10**.
- Via the jumpers **JP 11** to **JP 14,** the transfer rate of the four physical interfaces S1 to S4 is set.
- The **JP 15** jumpers can move up the address space by 1k (1/2 = 0 ... 3FFh (default), 2/3 = 400 ... 7FFh).

The board enables baud rates of up to 460 kbaud. The baud rate can be set separately for each interface.

Interrupt sharing is also possible, i.e. an interrupt can be shared by several logical interfaces.

⚠ ***Caution:*** This applies only to Windows 98, ***not*** to Windows NT 4.0/ Windows 2000! If more interrupts are required under Windows NT 4.0/Windows 2000, use the PCI 8-fold RS232 interface board available from Dionex. This board does not require an additional IRQ assignment.

⚠ ***Caution***: This board is not a **plug and play** board. The board must be installed under Windows 98 or Windows NT/Windows 2000 (see below)!

These boards are usually installed and configured by the Dionex Service. If this is not the case or if it is necessary to change the current settings, you will find the required information on the 4-fold interface board below the following topics.

- **Selecting the I/O-Address**
- **Interrupt Assignment**
- **Interrupt Through-Switching**
- **Setting the Baud Rate**
- **Installation under Windows**

Caution: Use a ballpoint pen to set the switches. Do not use a pencil, as graphite particles could cause a short circuit in the switch.

To avoid conflicts, use the default settings whenever possible.

Selecting the I/O-Address

The interface board is fitted with a DIP-switch marked **SW1**. Assigning ON and OFF states to the positions 1 to 5 determines the I/O-addresses of the logical interfaces in the DOS or UNIX mode.

The address is set via the switches of positions 1 to 3. Changing from DOS mode to the UNIX mode is via the positions 4 and 5 (DOS: 4=ON, 5=OFF; UNIX: 4=OFF, 5=ON).

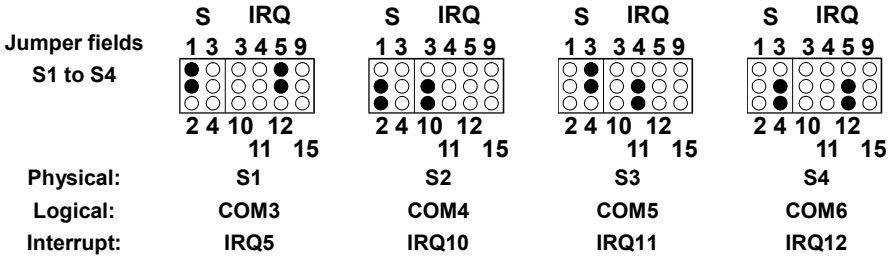
In the DOS mode (4=ON, 5=OFF), the address of the logical interface can be changed as follows (bold: default).

1	2	3	S1	S2	S3	S4
ON	ON	ON	3F8h (COM 1)	2F8h (COM 2)	3E8h (COM 3)	2E8h (COM 4)
OFF	ON	ON	2F8h (COM 2)	3E8h (COM 3)	2E8h (COM 4)	2F0h (COM 5)
ON	**OFF**	**ON**	**3E8h (COM 3)**	**2E8h (COM 4)**	**2F0h (COM 5)**	**3E0h (COM 6)**
OFF	OFF	ON	2F0h (COM 5)	3E0h (COM 6)	2E0h (COM 7)	260h (COM 8)
ON	ON	OFF	3F8h (COM 1)	2F8h (COM 2)	3E8h (COM 3)	2E0h (COM 7)
OFF	ON	OFF	2F8h (COM 2)	3E8h (COM 3)	2E0h (COM 7)	2F0h (COM 5)
ON	OFF	OFF	3E8h (COM 3)	2E0h (COM 7)	2F0h (COM 5)	3E0h (COM 6)

Interrupt Assignment

After addressing the logical interfaces (see: Selecting the I/O-Address), the physical interfaces (COM1 to COM 8) are assigned to the logical interfaces by allocating interrupts.

This is achieved by setting the jumpers **JP 1**, **JP 3**, **JP 5**, **JP 7**, and **JP 2**, **JP 4**, **JP 6**, **JP 8**. The board should have the following default settings:

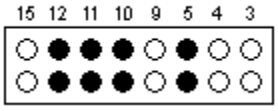


Under Microsoft Windows, the ports COM3 to COM6 are available to connect various HPLC instruments. COM1 and COM2 should be reserved for other functions (e.g. serial mouse port at COM1).

Interrupt Through-Switching

Each adjusted interrupt of the serial interface must be switched through to the ISA bus via the JP 10 interrupt enable jumper field. Through switching is only possible for interrupts that were previously assigned to an interface (see: Interrupt Assignment).

The default settings for I/O-addressing and the interrupt assignment determine how the positions 5, 10, 11, and 12 must be connected to switch through the interrupts 5, 10, 11, and 12.



Interrupt enable jumper field JP 10

Setting the Baud Rate

For each interface, a separate baud rate can be determined. The settings are via the baud rate multipliers **JP 11** to **JP 14**. The positions 1, 2, and 3 correspond to the simple, double, and fourfold basic frequency (1.8432 MHz, 3.686 MHz, and 7.372 MHz).

Caution: The Dionex Chromatography Management System only uses the basic frequency. For correct operation, the jumpers 11 to 14 must always be set to position 1! If this is not the case, serious conflicts in data transfer occur. Incorrect control and loss of data will result.

Installation under Windows

Windows 98

- Click the **Start** button, move to **Settings,** and select **Control Panel**.
- Double-click **Add New Hardware** and follow the instructions on the screen.
- Do *not* search for new hardware (**No**).
- Double-click the hardware type **Ports (COM & LPT)**.
- Select **Standard Port Type / Communications Port**.
- Click **Next** to install the corresponding driver.

Windows 98 now confirms that the installation is completed. You are prompted to restart the computer.

- **Do not restart your computer at this point!**

So far, Windows 98 only installed one interface, i.e. one (1) COM port! If you want to use several ports of the serial interface car, you have to repeat the entire procedure several times. The maximum is four times.

- Change to Control Panel / **System**.
- Open the tab dialog box **Device Manager**.
- Double-click **Ports (COM & LPT)**.

Double-click the last **COM port** in the list (when there are four additional ports installed, this is usually COM6, as the ports COM1 and COM2 are part of the standard installation).

- Open the tab dialog box **Resources**.
- Under **Setting based on** select **Basic Configuration 8**.
- Click **Input/Output Range**.
- Select **Change Setting**.
- In the **Value** field, enter the I/O-range (I/O-address) set on the board.
- Click **OK**.
- Click **Interrupt Request**.
- Select **Change Setting**.
- In the **Value** field, enter the interrupt value that is set on the board.
- Click **OK** twice.
- Repeat the entire procedure for each additional interface (e.g. COM5, COM4, and COM3).
- The port settings (baud rate, data bits, etc.) of the now correctly configured interfaces must not be set here. These settings are performed in the Dionex Chromatography Management System.

Now the installation of the interface board under Windows 98 is complete. Close the Control Panel and restart the computer, so that the new settings become effective.

Windows NT / Windows 2000

The installation of serial interfaces under Windows NT/Windows 2000 is considerably easier than under Windows 98.

- Click the **Start** button, move to **Settings,** and select the item **Control Panel**.
- Double-click **Ports**.
- Via the **Add** button, enter the required COM ports.

- Select **Settings** and **Advanced** to enter the interrupts and I/O-addresses that are set on each board via jumpers.
- Complete the procedure with **OK** and restart the computer.

It is not necessary to enter the port settings (baud rate, data bits, etc.) of the now correctly configured interfaces in Windows NT/Windows 2000. This is performed in the Dionex Chromatography Management System.

Installing the Serial PCI Interface Board (VScom)

Installing the Board

- Switch off the PC and disconnect the power cord.
- Remove the PC housing and find a free PCI slot. Carefully insert the board into the free PCI bus slot.
- Replace the PC housing, reconnect the power cord, and switch on the PC.

Depending on the environment (Windows 98 or Windows NT/Windows 2000), see the topics below for installation instructions:

Installing the VScom Board under Windows NT/Windows 2000

Installing the VScom Board under Windows 98

Also, see: **Installing the Serial PCI-Interface Board (Equinox)**

Should problems arise during the installation, see **Troubleshooting** for possible solutions.

Installing the VScom Board under Windows NT/Windows 2000

Device Driver Installation

To install the VScom board under Windows NT, insert the PCI board, and then start the program **DrvConf.exe** from the supplied diskette. DrvConf will recognize the new VScom PCI board and the already installed ports.

- As soon as the installation of the new board is complete, the configuration window will be displayed.
- Use this window to select the required board and change the configuration of individual ports. The following settings are possible below **Port Settings**:

Name: Choose the COM port assignment. Supported settings are **COM5** to **COM255**. **COM1** to **COM4** are assigned to specific addresses and cannot be selected.

Address: The addresses for ports of the boards VScom 400 PCI and VScom 800 PCI are automatically assigned by the BIOS (setting **PCI Automatic**) and cannot be changed.

IRQ: The interrupt of the board is assigned by the PCI BIOS and cannot be changed (**PCI Automatic**).

UART: The port is supplied with an UART of this type. Usually, it is not possible to change this parameter. It is recognized by the program and is only displayed.

Caution: For operating the PCI board with the Dionex Chromatography Management System, enter **Low (up to 115 kbps)** as the **Speed Mode** and choose **Overspeed**: **1** in the configuration window.

- After you have completed all settings, confirm them by pressing **OK**. The configuration program **DrvConf.exe** will then use these settings for the VSCom PCI board, copy the required device driver software and restart the system.
- After the restart, the ports of the new VScom PCI board are available in the system. You can now access the board under Windows NT.

Should problems arise during the installation, see **Troubleshooting** for possible solutions.

Installing the VScom Board under Windows 98

Device Driver Installation

When you install the VScom board under Windows 98, the following message will appear on the screen as soon as you have inserted the PCI board and after you have started Windows:

"New hardware component detected:

PCI Network Controller

Select the device driver for the new hardware component"

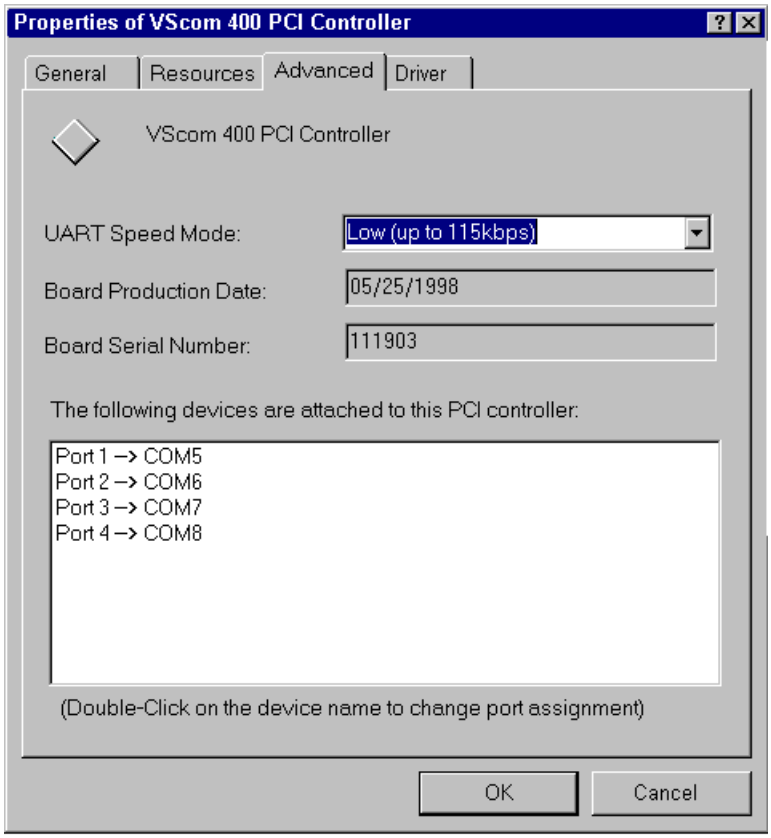
Proceed as follows:

- Insert the supplied diskette into the floppy drive.
- Select: **Device driver on Hardware manufacturer diskette**.
- Windows 98 then prompts you for the path. Normally **A:** is suggested. If this is your floppy drive, simply click **OK**.
- Windows 98 then copies and installs the device driver software for the VScom PCI board. After that, the software for the port device driver will be installed. The following message will appear on your screen: **New hardware component detected** and **VScom PCI Port #1**. Simply click **OK** when Windows 98 prompts you for the device driver diskette. Finally, all ports of the VScom PCI board will be installed.
- Windows 98 then continues the normal boot procedure.

At this point, you can check whether the installation was performed successfully. Check whether **VScom xxxPCI Controller** is entered below **Multi-function boards** in the **Device Manager** (xxx = VScom Model number). To open the device manager, click START > SETTINGS > CONTROL PANEL > SYSTEM > DEVICE MANAGER.

Port Setting: Speed and Assignment

To set the parameters for each port, choose the **Properties** of the **VScom xxxPCI Controller** (from **Multi-function boards** in the **Device Manager**). On the **Advanced** tab, you can set the speed and the assignment of the ports.



Caution: For operating the PCI board via the Dionex Chromatography Management System, enter **Low (up to 115 kbps)** on this sheet.

On the same sheet, you can change the names of the COM ports. Double-click the name you wish to change. The window **Change Port Name** will appear. Possible settings are: **COM1** to **COM99**.

If you have configured the remaining port names automatically in ascending order, choose the **Automatically renumber succeeding ports** option. All previously assigned COM port names will be ignored and will be replaced with the next free name

Should problems occur during the installation process, see **Troubleshooting** for possible solutions.

Troubleshooting

1. Use a Different PCI Slot

With some of those boards, problems might occur during the installation process. If the board driver does not recognize the board, it should be installed into the nearest PCI slot to the main board. Then, it should be possible to install the board without further difficulties.

2. BIOS Reset

You may as well reset the BIOS. Depending on your PC, this is done under either **Reset PCI Configuration** or **Reset Plug & Play Configuration**. For **DELL** PCs please proceed as follows:

- When booting the PC, press the F2 key to change to the BIOS Setup.
- Activate the LEDs **Num Lock**, **Caps Lock**, and **Scroll Lock** on the keyboard with the corresponding keys
- Enter ALT-E and ALT-F afterwards.

Installing the Serial PCI Interface Board (Equinox)

The Equinox boards are identical except for their components. Both boards have no jumpers and no DIP-switches. The boards both have a 78-pin output to which an additional cable is connected providing four (eight) serial interfaces. As soon as the board is installed, the COM port assignment and each single port are tested with a utility program supplied by Equinox.

Installing the Board

- Switch off the PC and disconnect the power cord.
- Remove the PC housing and find a free PCI slot. Carefully insert the board.
- Replace the PC housing, reconnect the power cable, and switch on the PC.

As PCI interface boards are **Plug and Play** boards, Windows 98 will attempt to install the inserted board.

- If this is the case, cancel the Windows 98 installation procedure.
- Instead, insert the supplied Equinox CD into your CD-ROM drive. Following the autostart of the CD, decide whether to perform the Windows NT/Windows 2000 or the Windows 98 installation.

Installing the Equinox Board (Board Version 3.32) under Windows NT/2000

Installing the Equinox Board (Board Version 2.30) under Windows 98

Also, see: **Installing the Serial Interface Board (VScom)**

Installing the Equinox Board (Version 3.32) under Windows NT/Windows 2000

After selecting the Windows NT / Windows 2000 installation on the Equinox CD, choose the link **Equinox SST Driver Windows NT 4.0**, **Windows NT 3.51, or Windows 2000**.

To perform the software installation, follow the instructions of the automatically displayed help text.

In contrast to Windows 98, the assignment of the COM port names and the installation of the logical COM ports are performed automatically under Windows NT/Windows 2000. Simply specify the port name with which to start (we recommend COM 11) and the number of ports to install (4 or 8).

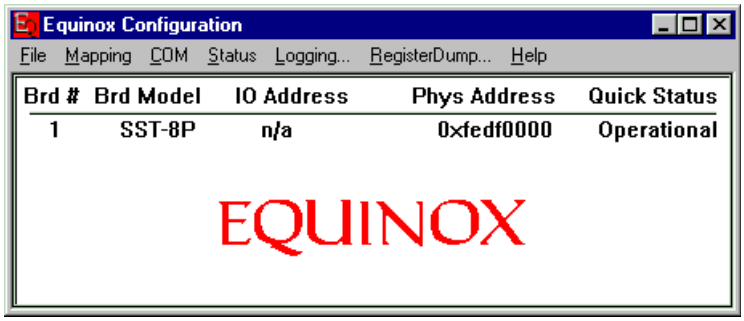
Finally, test the ports as described under **Installing the Equinox Board under Windows 98 (Board Version 2.30)** under **Functional Test**.

Installing the Equinox Board (Version 2.30) under Windows 98

After selecting the Windows 98 installation on the Equinox CD, choose the link **Finish Win98 Installation** and follow the instructions of the Software Wizard. After restarting Windows 98, the software installation of the board is completed. After that, the COM ports must be configured.

COM Port Assignment and Port Test

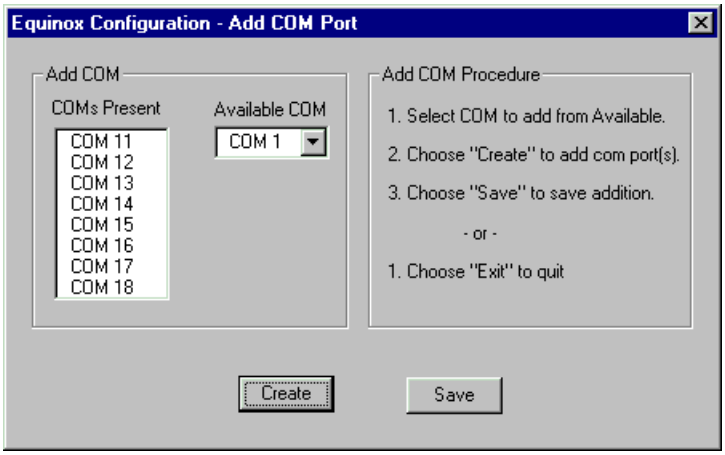
As soon as the software installation of the board is completed, the **Equinox Utilities** will be available in the start menu. Open the submenu and choose **Equinox Configuration**. The following window will appear.



If the board functions correctly, the **Quick Status** will indicate the status **Operational**. If this is not the case, detailed information is available via the **Status** option. NOTE: If the board is not recognized correctly, you may have to use a different PCI slot.

Installing further logical COM ports

Via the **COM** option, choose the **Add Logical COM ...** command to assign each port a specific COM port designation.



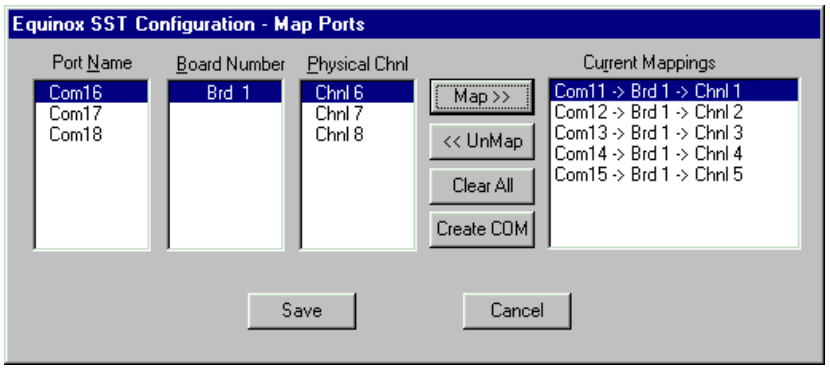
Via **Available COM**, choose a COM number and then press **Create**. Perform this four times for the 4-fold board, and eight times for the 8-fold board. NOTE: Start with COM 11. You will thus prevent overwriting an existing COM port assignment (e.g. COM1 = mouse port)!

In the field **COMs Present**, the designations COM11 to COM14 (4-fold board) or COM11 to COM18 (8-fold board) are displayed. Save the settings using the **Save** command.

If error messages appear (e.g. **Can't save to registry**), you can ignore them at this point. So far, they have not impaired the functionality of the board.

Connecting logical COM Ports with the Physical Channels

Via **Mapping**, choose the **Map Port** command. You will see the following dialog:



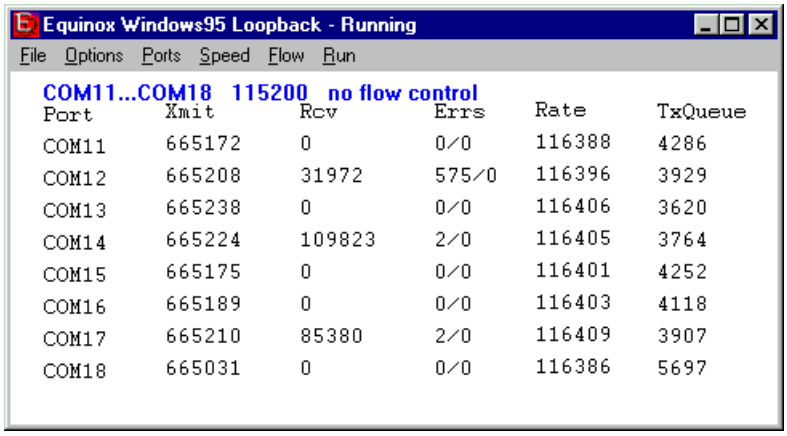
The list box **Port Name** shows all previously installed logical COM ports (e.g. COM11 to COM18). Via **Map**, the logical ports can be assigned physical channels (by pressing the button four or eight times). The result of these mappings is displayed in the list box **Current Mappings**. Save these settings via **Save**. Any error messages can be ignored.

After restarting Windows 98, the additional four or eight COM ports should be available.

Functional Test

The **Eqnloop** utility serves to test the functionality of the ports. Via **Equinox Utilities**, choose the **Equinox Eqnloop** command. In the **Loopback** dialog of the **Ports** menu, specify the number of the first COM port (number **11** in these instructions) under **First**. Via the **Count** command, specify the number of COM

ports that should be tested (4 or 8). You will see the following dialog. Start the test via the **Start** command in the **Run** menu.



As soon as you plug the included 25-pin loop-back connector in one of the ports, you will see a constantly changing value in the **Rcv** column. This is an indication for the optimum functionality. Repeat the test with all ports.

Installing the License Server

The optionally available ➢*License Server* of the Dionex Chromatography Management System (Dionex CMS) can be installed on any network PC fulfilling the following conditions:

- The operating system is Windows 98, Windows NT 4.0, or Windows 2000.
- LAN connection is via TCP/IP or IPX/SPX

Standalone

Copy the distribution files (17 in total) to any directory of your choice.

Note: If you do not see all 17 files in the Windows Explorer, make the missing ones visible via the **View** menu. Select **Options** to open the corresponding dialog box and select the **Show All Files** option.

The default path is **C:\Program Files\Softron\Chromeleon License Server**. Copy the **CmLicSrv.ini** license file that is shipped with the program to this directory. Your licenses of the will be available via the network provided the **CmLicSrv.ini** file is available in the above-mentioned directory.

To install the License Server, call the **CmLicMon** License Server Monitor once from the command line (DOS box) via the " **/install**" parameter (observe the space in front of the slash). Select **Start** > **Run** and browse for the **CmLicMon.exe** file in the opening dialog box. Pressing **Open** automatically writes the following entry into the **Run** box (if the CmLicMon.exe file was copied to the above default directory)

```
"C:\Program Files\Dionex\Chromeleon License Server\CmLicMon.exe"
```

Tip: The entry is given in quotation marks if spaces are used in the directory names. If no spaces are used, the quotation marks will be omitted, as they are not required.

Following the above entry, enter `/install`.

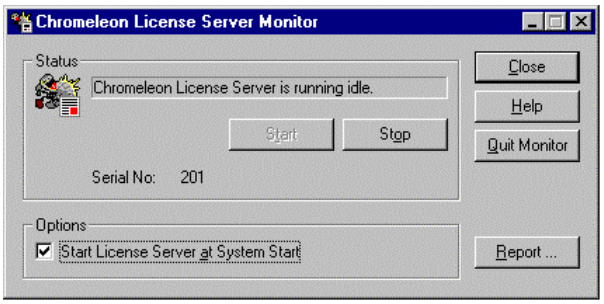
Note: Do not forget to enter the space in front of the slash!

Pressing **OK** executes the call.

Under Windows NT/Windows 2000, administrator privileges are required to perform this step.

Optionally, a link to the **CmLicMon** monitor program can be included in the Autostart directory. This will automatically start the monitor program whenever the system boots.

If you wish to start the License Server automatically as well upon booting your computer, open the monitor program and click **Start License Server at System Start**.



A configuration file for the License Server is supplied together with the distribution. However, this file needs to be adapted to local requirements. Replace the computer names PC_XX in the [Servers] section of the file **CmLicSrv.ini** by the names actually used in your network (e.g. ALPHA, BRAVO...). This is to assign serial number/➢*Key Code* pairs to the servers of the Dionex Chromatography Management System:

```
[License Server]
Serial Number = 4711
Key Code = 112233-445566
Pal Location = 5

[Servers]
ALPHA:        1/111111-111111
BRAVO:        2/222222-222222
CHARLIE:      3/333333-333333
DELTA:        4/444444-444444
ECHO:         5/555555-555555
FOXTROT:      6/666666-666666

[Clients]
 Max Clients = 10

[Checksum]
Checksum = 0x00005E77
```

☞ ***Tip***: If you have a hard-protect installed (i.e., the entry in the INI file

is: Pal location = 1), an I/O address must be specified. Enter the line "Pal Address = 0x030f". Depending on the jumper settings on the hard-protect, other available options are: 0x031f, 0x032f, and 0x033f. If the "Pal Address =" line is missing in the INI file, 0x030f is the default. Do **not** modify any other settings!

License Server and Dionex CMS Server installed on one PC

Install the Dionex Chromatography Management System (Dionex CMS) on your PC. The default path is **c:\chromel\bin**. Copy the **CmLicMon.exe** and **CmLicSrv.ini** files (both shipped together with the program) to this directory as well.

To install the license server service of the Dionex Chromatography Management System, start the **CmLicMon** License Server Monitor from the command line (DOS box) via the **/install** parameter:

C:\Chromel\Bin>cmlicmon /install

Under Windows NT, administrator rights are required for this step.

Proceed with the installation as described under **Standalone**.

If problems occur during the installation of the license server, see **Troubleshooting (License Server)** for possible remedial actions.

Troubleshooting (License Server)

- **The license server of the Dionex Chromatography Management System does not start**

  Under Windows 98

  Start the **CmLicSrv** program by selecting the **/console** option in the DOS command line.

  ```
  C:\Program Files\Dionex\Chromeleon License Server>cmlicsrv /console
  ```

  Following a list showing all network protocols that are available for RPC, the **CmLicSrv.ini** configuration file is displayed. Was the file found and completely processed? Did you modify entries in the file apart from the computer names? If **Listening for Clients** is not displayed at the end of

the file, the ➢*License _Server* cannot be initialized. Repeat the installation with **`cmlicmon /install,`** using administrator rights, if necessary.

Under Windows NT

First, check the Event Viewer of your system:

Start -> Programs-> Administrative Tools (Common) -> Event Viewer -> Log-> Application

CmLic Srv logs the server start and indicates possible errors. If the information given in the Event Viewer is not sufficient, you can activate extended output.

Start the CmLicSrv program via the Control Panel and not via the license server monitor.

Start -> Settings -> Control Panel-> Services

Enter **/console** as startup parameter and start the **Chromeleon License Server** service by pressing the **Start** button. Among others, all detected entries of the **CmLicSrv.ini** license file, possible errors, and all connection attempts of the Chromeleon (or PeakNet) servers and Chromeleon (or PeakNet) clients are logged.

- **The License Server of the Dionex Chromatography Management System remains in the Demo Mode**

  Check whether the supplied hardware protection module (dongle or hard protect) is correctly installed. The serial numbers of the module and in the [License Server] section of **`CmLicSrv.ini`** must be identical.

  Check whether the **Pal Location** entry in the [License Server] section of **`CmLicSrv.ini`** has been changed. "5" is the correct entry for dongles while "1" corresponds to hard-protects.

- **The Server of the Dionex Chromatography Management System remains in the Demo Mode**

  In the server configuration of the Dionex Chromatography Management System, ensure that the computer name for the license server is correct. Check whether the correct RPC protocol is used. Also check whether the PC on which the license server is installed can be accessed via the network, e.g. for a TCP/IP network with **`ping servername`** or by opening a network share in the Windows Explorer. Check whether a line for the server of the Dionex Chromatography Management System is provided in

CmLicSrv.ini and ensure that the computer name is spelled correctly in the [Servers] section.

- **The Server of the Dionex Chromatography Management System starts, however, the device drivers complain that a device control feature is missing when loading**

  The starting sequence for the two server services, the Chromeleon (or PeakNet) Driver and the Chromeleon (or PeakNet) Server, is not correct. Uninstall the services via the Server Monitor of the Dionex Chromatography Management System: **C:\Chromel\Bin>cmmon /deinstall**. Restart the computer and reinstall the services via the Server Monitor of the Dionex Chromatography Management System:

  C:\Chromel\Bin>cmmon /install

- **The Client of the Dionex Chromatography Management System remains in Demo Mode**

  In the client of the Dionex Chromatography Management System, ensure that the computer name for the license server is correct.

  Check whether the correct RPC protocol is used.

  Also check whether the PC on which the license server is installed can be accessed via the network, e.g. for a TCP/IP network with **ping servername** or by opening a network share in the Windows Explorer.

  Check in the License Server Monitor report of the Dionex Chromatography Management System whether all licenses for the clients were used. Restart the license server, if necessary.

- **Network Failure**

  In normal circumstances, a network failure does not cause any damage. Both, the Server and the Client of the Dionex Chromatography Management System Server save the license information locally for up to 7 days. Normally the user can continue working during this period even if the License Server cannot be accessed. Only after this period, the server of the Dionex Chromatography Management System shuts down and the client runs in demo mode.

  If the connection to the License Server of the Dionex Chromatography Management System is disrupted during active operation or if the connection is not available when the system is started, this is logged in the daily audit trail. In this case, a dialog box is displayed in the Client

indicating the remaining time. In addition, it is also logged into the audit trail when the connection to the CMLS is available again. The two audit trail warnings look as follows:

09:40:46 Warning: Chromeleon Server failed to retrieve a license from the license server CCHROMEL! Your local license will expire in 167 hours.

09:41:16 Chromeleon Server succeeded to retrieve a license from the license server CCHROMEL! Your local license has been updated.

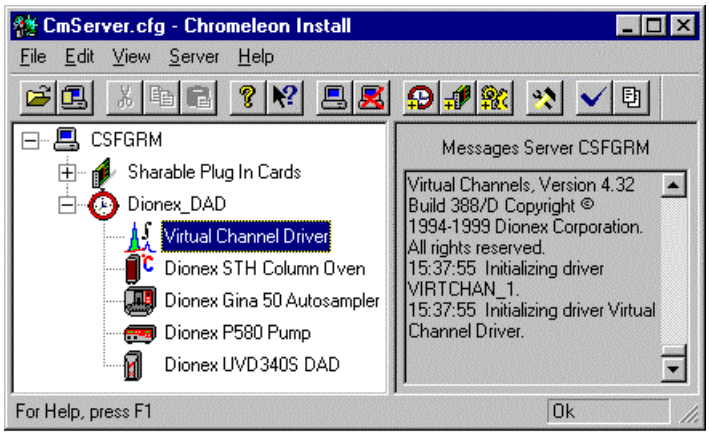
- **Could not create "Chromeleon Operators" group - No mapping between account names and security IDs was done**

  During the installation of CmLicSrv on an NT Backup Domain Controller the error **Could not create "Chromeleon Operators" group - No mapping between account names and security IDs was done (8b2)** might occur when calling in CmLicMon.exe /install. Remedial action: Create the group via the NT User Manager before running CmLicMon.exe /install.

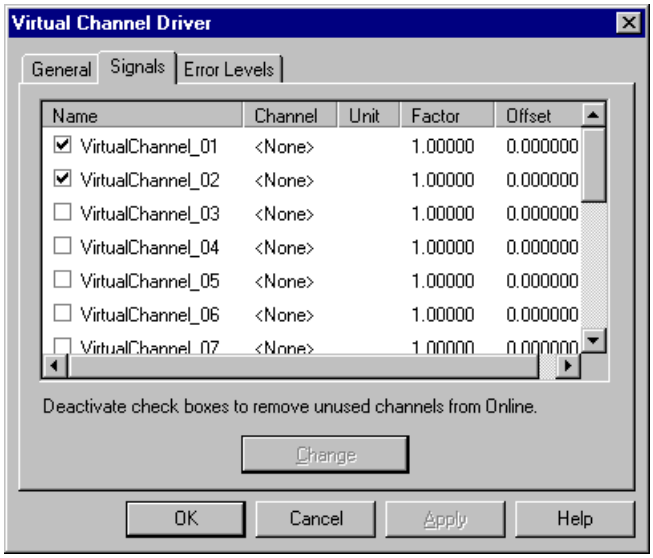
Also, see: **Installing the License Server**

Installating the Virtual Channel Driver (VCD)

The ➢*Virtual Channel Driver (VCD)* of the Dionex Chromatography Management System is a standard device driver of the Dionex Chromatography Management System that must be assigned to a timebase in the Server Configuration of Dionex Chromatography Management System. As standard, 16 virtual channels are available. If more virtual channels are required, several instances of the driver are possible:



If necessary, the standard channel names (`VirtualChannel_XX`) can be changed in the *Signals* configuration dialog after the installation:



This terminates the installation.

Also, see

Installing the Virtual Channel Driver: Configuration

Installing the Virtual Channel Driver: Channel Configuration

Installing the Virtual Channel Driver: Channel Types

Configuration

The ➢*Virtual Channel Driver (VCD)* offers the two properties *SamplingStep* and *LagThreshold*, which apply to all channels.

SamplingStep defines the time interval after which the VCD re-evaluates the expressions that are assigned to the channels. Only then, the signal of the virtual channel will be influenced by the modified terms in the expression. The smaller the interval, the more precise the recording of the modifications, yet the higher the workload of the processor.

Neither Windows 32 nor Windows NT/2000 are real-time operating systems. Therefore, a *precise* sampling rate cannot be ensured by a pure software solution such as the VCD. By comparing the two values, the VCD tries, however, to keep the channel time deviation (= number of generated data points multiplied by the *SamplingStep*) as small as possible against the time

that actually passed. If this difference exceeds or falls below the time interval defined by *LagThreshold*, an additional data point will be interpolated or a data point will be omitted respectively to bring the channel time up to the real time again. The longer the interval, the fewer data will be falsified, yet the longer the time deviation (especially with long acquisition times!).

Internally, a 100Hz signal is generated from the signal that was recorded with the data rate previously defined via *SamplingStep*. Then, the 100Hz signal is forwarded to the compressor. For digital channels, the last calculated value is repeated sufficiently often; in other cases, the last three calculated values are parabolically interpolated.

Also, see:

Installing the Virtual Channel Driver: Installation

Installing the Virtual Channel Driver: Channel Configuration

Installing the Virtual Channel Driver: Channel Types

Channel Configuration

The ➢*Virtual Channel Driver (VCD)* of the Dionex Chromatography Management System needs to know the expressions to be recorded. They are specified directly in the ➢*Program* (for information on the syntax please refer to: **How to ...: Device Control Virtual Channel Commands**).

For optimizing the signal recording, each virtual channel must have a type assigned. At present, three types are defined:

Analog	Suitable for expressions consisting of other analog signals	`UV_VIS_1/UV_VIS_2`
Digital	Suitable for digital expressions	`P580Relay_1.State AND P580Relay_2.State`
Fixed	Suitable for expressions that change slowly	`Pump.%A`

The selected type affects the settings of *Step*, *MaxAutoStep,* and *Average* of the respective signal as well as the selection of appropriate raw data compression. With the standard compressor of the Dionex Chromatography Management System, the meaning of these three parameters is the same as with normal signal channels. With the step compressor, they are irrelevant as this compressor type always uses a fixed step of 0,01s for sampling.

The following values are default:

	Step	MaxAutoStep	Average	Compression
Analog	Auto	5.1s	On	Standard compressor of the Dionex Chromatography Management System
Digital	Fixed, 0.01s			Special compressor for step signals
Fixed	Fixed, 0.01s	5.1s	Off	Standard compressor of the Dionex Chromatography Management System

For analog and fixed channels, the values for *Step*, *MaxAutoStep,* and *Average* can be changed after setting the type. For fixed channels, identical settings for the step rate and the *SamplingStep* are recommended to ensure that the compressor only records the originally sampled datapoints.

Use the *Formula* commands to specify the expression to be recorded. All expressions that are available in the condition of a *BeginTrigger* command can be used, i.e., arithmetic and logical operations. However, the expression must be numerical. While the program is executed, the property *FormulaCur* states the last calculated value of the expression (which is different after each *SamplingStep*.) The resulting minimum and maximum values of the expression are indicated in *FormulaMin* and *FormulaMax* respectively.

Similar to other signal channels, the property *Value* allows viewing the current (perhaps interpolated) signal value (changes every 0.01s).

The *Equate* property allows you to assign the virtual channel an additional user-defined name during the program run. You can use *Log* system command to write this to the Audit Trail.

During data acquisition, it is not possible to change the **Step**, **MaxAutoStep**, **Average**, **Formula**, and **Type** properties. The **FormulaMin**, **FormulaMax2**, and **2FormulaCur** properties are **read-only**.

Also, see:

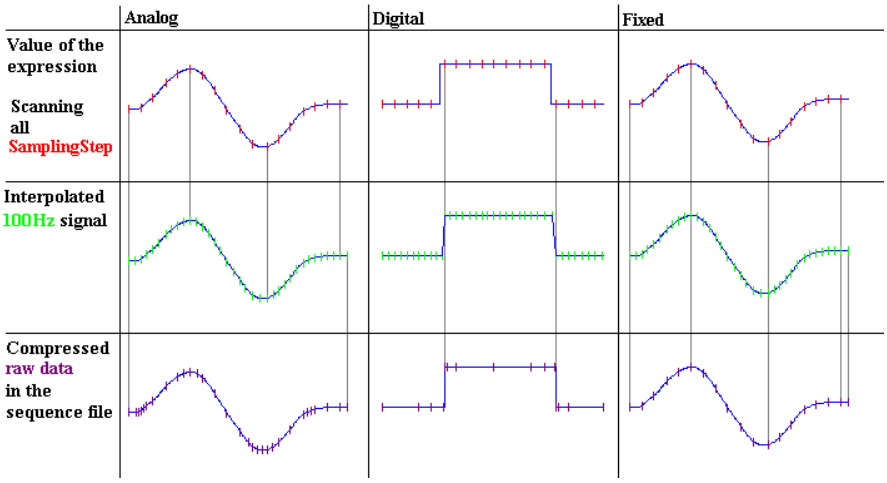
Installing the Virtual Channel Driver: Installation

Installing the Virtual Channel Driver: Configuration

Installing the Virtual Channel Driver: Channel Types

Schematic of the Channel Types

For a better understanding and to avoid artifacts please find below the schematic representation of different signal conversions:



Also, see:

- **Installing the Virtual Channel Driver: Installation**
- **Installing the Virtual Channel Driver: Configuration**
- **Installing the Virtual Channel Driver: Channel Configuration**

Installing and Controlling Third-Party Instruments

In addition to the Dionex ➢*Device Drivers*, the Dionex Chromatography Management System offers numerous drivers for controlling third-party instruments. These instruments are not part of the Dionex product range. Support is available for instruments from the following manufacturers:

ABI (see APPLIED BIOSYSTEMS)

AGILENT (formerly HP)

AMERSHAM PHARMACIA BIOTECH (see PHARMACIA)

ANTEC

APPLIED BIOSYSTEMS

BERTHOLD

BIO-RAD

CTC ANALYTICS

Dostmann

ESA

FINNIGAN

FISONS

GILSON

HEWLETT PACKARD (see Agilent)

ISCO

JASCO

KNAUER

KONTRON

KRATOS

LKB (see PHARMACIA)

MERCK HITACHI

NELSON Interfaces

PHARMACIA

RAININ/VARIAN (Pumps)

SOMA

THERMOQUEST

TSP

VARIAN (GC)

In addition, a **Generic Device Driver** is available which assists you in developing your own device driver.

Note: As programming device drivers for third-party instruments requires a considerable effort and as not all instruments are designed for direct control, support may be limited to certain functions.

For information on cables, pin assignments, and Dionex part numbers (if available), see **Cables and Pin Assignments** in the appendix of these Installation Instructions.

AGILENT (formerly HP)

The Dionex Chromatography Management System supports controlling the following Agilent (formerly HP) instruments:

- HPLC Systems **HP1050** and **HP1100** (see as well **Hints on HP1100**),
- Gas Chromatographs **HP5890** and **HP6890** as well as
- GC Autosampler **HP7673** and **Autosampler for HP6890 + Controller Box HP G1512**.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

AGILENT (formerly HP): HP1050 - Overview

Device Type:	HPLC System
Device Drivers:	HP79852 Gradient Pump: **HP1050 Gradient Pump** (supports three eluents and two relays) (tested) for firmware version 3.2) HP79855 Autosampler: **HP1050 Autosampler** (supports two relays) (tested for firmware version 4.2)
Supported Hardware Options:	HP79852 Gradient Pump HP79855 ➢*Autosampler*

What is required?

License:	Extended Device Control
Connection:	Null modem cable (Dionex part no.: 8914.0103A (25-pin to 9-pin) or 8914.0129 (9-pin to 9-pin), for details see **Null Modem Cable**) in the appendix of these Installation Instructions.
Control Panel:	HP1050S.pan

Further Information

For information on how to install the HP1050 HPLC system, see **Agilent (formerly HP): HP1050 - Installation**.

For an overview on the different HP instruments for which Dionex device drivers are available, see **Agilent (formerly HP)**.

AGILENT (formerly HP): HP1050 - Installation

Hardware Installation

Device Settings

Having switched on the instrument and upon completion of the initialization, perform the following steps according to the Agilent Operating Instructions to enter the device settings:

- Press the <CTRL> key: **Date & Time** appears.
- Press the <Next> key: **Configuration** appears.
- Press the <Enter> key.
- Press the <Next> key until **Communication** appears.
- Press the <Enter> key: **Interface** appears.
- Press the <Right> key.
- Press the <Next> key until **Serial** appears.
- Press the <Enter> key.
- Press the <Next> key until **Serial Mode** appears.
- Press the <Right> key.
- Press the <Next> key until **A** appears. (This sets the communication parameters as follows: 7 Data Bits, Even Parity, and 2 Stop Bits).
- Press the <Enter> key.
- After the <Next> key, **Baudrate: 9600** appears.
- Press the <Next> key and select **XON/XOFF: Off** (disabled).

To be able to execute flow ramps with the 1050 gradient pump, ensure that the **Remote Mode** is set to **Local**:

- Press the <CTRL> key: **Date & Time** appears.
- Press the <Next> key: **Configuration** appears.

Device Settings (Cont'd)

- Press the <Enter> key.
- Press the <Next> key until **Remote** appears.
- Press the <Right> key.
- Press the <Next> key until **Local** appears.
- Press the <Enter> key.

Restrictions:

To ensure smooth handling of sample injections, a minimum time of 2 minutes is required between two injections. This is checked with the ReadyCheck of each program. If the time remains under 2 minutes, an error message will be displayed.

Software Installation

Install the **HP 1050 HPLC System** ➢*Device Driver* in the  **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **HP1050 Gradient Pump** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port.

   On the *Solvents* tab, specify the number and names of the eluents that are delivered by the pump.

   On the *Relays* tab, check a box to enable or disable the corresponding relay.

   You do not need to change the presetting on the *Error Levels* tab.

5. Add the **HP1050** ➢*Autosampler* under the same timebase.
6. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port.

   On the *Rack* tab, check the rack used.

   On the *Relays* tab, check a box to enable or disable the corresponding relay.

   You do not need to change the presetting on the ➢*Error Levels* tab.
7. To control the HP1050 HPLC system connect the **HP1050S** control panel in the client of your Dionex Chromatography Management System to the corresponding timebase.

Application

Nothing particular known.

Troubleshooting

Nothing particular known.

Further Information

For an overview on the HP1050 HPLC system, see **Agilent (formerly HP): HP1050 - Overview**.

Note: The Dionex device drivers for HP1050 have been tested successfully with the following firmware versions:
HP1050 GP rev 3.2 and HP1050 S rev 4.2.
Should you have problems with firmware versions lower than the ones indicated, a firmware update might help.

For an overview on the different HP instruments for which Dionex device drivers are available, see **Agilent (formerly HP)**.

AGILENT (formerly HP): HP1100 - Overview

Device Type:	HPLC system
Device Driver:	**HP 1100 HPLC System**
Supported Hardware Options:	• HP1100 LC Diode Array Detector (tested for firmware version A.03.61) • Variable Wavelength Detector (VWD - firmware version A.03.80) • Pump: High-pressure gradient pump, optionally with solvent selection valves (Solvent Selection Valves, FW: A.03.60), Low-pressure gradient pump (A.01.06) or Isocratic pump • Degasser • Sample thermostat (A.03.61) • Injection unit (A.03.61) • Column compartment with column thermostat (optionally) + column switching valve (A.03.60).

What is required?

License:	Extended Device Control PDA License (for HP1100 LC Diode Array Detector)
Connection:	IEEE cable CAN cable for each module (The cables are available via Agilent only.)
Hardware Prerequisites:	IEEE board in the server PC of the Dionex Chromatography Management System (The board is available via Agilent or NI only.)
Control Panel:	HP1100.pan

Further Information

For information on how to install the HP1100 HPLC system, see **Agilent (formerly HP): HP1100 - Installation**.

For an overview on the different HP instruments for which Dionex device drivers are available, see **Agilent (formerly HP)**.

AGILENT (formerly HP): HP1100 - Installation

Hardware Installation

Device Connection: The device driver communication with the HPLC system is via IEEE. Therefore, an IEEE board must be installed in the server PC of the Dionex Chromatography Management System. The PC is connected to the HPLC system via an IEEE cable. If the system includes a photodiode array detector, we recommend connecting the PDA directly to the PC via the IEEE cable. All other modules are then connected to the PDA via CAN cables.

Device Settings: In addition, a corresponding VISA library must be installed. The library is shipped as part of the IEEE board package and is available from manufacturer. After installation, run the I/O configuration application once to configure the library.

Communication with the HPLC System HP1100 is possible both, via Agilent IEEE boards or IEEE boards from National Instruments (NI). For information, see:

Agilent (formerly HP):

HP1100 - Installing and Configuring the HP IEEE Board and the VISA Library

HP1100 - Installing and Configuring the NI IEEE Board and the VISA Library

Restrictions: Not known.

Software Installation

Install the **HP 1100 HPLC System** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. First, turn on all HP1100 modules.
2. Start the server of the Dionex Chromatography Management System.
3. Start the **Server Configuration** of the Dionex Chromatography Management System.

4. Add the **HP1100 HPLC System** under the desired timebase (via the **Add Device** command of the context menu).
5. The following settings are required on the different tabs (the links are available in the Online Help only):

   You do not need to change the settings on the *General* tab.

   On the *Components* tab, select the installed devices as well as an HPIB address and press **Scan CAN**.

   On the *Options* tab, specify the options installed.

   On the *Solvents* tab, specify the number and names of the eluents that are delivered by the pump.

   On the *Rack and Syringe* tab, specify the used rack and syringe.

   You do not need to change channel assignment of the ➢*Signals* tab.

   You do not need to change the presetting on the ➢*Error Levels* tab.
6. Turn off the detector and turn it on again. Wait approx. 15 s until the firmware is active again.
7. In the Server Configuration, press **OK** in the **HP1100 HPLC System** dialog box. The server configures and automatically reconnects all HP1100 modules.
8. To control the HP1100 HPLC system connect the **HP1100** control panel in the client of your Dionex Chromatography Management System to the corresponding timebase.

Application

Hints for installing several HP1100 systems via one IEEE board

If you plan to connect more than one HP1100 system to the IEEE interface all individual modules must have **different HPIB addresses**, i.e., all addresses must be listed in the **Show Devices** dialog box. This is especially important with the modules of the different HP1100 systems that are connected via IEEE cables to the IEEE board.

If two HP1100 systems are connected to the IEEE board via their detectors, the detector of the first system might get e.g. the HPIB address 26 and the detector of the second system the HPIB address 27.

Troubleshooting

Nothing particular known.

Further Information

For an overview on the HP1100 HPLC system, see **Agilent (formerly HP): HP1100 - Overview**.

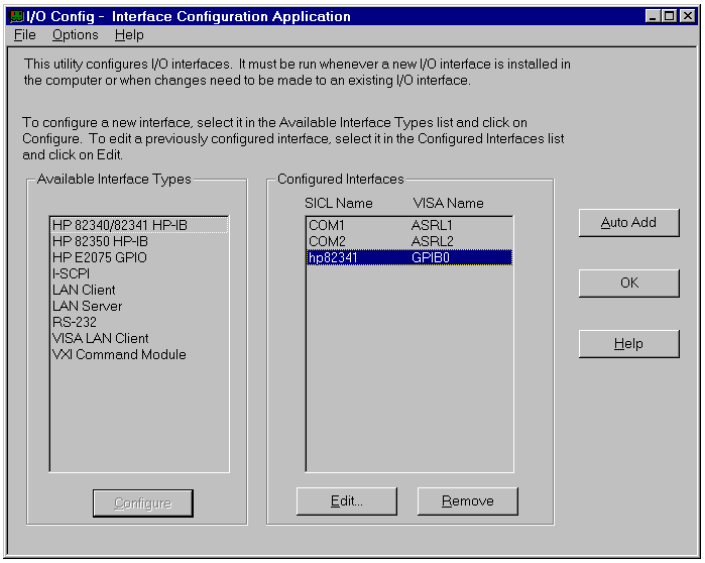
For more information on the HP1100 HPLC system, see **Hints on Programs for the HP1100 HPLC System**.

For an overview on the different HP instruments for which Dionex device drivers are available, see **Agilent (formerly HP)**.

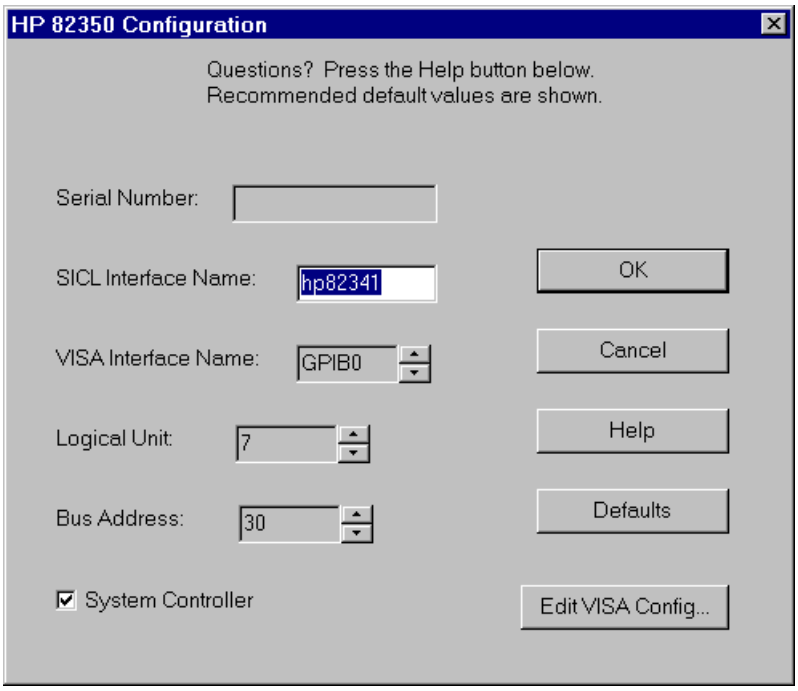
AGILENT (formerly HP): HP1100 - Installing and Configuring the HP IEEE Board and the VISA Library

HP-PCI (HP 82350A) and HP-ISA (HP 82341C)

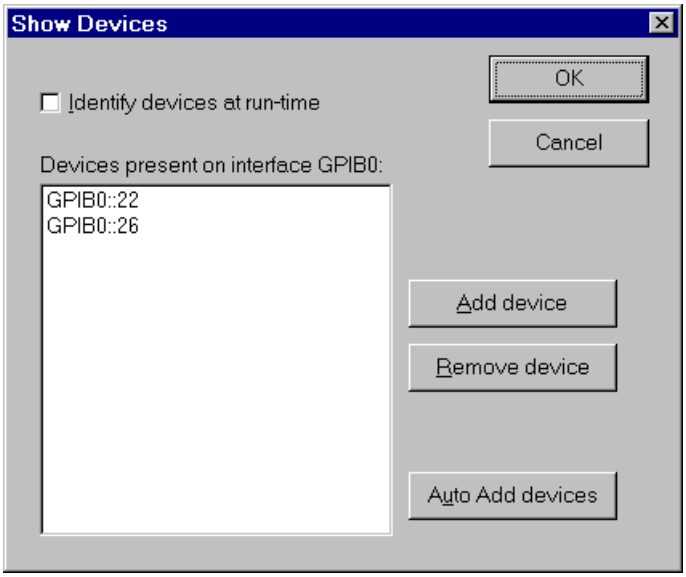
The I/O configuration attempts to find all installed interfaces suitable for VISA communication:



Highlight your IEEE board (hp8234x) in the list of configured interfaces and click **Edit**.

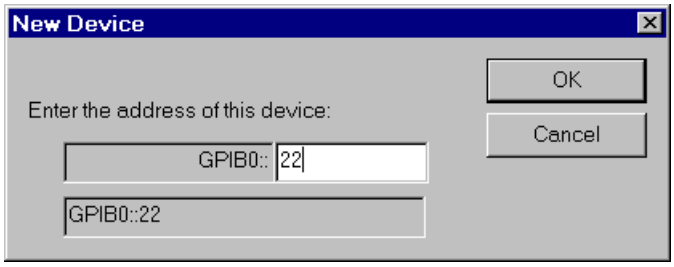


Ensure that the VISA interface name starts with GPIB, as shown. Also ensure that the bus address does not conflict with the HPIB address(es) you plan to use for your module(s) Generally, 30 is a suitable default value. Enable the **System Controller** checkbox and click **Edit VISA Config...**.



Ensure that the **Identify devices at run-time** checkbox is **disabled** and use the **Add Device** button to manually add the HPIB address you will be using for your module(s). For information on the default HPIB address of each module see the corresponding Agilent manuals.

Caution: If you plan to connect more than one HP1100 system to one IEEE interface, ensure that all modules use different HPIB addresses and that all addresses are listed here! This is especially important when using IEEE cables to connect the modules to the IEEE board.



Close all dialogs with **OK**. You may be asked to reboot your system.

We recommend using the following IEEE cards:

- HP 82350A (PCI-IEEE) Rev. B
- HP 82341C (ISA-IEEE)

together with the following VISA library:

- HP E2094H VISA 1.1 Rev H.01.02.

☞ ***Tip***: The HPIB board 82335 is not compatible with the Dionex Chromatography Management System.

For information on the respective HPLC system, see **Agilent (formerly HP) HP1100 - Overview**.

For information on how to install NI-IEEE boards and the VISA library, see **Agilent (formerly HP): Agilent (formerly HP): HP1100 - Installing and Configuring the NI-IEEE Board and the VISA Library**.

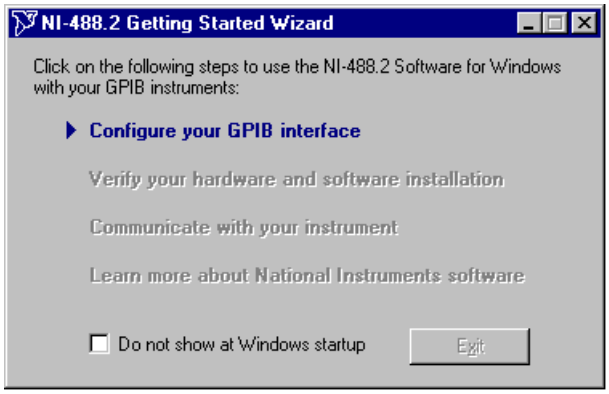
AGILENT (formerly HP): HP1100 - Installing and Configuring the NI IEEE Board and the VISA Library

NI-PCI (GPIB and GPIB+)

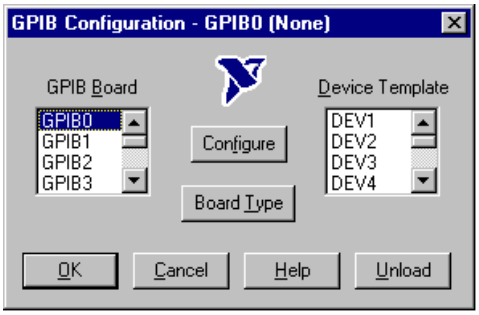
Instead of the Agilent IEEE boards IEEE boards from National Instruments (NI) can be installed:

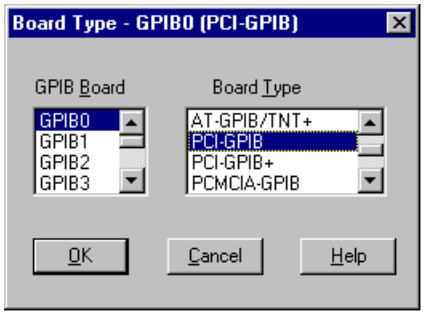
Insert the supplied CD. The setup program (CD:\AutoRun.exe) starts automatically. Select **Install NI-488.2 Software for Windows** and follow the instructions of the installation wizard. You can manage without the **Development Files and Samples** component. If the installation wizard prompts you, uninstall any existing installation first.

Having installed the board in the PC, another wizard guides you through the configuration steps:

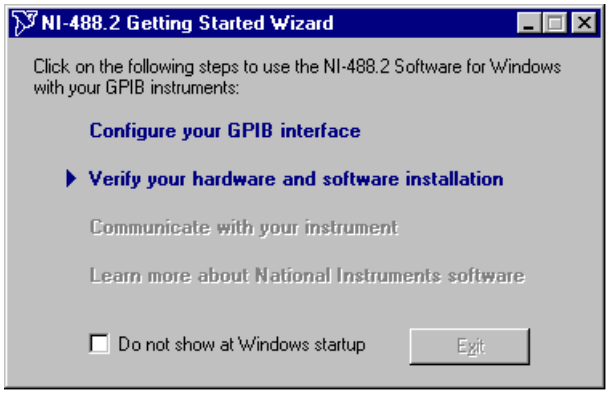


Configure the GPIB0 board according to the installed board type:

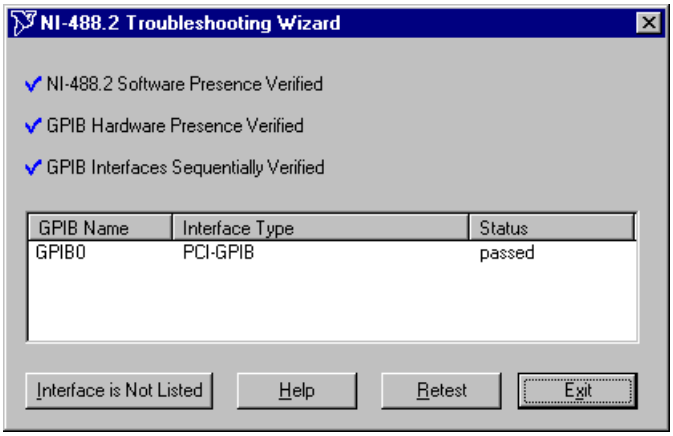




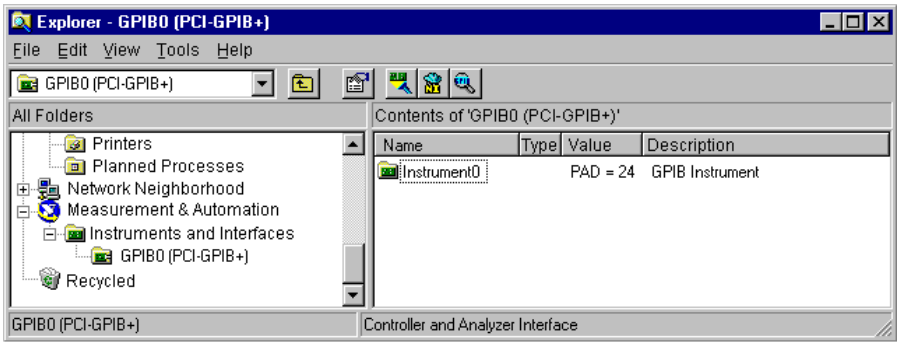
No additional settings are required. The second step checks the installation:



After the successful test



you can exit the Getting Started Wizard. Right click **Measurement & Automation\Instruments and Interfaces** to open the context menu and select **Scan for Instruments**. Then, the HP1100 modules that are connected to the IEEE bus must be listed:



For information on the respective HPLC system, see **Agilent (formerly HP): HP1100 - Overview**.

For information on how to install the HP IEEE boards and the VISA Library, see **Agilent (formerly HP): Agilent (formerly HP): HP1100 - Installing and Configuring the HP IEEE board and the VISA library**.

AGILENT (formerly HP): Hints on Programs for the HP1100 HPLC System

Hints on ➢*Program* development for the HP1100 HPLC system

- **Flow ramps** (commands: ⇒*Flow*, ⇒*%A, %B, %C, %D*) cannot be executed manually at negative times (t < 0) or in programs without an **Inject** command. (The HP1100 pumps do not support this.)
- The ⇒*Inject* command and all **sample preparation** commands are only accepted at the time t = 0. The HP1100 ➢*Autosampler* executes these commands as a block during the transition from Prerun to Run following a possibly specified **UV.Autozero** command.
- Interpretation of the **Inject** command **with explicit sample preparation**: If sample preparation commands are specified the position of the required inject command among these commands is irrelevant. The actual inject occurs either explicitly via the **Valve ValvePosition=MainpassOnStart** command or automatically at the end of the sample preparation if the command is not given.

- Changes of the **parameter of the 3D-field** may result in an automatic autozero of the PDA. During the execution of the autozero (see Property UV.NotReadyCauses(Prepare)) no further command must be given that would result in another autozero. If necessary, this can be achieved via the command **Wait UV.Ready**. During the execution of the autozero no Run must be started. Therefore, the Program Wizard adds a Wait UV.Ready before the Inject command.

Hints on manual program creation

Programs for the HP1100 that were developed manually should include a ⇒*Wait* command before the **Inject** command for each module:

```
0.000  UV.Autozero
       Wait  UV.Ready and ColumnComp.Ready and
       Sampler.Ready and Pump.Ready
   Inject
   3DFIELD.AcqOn
   UV_VIS_1.AcqOn
   UV_VIS_2.AcqOn
   UV_VIS_3.AcqOn
   UV_VIS_4.AcqOn
   UV_VIS_5.AcqOn
```

(These commands are automatically inserted if the Program Wizard is used).

Note: Generally, a time should be given at the beginning of a program (pump and detector presetting, e.g. at the time "-1.000") thus defining a time for each command.

For further information on how to install the HP1100 HPLC system, see **Agilent (formerly HP): HP1100 - Installation**.

AGILENT (formerly HP): HP5890 - Overview

Device Type: Gas chromatograph

Device Driver: **HP 5890 Gas Chromatograph**

Supported Hardware Options:

- Up to two injectors (optionally with oven)
- Up to two detectors (optionally with oven):
  Flame Ionization Detector (FID)
  Thermal Conductivity Detector (TCD)
  Nitrogen Phosphorus Detector (NPD)
  Flame Photometric Detector" (FPD)
  Electron Capture Detector (ECD)
- Oven (column thermostat)
- Auxiliary Heater (additional oven)
- Electronic Pressure Programming
- **Purge A** and **Purge B** valves
- 4 valves of the HP5890 series II

What is required?

License: Device Control

Connection: Special RS232 cable (also, see **HP5890: RS232 Cable** in the appendix of these Installation Instructions)

(The cable is not available from Dionex; it has be ordered from Agilent and **modified**!)

Hardware Prerequisites: Data acquisition requires an A/D converter, e.g. a ➢*UCI-100 Interface*, a Dionex UI20 (Dionex part no. 46017), or any other A/D converter that is supported by the Dionex Chromatography Management System, e.g. PE Nelson Boxes including the corresponding signal cables.

Interface Board:

Series I (serial numbers below 2443A-003099):
Interface board - Agilent part no. 19254A-001

Hardware Prerequisites: (Cont'd)

Series II (serial numbers above 2443A-003099): Interface board - Agilent part no. 19254A or 19242-60030A

Caution: Do not use the combined HP-IB/RS232 Interface Boards (Agilent part no. 19257), which are also available from Agilent.

Usually, the interface board is not part of the default GC equipment. It is installed instead of the INET port. Installation, however, is possible in instruments only that have one of the following EPROM versions:

HP5890 GC Series I: 05890-80150 or higher

HP5890 GC Series II: 05890-80300 or 80320

Serial Interface Board

Serial interface board with 4 COM ports
Dionex part no. 5906.2094 or

Serial interface board with 8 COM ports
Dionex part no. 5906.2095 or

Serial interface board with 8 COM ports
Dionex part no. 5906.2096

***Control Panel*s:**

HP5890.pan or
HP5890 one Detector.pan

Further Information

For information on how to install the HP5890 GC, see **Agilent (formerly HP): HP5890 - Installation**.

For an overview on the different HP instruments for which Dionex device drivers are available, see **Agilent (formerly HP)**.

AGILENT (formerly HP): HP5890 - Installation

Hardware Installation

RS232 Board Installation:

First, switch off the GC and disconnect the unit from the mains. Then, remove the right side control panel on the right of the GC. You can now access the GC motherboard.

Draw the INET board (if there is one) out of the slot and replace it by the appropriate interface board. A symmetrical connector is used for the serial cable. The connector is located in the housing recess on the top right below the cover (where the INET port was previously located). As the connector is symmetrical, the socket of the connecting cable can be placed either way. The relevant pins on the 25-pin MinD connector will always be correctly connected.

- Connect the analog cable (Agilent part no. 05890-60780) to the selected channel of the UCI-100 (e.g. Signal 1 = Detector 1; Signal 2 = Detector 2).

☞ ***Tip***: A separate cable is required for each detector!

Device Connection:

Connect the RS232 cable (12-pin connector) to the HP RS232 board.

Then connect the 25-pin female connector to the serial COM port cable of the PC.

Device Settings:

After closing and switching on the instrument, the baud rate is set to 9600 baud on the instrument. To do this, press **CLEAR** on the GC keyboard, and then press the "." key. The display will show **CALIB AND TEST [0-9]**. Press **3** and **Enter**. The display should show **CONFIGURE NETWORK**. Enter **1** and press **ENTER**. This sets the baud rate to 9600 baud. The setting becomes effective after resetting the instrument ("**CLEAR**","." "**5**," "**ENTER**").

Device Settings: (Cont'd) When using the HP7673 autosampler, the two instruments are usually connected via an additional cable. Remove this cable at both ends.

It is now possible to use the new Agilent autosampler (of the HP6890 system). For details, see **Autosampler Series 6890**.

Restrictions: Not known.

Software Installation

Settings required under Windows 98 (not NT/2000!)

The parameters of the serial port need to be changed. The receive buffer must be set to **Low**. Proceed as follows:

Open the **Control Panel** via **Start** and **Settings**. Select **System** and the **Device Manager** dialog tab. Open the **Properties** of the respective COM port. On the **Port Settings** dialog tab, click **Advanced** and set the receive buffer as low as possible.

Server Configuration

For information on how to install the HP5890 GC in the Server Configuration, see **HP5890 - Server Configuration**.

Application

Entering a Temperature Gradient

Entering a temperature gradient is either directly (via the **Flow** command from the **Control** menu; GC-tab) or via a PGM file.

Under the Dionex Chromatography Management System, a temperature profile is possible with a maximum of three ascents or descents (the HP5890 GC cannot store more steps!). The maximum temperature change (ascent) is 70°C per minute.

When entering a temperature gradient in the ➢*Program*, the so-called "base point philosophy" is used (similar to entering a flow or percent gradient in HPLC). Each **Temperature** command serves as a base point for the gradient program. Understandably, no gradient is executed before the Inject command. Temperature gradients can only begin after the Inject command. If the program does not contain an Inject command, this does not apply.

Temperature Settings

Temperature control of the injector, oven, and detector can be activated and deactivated via the following commands:

```
0.00      InjectorA.TempCtrl = On     or = Off
0.00      InjectorB.TempCtrl = On     or = Off
0.00      GC.TempCtrl = On            or = Off
0.00      DetectorA.TempCtrl = On     or = Off
0.00      DetectorB.TempCtrl = On     or = Off
```

To set the temperature of a single module e.g. to 80°C, the following command must be entered:

```
0.00      InjectorA.Temperature = 80
0.00      InjectorB.Temperature = 80
0.00      GC.Temperature = 80
0.00      DetectorA.Temperature = 80
0.00      DetectorB.Temperature = 80
```

The temperature of the injector system and the detector should always be approx. 15 - 20°C above the current oven temperature. Reaching the nominal temperature on the instrument can take some time. Please note that the oven heats faster than the injector and the detector system. As soon as the temperature is reached, the GC sends a **Ready** signal. Only after this, injection is possible via the autosampler.

Example:

The following program waits until the nominal temperature of 150°C is reached, before the ⇒*Inject* command is executed:

```
0.000   GC.Temperature = 150
  Wait  GC.Ready
  Inject
......  ..............
```

Caution: After receiving the nominal temperature value from the Dionex Chromatography Management System, the instrument implements the desired value as fast as possible. If the value is "almost" reached, the **Equilibration Time** passes until the instrument sends the confirmation message to the Dionex Chromatography Management System. The duration of this time interval can be set via the **Equilibration Time** parameter in the Dionex Chromatography Management System.

Troubleshooting

Should you have special questions, please contact the Dionex Service.

Further Information

For an overview on the HP5890 GC, see **Agilent (formerly HP): HP5890 - Overview**.

For information on how to install the HP5890 without controlled autosampler, see **Agilent (formerly HP): HP5890 - without Autosampler**.

For an overview on the different HP instruments for which Dionex device drivers are available, see **Agilent (formerly HP)**.

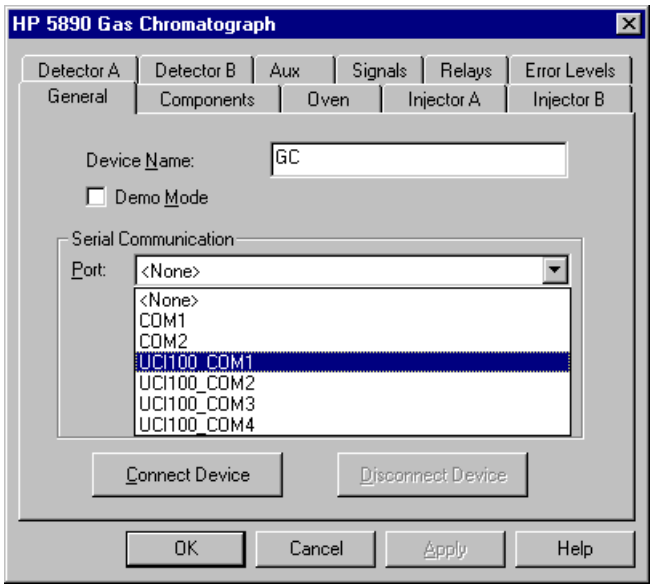
AGILENT (formerly HP): HP5890 - Server Configuration

Server Configuration Settings

Install the **HP 5890 Gas Chromatograph** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **HP 5890 Gas Chromatograph** under the desired timebase (via the Add Device command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

You do not need to change settings on the *General* tab.



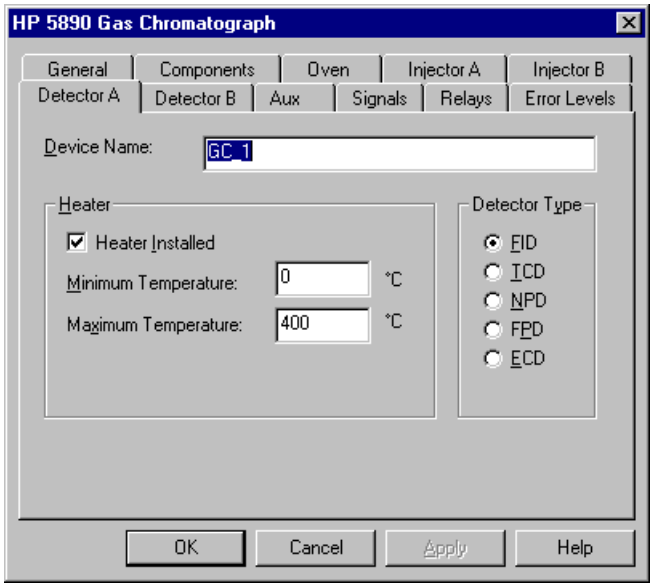
On the *Components* tab, select the installed devices.

On the *Oven* tab, set the limits for the controllable temperature range.

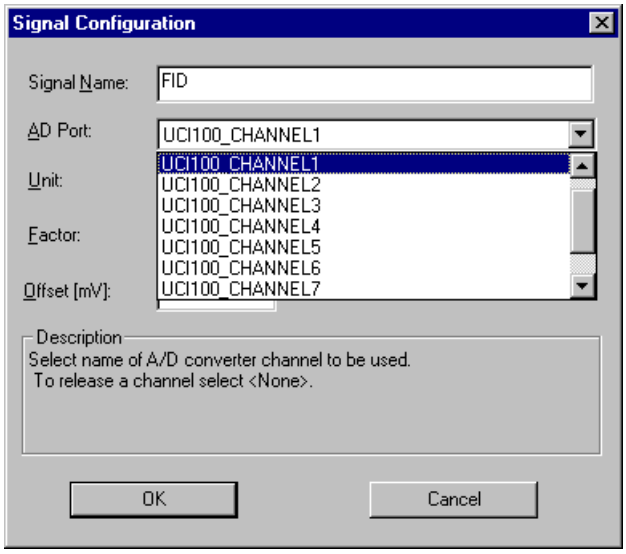
On the *Injector* tab, you can set up the temperature control for the injector oven.

On the *Detector* tab, specify the installed detector and its temperature control.

The *Aux* tab allows you to set up the temperature control for the **Auxiliary Device**.

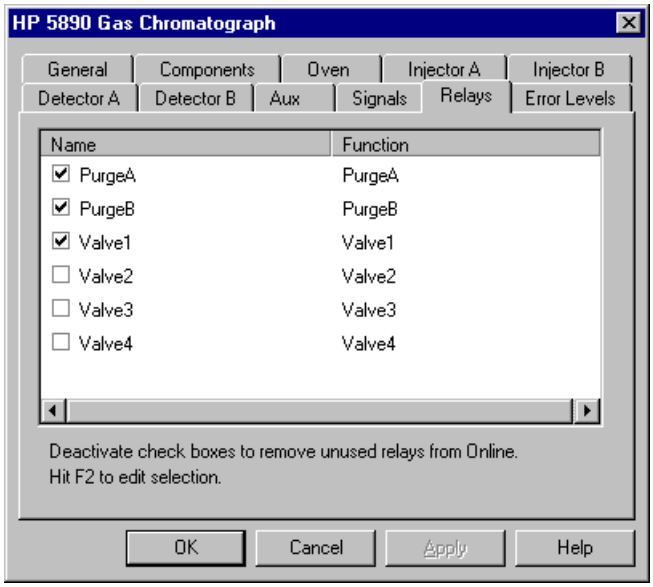


Open the **Signal Configuration** dialog box from the *Signals* tab by double-clicking the respective channel.



Assign a channel to the signal and name the signal in the **Signal Name** field according to the selected detector type.

Remove all unavailable relays on the ➢*Relays* tab:



You do not need to change the presetting on the ➢*Error Levels* tab.

5. To control the HP5890 GC connect the **HP5890** control panel or (in case of just one detector) the **HP5890 one Detector** control panel in the client of your Dionex Chromatography Management System to the corresponding timebase.

Further Information

For an overview on the HP5890 Gas Chromatograph, see **Agilent (formerly HP): HP5890 - Overview**.

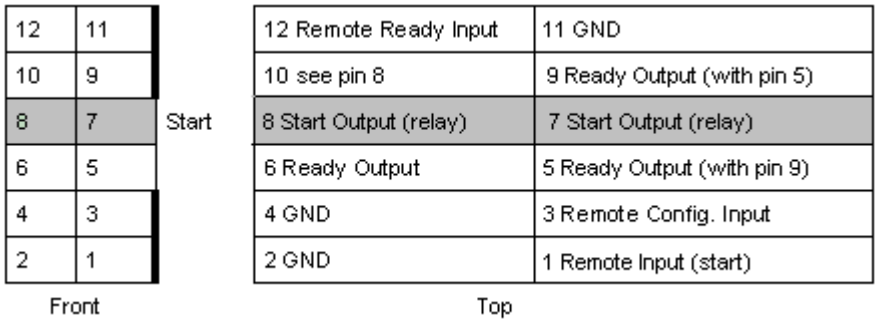
For information on how to install the HP5890 Gas Chromatograph, see **Agilent (formerly HP): HP5890 - Installation**.

AGILENT (formerly HP): HP5890 - without Autosampler

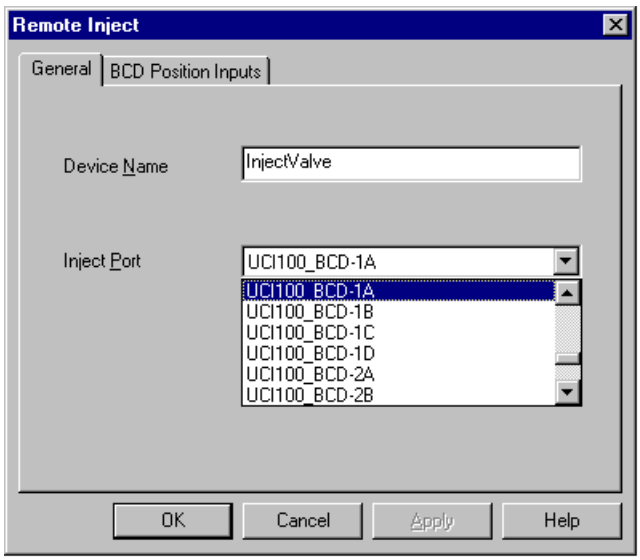
If there is no controlled autosampler available, the Inject Response has to be read from a remote input or a "remote start" of the A/D converter into the Dionex Chromatography Management System to start the sample.

No autosampler installed

In order to be able to synchronize the Inject Response with the program start at the GC and the data acquisition at the Dionex Chromatography Management System, use the remote start cable of the HP5890 (Agilent part no. 05890-061080).



- To start data acquisition at an Inject Response, connect pins 7 and 8 to the ➢*Remote Input* of the Dionex Chromatography Management System. (This relay is potential-free. Therefore, the polarity is not relevant if there is only one remote input of the Dionex Chromatography Management System connected.
- Install the ➢*Remote Inject* driver in the **Server Configuration**.
- Assign a remote input to the inject port of the Remote Inject:



- Connect pins 7 and 8 of the transmission cable with the cables of the digital input.
- The Dionex Chromatography Management System recognizes in the **Inject** command line of a program file whether the state of the **Remote Inject** changes and starts data acquisition as soon as the **Run** button is pressed on the GC.
- Further functions of the transmission cable can be connected, if requested.

Non-controlled autosampler installed

With non-controlled autosamplers, such as Headspace Injectors, connect the **Inject Marker** output of the autosampler to the remote input of the Dionex Chromatography Management System at **Remote Inject** instead of the remote start cable (polarity!).

The remote start cable of the HP5890 GC is not required!

For information on how to install the HP5890 gas chromatograph, see **Agilent (formerly HP): HP5890**.

AGILENT (formerly HP): CIS3

When operated under the Dionex Chromatography Management System the CIS3 Injection System has to be controlled via relays and inputs, as there is not separate driver available.

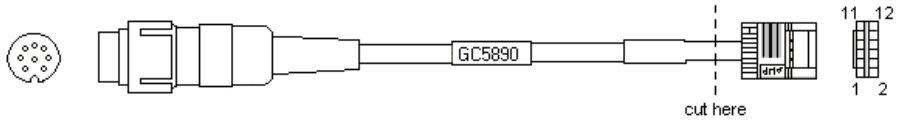
Hardware

To control the CIS3, one relay and one remote input are required. These are made available via

- A 4 channel relay board (Dionex part no. 5919.000) or
- A 16 channel relay board (Dionex part no. 5919.010) and
- A remote input of the Dionex A/D board

Wiring

Connector 1 (CIS)	Signal Name	Color	Connector 2 HP5890 (used by CM Relay & Inputs)	Signal Name	Relay or inputs used by CM
1	Start Input	Yellow	8 (removed)	Start Output	Relay (CIS_Start)
2					Not used
3	Ready Output 0	Brown	12 (removed)	GND	Input (CIS_Ready)
4	Ready Input	Gray	6 (removed)	Ready Output	Not used
5			2, 5, 7 connected (removed)		Not used
6					Not used
7	GND	Green	4 (removed)	GND	Relay (CIS_Start)
8	Ready Output 1	Pink	11 (removed)	GND	Input (CIS_Ready)



- Cut the 12-pin connector at the line (see figure) to connect the relays and inputs.

- Connect the relay (CIS_Start) with CIS cable pins 1 (yellow) and 7 (green). The polarity is not relevant.
- Connect the relay (CIS_Ready) with CIS cable pins 2 (brown) and 8 (pink). The polarity is not relevant.
- Affix the cable with shrinking tube or something similar.

Settings in the Dionex Chromatography Management System

- Install relay (CIS_Start) in the **Server Configuration**; **Function:** The relay has two functions for the CIS3: First, it loads the internal CIS3 program into its memory. Second, it starts the CIS3 program.
- Install Digital Input (CIS_Ready) in the Server Configuration; **Function**: Setting the **Wait for Ready** signal for the Dionex Chromatography Management System to pause the HP7673 sampler until the initial condition of the CIS3 is reached.
- In addition, add the corresponding commands to your ➢*Program*.

Program

The **Wait CIS_Ready** and **CIS_Start** settings must be used at the beginning of the program.

```
-0.100   Wait CIS_Ready = 0
;waits until the CIS cooled down to the initial settings
-0.050   CIS_Start.On    Duration = 1.000
;starts the CIS cycle

0.000 Inject

;The CIS_Start command must be given in the PGM file in the line after
the Inject command:
   CIS_Start.On   Duration = 1.000
;starts the CIS temperature program

   FID.AcqOn
;depends on the detector used (in this case: FID)

0.500 FID.AcqOff
;depends on the detector used (in this case: FID)
   end
```

Further Information

For an overview on the HP5890 Gas Chromatograph, see **Agilent (formerly HP): HP5890 - Overview**.

For information on how to install the HP5890 Gas Chromatograph, see **Agilent (formerly HP): HP5890 - Installation**.

AGILENT (formerly HP): HP6890 - Overview

Device Type: Gas chromatograph

Device Driver: **HP 6890 Gas Chromatograph**

Supported Hardware Options:

- Up to 2 **Inlets**
  Options:
  - Purged Packed EPC
  - Cool On-Column EPC
  - Split/Splitless EPC
  - Purged Packed
  - Cool On-Column
  - Split/Splitless
  - ACI
  - manual ACI
  - PTV
  - Gerstel PTV
  - <other PTV>
  - PCM
  - Gerstel CIS3
  - <JIB>
  - Volatiles
  - Unknown/Other
- **Column Oven**
- **Sampler** optionally with
  - up to 2 injectors (with 5 µl, 10 µl, 5 nl, or 10 nl)
  - Tray
  - Bar Code Reader
- Up to 2 **Detectors** (optionally with oven):
  Flame Ionization Detector (FID)
  Thermal Conductivity Detector (TCD)
  Electron Capture Detector (ECD)
  Nitrogen Phosphorus Detector (NPD)
  Flame Photometric Detector (FPD)
  micro Electron Capture Detector (µ-ECD)
- 8 valves

What is required?

License: Device Control

Connection: RS232 null modem cable (Dionex part no. **8914.0103A** also, see **Null Modem Cable (RS232)**

HP6890: A/D Cable

Hardware Prerequisites: Data acquisition requires an A/D converter, e.g. a ➢*UCI-100 Interface*, a Dionex UI20 (Dionex part no. 46017) or any other A/D converter which is supported by the Dionex Chromatography Management System, e.g. PE Nelson Boxes including the corresponding signal cables.

Interface Board:

Series I (serial numbers below 2443A-003099):
Interface board - Agilent part no. 19254A-001

Series II (serial numbers above 2443A-003099):
Interface board - Agilent part no. 19254A or 19242-60030A

Caution: Do not use the combined HP-IB/RS232 Interface Boards (Agilent part no. 19257), which are also available from Agilent!

Usually, the interface board is not part of the default GC equipment. It is installed instead of the INET port. Installation, however, is possible in instruments only that have one of the following EPROM versions:

HP5890 GC Series I: 05890-80150 or higher

HP5890 GC Series II: 05890-80300 or higher

Serial Interface Board

Serial interface board with 4 COM ports
Dionex part no. 5906.2094 or

Hardware Prerequisites: (Cont'd)	Serial interface board with 8 COM ports Dionex part no. 5906.2095 or Serial interface board with 16 COM ports Dionex part no. 5906.2096
Control Panels:	HP6890.pan or HP6890 Single Injector.pan

Further Information

For information on how to install the HP6890 GC, see **Agilent (formerly HP): HP6890 - Installation**.

For information on how to install the HP6890 GC with the HP1512 Controller Box, see **Agilent (formerly HP:) Autosampler for HP6890 + Controller-Box HP G1512**.

For an overview on the different HP instruments for which Dionex device drivers are available, see **Agilent (formerly HP)**.

AGILENT (formerly HP): HP6890 - Installation

Hardware Installation

Device Connection:	RS232 null modem cable (Dionex part no. **8914.0103A**; also, see **Null Modem Cable (RS232)** in the appendix of these Installation Instructions). The PC must be connected to the **Modem** port (RS232C) of the gas chromatograph (**Site Preparation and Installation Manual**, page 44, No. 4 in the illustration).
Device Settings:	(Also, see the **Site Preparation and Installation Manual** supplied with the GC.) 1. Press the [Options] key. 2. Use the arrow keys to select the line **Communication** (**<** on the right margin).

Device Settings: (Cont'd)

3. Press the [Enter] key.
4. The first five settings must correspond to the device driver settings (see the **General** tab of the instrument in the **Server Configuration** of the Dionex Chromatography Management System. **Caution**: The order of the settings is different here! Please note that **End of command** must be set to **LF**.

   The communication settings must be as follows:

Baud rate	9600
Handshake	XonXoff
Parity	None
Data bits	8
Stop bits	1
End of command	LF

   To change the settings, move the **<** selection to the line to edit, and then press **Mode/Type**. Now, move the **<** to the required value and press the [Enter] key.

Restrictions: Not known.

Software Installation

Install the **HP 6890 Gas Chromatograph** ➢*Device Driver* in the **Server Configuration** of the Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **HP 6890 Gas Chromatograph** under the desired timebase (via the Add Device command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only).

   On the *General* tab, select a free COM port.

On the *Options* tab, specify the limits for the controllable temperature range of the column oven. In addition, enable the EPC (Electronic Pneumatic Control) option if you are using an electronic pneumatic control unit.

The *Front/Back Inlet* tab allows you to set up the temperature control for the **Inlet**.

☞ ***Tip***: The Programmable Temperature Vaporizing Inlet (PTV) is available in various variants from Agilent (OEM version) or the manufacturer, Gerstel, (under the name of **Cooled Injection System CIS**). Ensure that the correct variant is selected during the installation.

The Volatile Interface is currently not supported.

On the ➢*Sampler* tab, indicate the installed autosampler components: Tray, Bar Code Reader, Front/Back Injector + syringe type.

On the ➢*Front/Back Detector* tab, specify the installed detector(s) and its/their temperature control.

Open the **Signal Configuration** dialog box from the ➢*Signals* tab by double-clicking the respective channel. Assign a channel to the signal and name the signal in the **Signal Name** field according to the selected detector type.

On the ➢*Relays* tab, remove all relays that are not used.

You do not need to change the presetting on the ➢*Error Levels* tab.

5. To control the HP6890 GC connect the **HP6890** control panel or (in case of just one injector) the **HP6890 Single Injector** control panel in the client of your Dionex Chromatography Management System to the corresponding timebase.

Application

Notes on the Device Driver:

General

Experienced HP6890 users should be able to control the instrument without any problems. In the Dionex Chromatography Management System, short descriptions of the GC commands are available in the corresponding Command dialog box or the Properties/Link box.

In the Dionex Chromatography Management System, pressure is always stated in bar. Selecting a different pressure unit is not supported. For further information, please contact the Dionex Service.

Column

It is possible to enter column dimensions and connections. However, entering the calibration is currently not possible. If column dimensions are not defined, certain commands cannot be executed (e.g.: Velocity, MakeupMode = Combined, etc.).

It is not recommended to enter the column dimensions and connections in a sample program. However, the parameters should be included in the Audit Trail via the Log command.

Valves

Special valve types (Multiposition, Gas Sampling) are currently not supported. For further information, please contact the Dionex Service.

Aux

Aux are currently not supported. For further information, please contact the Dionex Service.

Sampler

The extended capabilities of the HP7683 sampler (e.g. solvent prewashes) are now supported. These were not supported with the model 7673.

When connecting the instrument for the first time, some (or many) error messages may appear starting with **Error log at**. These are previous errors recorded by the sampler. You can simply ignore them. Future versions will show new errors only.

Barcode Reader: If **UseBCR= On**, the barcode of the sample is read during the Inject command and is logged in the Audit Trail.

Application

Entering a Temperature Gradient

Entering a temperature gradient is performed either directly (**Flow** command from the **Control** menu; GC-tab) or via a ➢*PGM File*.

For the HP6890, a temperature profile can be entered with a maximum of six ascents or descents (the HP6890 GC cannot store more steps!). The maximum temperature change (ascent) is up to 120°C per minute, depending on the oven type.

Gradients are entered in the Program Wizard or online in the typical format for GC applications (the starting and end temperatures are entered as well as the modification rate). In the program, however, the so-called "base point philosophy" is used (similar to entering a flow or percent gradient in HPLC). Each **temperature** command serves as base point of the gradient program. The Wizard automatically converts the entered rates into the base point representation.

However, no gradient is executed before the Inject command. Temperature gradients can only begin after the Inject command. If the program does not contain an Inject command, this does not apply.

Temperature Setting Commands

Temperature control of the oven, the two inlets and the two detectors can be activated and deactivated via the following commands:

```
0.000      FrontInlet.TempCtrl=On      Or = Off
0.000      BackInlet.TempCtrl=On       Or = Off
0.000      GC.TempCtrl=On              Or = Off
0.000      FrontDetector.TempCtrl=On   Or = Off
0.000      BackDetector.TempCtrl=On    Or = Off
```

To set the temperature of an individual module to 80°C, use the following command:

```
0.000      FrontInlet.Temperature = 80
0.000      BackInlet.Temperature = 80
0.000      GC.Temperature = 80
0.000      FrontDetector.Temperature = 80
0.000      BackDetector.Temperature = 80
```

Reaching the nominal temperature on the instrument can take some time. Please note that the oven heats faster than the injector and the detector system. As soon as the nominal temperature is reached, the GC sends a **Ready** signal. Only after this, injection is possible via the autosampler.

Example:

The following program waits until the nominal temperature 150°C is reached, before the Inject command is executed:

```
0.000   GC.Temperature = 150
  Wait  GC.Ready
  Inject
......  ..............
```

Caution: After receiving the nominal temperature value from the Dionex Chromatography Management System, the instrument implements the desired value as fast as possible. When the value is "almost" reached, the **Equilibration Time** passes until the instrument sends the confirmation message to the Dionex Chromatography Management System. The duration of this time interval can be set via the **Equilibration Time** parameter in the Dionex Chromatography Management System.

Troubleshooting

Should you have special questions, contact the Dionex Service.

Further Information

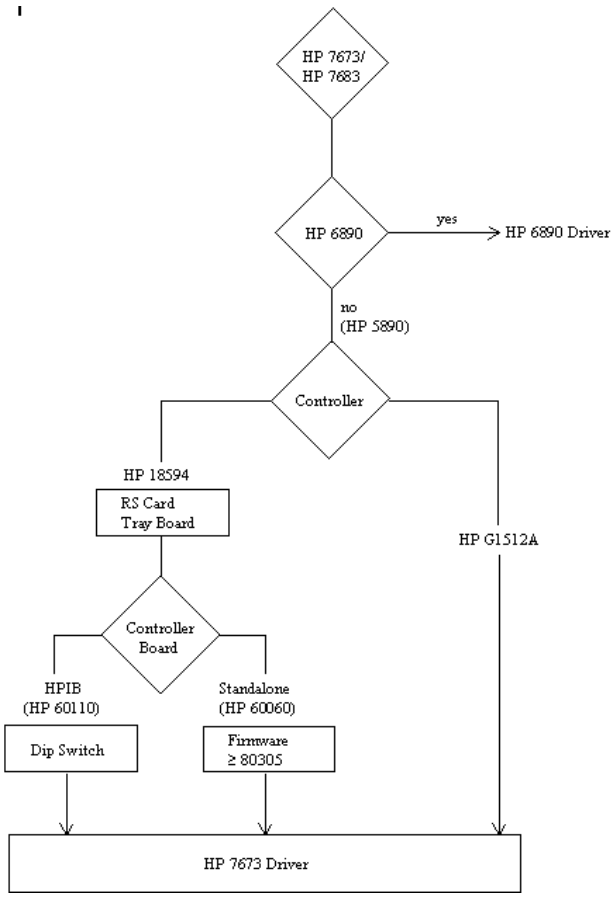
For an overview on the HP6890 GC, see **Agilent (formerly HP): HP6890 - Overview**.

For information on how to install the autosampler for the HP6890 GC with the HP1512 Controller Box, see **Agilent (formerly HP): Autosampler for the HP6890 + Controller-Box HP G1512**.

For an overview on the different HP devices for Dionex device drivers are available, see **Agilent (formerly HP)**.

AGILENT (formerly HP): GC-Autosampler - Flow Chart

The following chart describes the device drivers required for the respective applications:



For information on how to install the different autosamplers, see:

GC Autosampler **HP7673** and **Agilent (formerly HP): Autosampler for HP6890 + Controller Box HP G1512**

AGILENT (formerly HP): Autosampler for HP6890 + Controller Box HP G1512

Autosamplers of the GC Series HP 6890 (Controller Box HPG1512)

Instead of the Autosampler 7673 (for installation information on the HP7673 see **Agilent (formerly HP): HP7673**), which is no longer available since mid 1997, Agilent now supplies the autosampler of the HP6890 series and a corresponding controller box. The controller box (HPG1512) is capable of emulating the HP7673 controller box in **standalone operation**. The controller box of the system already contains all required plug-in cards, so that no conversion is possible. The DIP-switches on the rear panel of the box must be set as follows.

Left DIP-switch: set all switches to **0**, except the switch at the far right to **1**.

Right DIP-switch: set all switches to **0**.

After setting the switches, the controller box must be switched off and on again.

Connecting the Cables

- Use a serial standard interface cable (25-pin to 9-pin; Dionex part no. 8914.0103A) to connect the RS232 output of the controller board to the serial interface of the server PC.
- Connect the 9-pin end with the 9-pin to 25-pin extension cable (part no. 8914.0110).
- Finally, connect the 25-pin connector of the extension cable with the serial COM port cable of the PC.

The Controller Box of the HP6890 (HPG1512) behaves as the box of the HP7673. Nevertheless, the **HP 6890 Gas Chromatogram** ➢*Device Driver* can be used for controlling the autosampler. In the **Server Configuration** under **Sampler**, select the **Automatic Liquid Sampler Installed** option and select the specification according to your installation.

Caution: If you use an Agilent autosampler, the program files must be at least 2 min. long to allow the autosampler sufficient time until the next injection.

For a flow chart on the different HP autosamplers, see **Agilent (formerly HP): GC Autosamplers - Flow Chart**

For information on how to install the HP7673, see **Agilent (formerly HP): HP7673 - Overview**.

Further installation information is available for the following Agilent devices:

HPLC Systems **Agilent (formerly HP): HP1050** and **Agilent (formerly HP): HP1100 - Overview**

Gas Chromatographs **Agilent (formerly HP): HP5890** and **Agilent (formerly HP): HP6890 - Overview**.

AGILENT (formerly HP): HP7673

Controlling the HP7673 GC Autosampler requires the following hardware:

From Agilent:

- RS232-C-board for COMM Agilent part no.: 18594-60080
- Firmware version 80305 or higher

Tip: For the HP6890 Controller Box HPG1512, no RS232 board is required!

From Dionex:

RS232 cable (➢*Null Modem Cable*) DX part no.: 8914.0103A (25-pin - 9-pin, not 9-pin - 9-pin!)

Installation

The autosampler HP7673 corresponding to the Gas Chromatograph HP5890 consists of three parts: a controller (controller box and boards), a sample tray, and the injection unit with two injectors. As the injection unit has its own turret, the sample tray is not required. However, the Dionex Chromatography Management System currently supports this instrument only with the tray!

For operating the autosampler, the controller box is first fitted with the RS232-C board (Agilent part no.: 18594-60080). Connect the RS232 cable to the **COMM** position.

Insert the board in the **COMM** slot. Configure the board via the W1 baud rate jumper (9600 baud, 8 data bits, no parity, and 1 stop bit).

Then, the tray board (Agilent part no. 18594-60075) required for connecting the sample tray is inserted.

Finally, install a controller board (also, see the **Installing the Controller** chapter in the **HP7673 Automatic Sampler Operating Manual**). Choose either the HPIB board (18594-60110) or the standalone controller board (Agilent part no. 18594-60060).

- The HPIB-controller enables HPIB and RS232 communication. With the Dionex Chromatography Management System, only the RS232 communication is used. The communications parameters (8 data bits, no parity, 1 stop bit) must be set via the 5-fold DIP-switch.
- Set the required baud rate via the DIP-switches on the RS232 board:

DIP-switch	**1**	**2**	**3**	**4**	**5**
	1	0	1	0	0
Or	On	Off	On	Off	Off

- On the rear of the standalone controller, there is a (9-pin) SUB-D connector labeled Test. Ensure that the firmware is version 80305 or higher. The corresponding EPROM is shipped with the serial interface board (60080).

If you do not have the RS232-C Board or the Controller Board, you can order the missing board later. However, it may be preferable to purchase a new Controller Box Agilent G1512 (see below) instead.

Connecting the Cables

- Connect the injector and the controller box via the appropriate Agilent connecting cable.
- Connect the sample tray to the tray board.
- Use a serial standard interface cable (25-pin to 9-pin; Dionex part no. 8914.0103A) to connect the RS-232 output of the RS232 board to the serial interface of the server PC.
- Connect the 25-pin end to the RS232 output of the Controller Box.

- Connect the 9-pin end with the 9-pin to 25-pin extension cable (Dionex part no. 8914.0110).
- Finally, connect the 25-pin connector of the extension cable with the serial COM port cable of the PC.

Dionex Device Driver

Operating the autosampler requires the HP7673A.CDD device driver. As soon as this driver is located in the BIN directory, install the **HP 7673A GC Autosampler** device driver in the **Server Configuration** of the Dionex Chromatography Management System.

***Note**:* In contrast to controlling the autosampler HP7673 via the GynkoSoft data system, only a single device driver is required in the Dionex Chromatography Management System!

Please determine which controller board (standalone or HPIB) is used for controlling the autosampler HP7673. You can recognize the standalone board by the test connector and the HPIB board by the HPIB connector protected by a red cover when unused.

Also, define the injection system of the (front-/rear injector), the syringe size, and the injector inlet.

For information on how to install the HP7673 in the Server Configuration, see **HP7673 - Server Configuration.**

For a flow chart, regarding the different HP autosamplers, see **Agilent (formerly HP): GC Autosampler - Flow Chart.**

For information on how to install the Controller Box which is available since 1997 instead of the HP7673, see **Autosampler for HP6890 + Controller Box HP G1512A.**

Further installation information is available for the following Agilent devices:

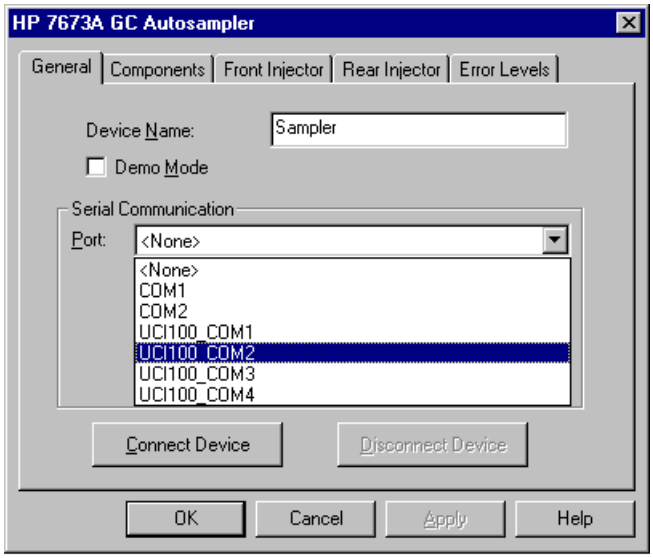
HPLC systems **Agilent (formerly HP): HP1050 - Overview** and **Agilent (formerly HP): HP1100 - Installation**.

Gas Chromatographs **Agilent (formerly HP): HP5890 - Overview** and **Agilent (formerly HP): HP6890 - Overview**.

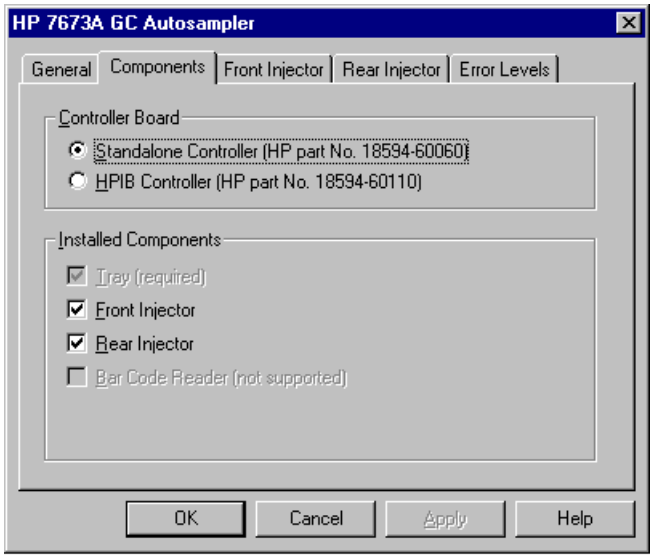
AGILENT (formerly HP): HP7673 - Server Configuration

Settings in the Server Configuration:

Select the HP Sampler 7673 and assign a free COM port on the **General** tab:



There are two versions of controller types available. For the HP7673 select the HPIB protocol if the operation of the autosampler is not possible with the standalone protocol. The HP6890 Controller Box must always be installed as standalone controller.



Finally, install all available components.

For information on how to install the HP7673 autosampler, see **Agilent (formerly HP): HP7673**

Further installation information is available for the following Agilent devices:

HPLC Systems **Agilent (formerly HP): HP1050 - Overview** and **Agilent (formerly HP): HP1100 - Overview**

Gas Chromatographs **Agilent (formerly HP): HP5890 - Overview** and **Agilent (formerly HP): HP6890 - Overview**.

ANTEC

If the electrochemical detector ANTEC **DECADE** is connected to the HPLC system via an RS232 interface, a 9-pin standard ➢*Null Modem Cable* and a mouse adapter (9-pin -> 25-pin), it can be operated directly from any the client of the Dionex Chromatography Management System.

***Note**:* Alternatively, a 9/25-pin cable (Dionex part no. 8914.0122 for a 25-pin port or Dionex part no. 8914.0138 for a 9-pin port) can be used for the connection with the following pin assignment:

Antec Decade		**PC**	
25-pin Sub-D Connector		25-pin Sub-D Connector	9-pin Sub-D Connector (UCI-100)
2	----------	3	2
3	----------	2	3
7	----------	7	5
4, 5, and 20 internally connected			

In addition to the correct installation and configuration of the detector via the **Server Configuration**, correct serial communication is only possible if the instrument is switched to remote operation. Perform the following steps:

- Switch the detector on and wait until the main screen is displayed. Detectors with the RS232 option (only these can be controlled by the Dionex Chromatography Management System), the instrument display shows on the lower right: RS232.
- Press the RS232 (F5) button on the instrument.

The detector is now in remote operation and can be controlled via the data system. All functions of the detector that are otherwise performed on the instrument or via the **Dialogue** software are now available under the Dionex Chromatography Management System. A distinction is made between the ➢*DC Mode*, the ➢*PULSE Mode*, and the ➢*SCAN Mode*.

- Open the **ANTEC.pan** control panel to operate the detector.
- Activate the switch **Connect** to start the detector.
- As soon as the remote operation is ensured, setting the parameters can be continued in the usual way.

- Details on the individual parameters can be accessed directly in the control panel via the F1 key. However, this requires basic knowledge in operating the detector. For further information, see the detector manual.

In contrast to the parameters, the measuring data is not communicated via the RS232 interface. For the data communication, the detector must be connected to the ➢*A/D Converter* via the outputs **Rec.** and/or **Int.**.

The integrator output (**Int.**) supplies an analog signal that is not manipulated and that accurately indicates the state of the working electrode. In contrast, the recorder output (**Rec.**) supplies a smoothed, electronically processed signal.

Please note that both outputs can be used in **DC mode**, but only the recorder output in **PULSE mode** and **SCAN mode**.

The Online Help illustrates the four **Server Configuration** pages on this detector type: *General*, *Signals*, *Relays*, and *Error Levels*.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

APPLIED BIOSYSTEMS

For controlling the **ABI 785A** UV detector (identical with Perkin Elmer 785A), the connecting cable (Dionex part. no. 8914.0119 for a 25-pin port or Dionex part no. 8914.0137 for a 9-pin port) must have the following pin assignment:

ABI 785A		**PC**	
Serial A			
9-pin Sub-D (male)		25-pin Sub-D (female)	9-pin Sub-D (female)
9	----------	2	3
5	----------	3	2
1	----------	7	5

The communications parameters must be set as follows: 9600 Baud, 8 Data bits, No Parity, 1 Stop bit, No Handshake.

Set the correct baud rate on the instrument itself. From the instrument's startup display, perform the following steps:

- Press **More** (F4 key).
- Press **Util** (F2).
- Press **More** (F4).
- Use the arrow keys to move the cursor to the BAUD parameter.
- Use the **Prev**. and **Next** keys to select the value 9600.
- Press **Done** (F4).
- Press **Exit** (F1).

This brings you back to the startup display.

As special parameters, the **Rise Time** as well as **Scan** and **SetRelays** (the latter are, however, not included in the ABI785A.PAN control panel) are available.

The Online Help illustrates the three **Server Configuration** pages on this detector type: *ABI_785A_UV-VIS_Detector*, *Generic*, and *Error Levels*.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

BERTHOLD

The Dionex Chromatography Management System is capable of controlling the BERTHOLD LB 507A and LB 509 Radioactivity Detectors. Select the **Berthold_LB_507_509** ➢*Device Driver* in the **Server Configuration**. Ensure that the LB507AB.GEN driver is available in the BIN directory and that the radioactivity detector is connected to the PC via a special cable (see below).

***Note**:* Before connecting the radioactivity detector to the Dionex Chromatography Management System, perform a reset at the device (see device manual).

Pin Assignment of the RS232 Connecting Cable

(Dionex part no. 8914.0114 for a 25-pin port or Dionex part no. 8914.0135 for a 9-pin port)

LB 507 A/LB 509		PC	
25-pin Sub-D Connector (female)		25-pin Sub-D Connector (female)	9-pin Sub-D Connector (female)
		1 = Shield	1 = Shield
2	----------	3	2
3	----------	2	3
5	----------	4	7
7	----------	7	5
6, 8, 20 internally connected		4, 5 internally connected	7, 8 internally connected

***Note**:* The model Berthold LB 508 has a completely different (binary) control protocol. Controlling this instrument is currently not possible via the Dionex Chromatography Management System.

Pin Assignment of the Rate-Meter Connector (Analog Output of the Detectors)

Pin	Direction	Function
1	Out	Analog1 lo
2	Out	Analog1 hi
3	Out	Analog2 lo
4	Out	Analog2 hi
5	Out	High lumin.
6	-	GND
7	-	-
8	-	-
9	Out	+15V

The Online Help illustrates the three **Server Configuration** pages on this detector type: *Berthold_LB_507_509*, *Generic*, and *Error Levels*.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

BIO-RAD

To control the BIO-RAD **AS 100** Autosampler, select the **BIO_RAD AS 100** *Device Driver* in the Server Configuration. Ensure that the **bras100.cdd** driver is available in the BIN directory.

Dionex Chromatography Management System - Options

Operating the Dionex Chromatography Management System requires the **Extended Device Control** Feature (**Options of the Dionex Chromatography Management System**). Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.

Connection

A standard ➢*Null Modem Cable* with all lines connected (the assignment of the Dionex null modem cable is slightly different!) as well as a gender changer from female to male and a 9-pin to 25-pin adapter are required for the AS 100 side.

AS 100		PC
25-pin Sub-D connector (male)		9-pin Sub-D connector (female)
1 = ground		
2 TXD	----------	RXD 2
3 RXD	----------	TXD 3
4 RTS	----------	RTS 8
5 CTS	----------	RTS 7
6 DSR		DTR 4
7 GND	----------	GND 5
20 DTR		DSR 6

Control via the Dionex Chromatography Management System

Controlling the AS 100 requires version 6.01 (or higher) of the Dionex Chromatography Management System. Before an injection is possible, the **Activity Code** string of the sampler must be "STOP". In addition, the **ReadForInject** property must be true (= 1). Otherwise, a **flush** command must be executed, i.e., a flush command is required between two injection commands!

Example for a typical AS 100 ➢*Program*

```
-0.1  Flow =   1.000
   Sampler.Temperature.Nominal = 5
   ; make sure that the sampler becomes ready for inject
   Sampler.Flush

 0.000   ; wait until sampler becomes ready for inject
   Wait  Sampler.ReadyForInject
   UV.Autozero
   Inject
   UV_VIS_1.AcqOn

10.000   UV_VIS_1.AcqOff

   End
```

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

CTC ANALYTICS

CTC ANALYTICS A200S (GC Autosampler; identical with Fisons A200S)

The design of the GC Autosampler A200S corresponds to the A200S from Fisons. Both instruments can be controlled via the Dionex Chromatography Management System. For this, select the **CTC_A200S_Sampler** ➢*Device Driver* in the **Server Configuration**. Ensure that the CTCA200S.GEN driver required for both instruments is available in the BIN directory and that the PC and the autosampler are connected via a serial connecting cable.

Please note, however, that instead of a so-called "null modem cable" a ➢*Modem Cable* (Dionex part no. 8914.0128 for a 25-pin port or Dionex part no. 8914.0144 for a 9-pin port) is used. Pins 2, 3, and GND are supported only. The sampler requires a 25-pin male connector on its side.

For controlling these two instruments, it is necessary to set the **Start Signal Source** parameter to **Remote** on the instrument. For details, see the Manual supplied with the instrument.

The Online Help describes the special page for this autosampler in the **Server Configuration** (*Sampler*).

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

DOSTMANN

Controlling the Dostmann **P550** Temperature Measuring Device is via the **Dostmann Thermometer P550** ➢*Device Driver*.

To connect the thermometer to the PC, connect the PC adapter cable (included in shipment) to the socket that branches off the power unit cable. Connect the PC adapter cable to a free serial port of your PC.

The thermometer digitally transmits the temperature data to the data system. To enable recording of data, a virtual channel must be installed. Install a ➢*Virtual Channel Driver* in the **Server Configuration**; also, see to **VCD: Installation**.

For further installation information, see the general operating instructions: **Connecting the Dionex Column Thermostat PQ Kit to CHROMELEON**.

ESA

ESA CouloChem II (Electrochemical Detector)

If the ESA **CouloChem II** electrochemical detector) is connected to the HPLC system via an RS232 interface, it can be operated directly from any ➢*Client* of the Dionex Chromatography Management System.

The instrument is connected via a serial RS232 cable (for the Dionex part nos., see ➢*Null Modem Cable*). The pin assignment must be as follows:

ESA CouloChem II		PC	
		COMx (25-pin)	COMx (9-pin)
2	----------	2	3
3	----------	3	2
5	----------	7	5
		Internal:	Internal:
		4 - 5	7 - 8

The interface parameters must be set as follows:

Baud rate:	4800
Data bits:	7
Stop bits:	1
Parity:	EVEN
Handshake:	NONE

In addition to the correct installation and configuration of the detector via the **Server Configuration** (**ESA CouloChem II ECD** ➢*Device Driver*), the instrument itself must be switched to remote operation. Perform the following steps:

- Switch on the detector. After the detector self-test is completed press the **MODE** key and then the arrow key ↑ until the text **SYSTEM MENUS** is shown on the display.
- Press **ENTER** until the text **ENTER REMOTE COMMUNICATIONS MODE** appears. Renewed pressing the **ENTER** key activates the remote mode.

The detector can now be remote controlled via the data system. All setting and analysis parameters of the ➢*DC Mode* and the ➢*PULSE Mode* are supported. There is a separate control panel for each mode.

All parameters of the **DC** mode can be set via the **ESA_DC.pan** control panel. In the window **ESA_PULSE.pan** all parameters of the mode **PULSE** can be reached.

- Open one of the two windows to operate the detector.
- Activate the switch **Connect**. You will now be notified that it is necessary to activate the remote mode on the instrument. If there is a serious error (e.g. power failure), this switch is deactivated. For the user this means that the ESA detector must be switched manually to remote operation again. Otherwise, it would be in an undefined start state. This is necessary because the ESA detector is not capable of reporting its status to the data system.
- As soon as the remote operation is ensured, setting the parameters can be continued in the usual way.
- Details on the individual parameters can be accessed directly in the control panel via the F1 key. However, this requires basic knowledge of how to operate the detector. For further information, see the detector manual.

In contrast to the parameters, the analysis data is not transferred via the RS232 interface. It is recorded via the ➢*A/D Converter* and is then forwarded to the system.

The Online Help illustrates the three **Server Configuration** pages on this detector type: *General*, *Signals*, and *Error Levels*.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**

FINNIGAN: aQa Mass Spectrometer

Controlling the aQa ➢*Mass Spectrometer* requires the following files:

FinMsAqa.cdd (for CmDriver.exe),

FinMsAqaX.cds (for CmServer.exe),

a message DLL (**messages.dll**), and

a configuration module (**TspCfg.cdc**).

The **demo.raw** file allows demo data creation.

Instrument Installation

aQa data acquisition cannot be started by the ➢*Xcalibur* software interfaces. Therefore, it is required to connect the Inject-Output-Signal of the LC ➢*Autosampler* to the Finnigan aQa User Interface IN1 digital input (use the black and red wires of the 3 wire cable that is shipped with the aQa mass spectrometer).

For information on the software installation required for data acquisition, see **How to ...: Actions Related to the aQa-MS Installing MS Components**.

Tip: The aQa mass spectrometer can be contacted via the TDAT board. If you are using a DELL PC, ensure to reserve the IRQ5 in the BIOS for this ISA board. In addition, also reserve DMA 1 and 0x300-0x307 as I/O address, if required by your BIOS.

TIC and SIM Channel Device Properties and Commands

These channels are standard data channels with the following properties:

Property	Min	Max	Purpose

MinMass	2.00	1636.00	Read only	Minimum mass recorded in this trace. (SIM channels only)
MaxMass	2.00	1636.00	Read only	Maximum mass recorded in this trace. (SIM channels only)
Polarity	Negative	Positive	Read only	Polarity
SourceVoltage	0 V	200 V	Read only	aQa max voltage. (SIM channels only)
SourceVoltage	0 V	200 V	Read only	aQa max voltage range. (TIC/TICF channels only)
Filter	n/a	n/a	Read only	Filter string as used in Finnigan aQa method.

☞ ***Tip***: No data compression is supported. Thus, neither the **Step** command, nor the **MaxAutoStop** or **Average** commands can be set. Manual data acquisition is not possible either. In addition, acquisition is started at time 0.000 and stopped at program end for all channels that deliver data according to an aQa method file. These channels appear neither in the Program Wizard nor in the control panel.

MS Device Properties and Commands

Property	Min	Max	Default	Purpose
Ready	Ready=1, Busy=0		Read only	Indicates whether the spectrometer is busy or idle.
Operation	On=1, Off=2, Standby=3		Off	Indicates whether the spectrometer is busy or idle.
Status	n/a		Read only	Indicates the spectrometer's operational status.
Range	1 (for exp(1) Counts)	10 (for exp(10) Counts)		Scaling range used for online signal plot during data acquisition. (Can be set only before data acquisition starts.)
Smoothing	None=-1, Gaussian=0, Boxcar=1	None		Smoothing algorithm. **Note**: This parameter is used by Xcalibur raw data extraction during online and post-run channel extraction.

Property	Min	Max	Default	Purpose
SmoothingPoints	3, 5, 7, 9, 11, 13, 15	3		Number of data points used for smoothing. **Note**: This parameter is used by Xcalibur raw data extraction during online and post-run channel extraction.
HardwareVersion	n/a		Read only	The mass spectrometer's hardware version. **Note**: This value is available only after the first raw data acquisition.
FirmwareVersion	n/a		Read only	The spectrometer's firmware version. **Note**: This value is available only after the first raw data acquisition.

Command	Purpose
Connect	Connects the device
Disconnect	Disconnects the device
Reset	Resets the device to the defaults

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

FISONS

The following Fisons instruments can be controlled:

Fisons Gas Chromatograph 8000

Fisons Autosamplers AS800 and A200S (for the latter, also see **CTC ANALYTICS**).

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

FISONS: Gas Chromatograph 8000 - Overview

Device Type:	Gas chromatograph
Device Driver:	**Fisons 8000 Gas Chromatograph**
Supported Hardware Options:	Fisons 8000 gas chromatographs or Mega 2 GC with: Electrometer EL800 Digital Flow and Pressure Controller (DFPC) with up to 2 injectors and up to 7 valves.

What is required?

License:	Device Control
Connection:	RS232 cable (for details, see **Fisons GC: Cable 8914.0126 / 8914.0142** in the appendix of these Installation Instructions)
Hardware Prerequisites:	Data acquisition requires an A/D converter, e.g. a ➢*UCI-100 Interface* with the corresponding signal cables Free RS232 port
Software Prerequisites:	• FisCfg.cdc configuration module • Message.dll
Control Panels:	Fis8000A.pan or Fis8000B.pan or Fis8000C.pan

Further Information

For information on how to install the Fisons 8000 Gas Chromatograph, see **Fisons: Gas Chromatograph** 8000 **- Installation**.

For an overview on the different Fisons instruments for which Dionex device drivers are available, see **Fisons**.

FISONS: Gas Chromatograph 8000 - Installation

Hardware Installation

Device Connection:	Device Connection is via an RS232 cable (for details, see **Fisons GC: Cable 8914.0126 / 8914.0142** in the appendix of these Installation Instructions)
Device Settings:	Communication is via the following interface parameters: 9600 baud, 8 data bits, No parity, 1 stop bit. The baud rate has to be set at the instrument as well. Proceed as follows: Simultaneously pressing the keys <SB TIME - PROG RESET - ACTUAL TEMP> sets the value to 9600 baud.
Restrictions:	Not known.

Software Installation

Install the **Fisons 8000 Gas Chromatograph** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Fisons 8000 Gas Chromatograph** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port.

   On the *Components* tab, enter the installed components. In addition, specify the maximum flow rate of the injector(s).

   The *Oven & Zones* tab allows you to set up the temperature control for the oven as well as three temperature-controlled heating zones for the GC. Two channels and two injectors are available.

Open the **Signal Configuration** dialog box by double-clicking the respective channel on the ➢*Signals* tab. Assign a channel to the signal and name the signal in the Signal Name field according to the selected detector type.

On the *Relays* tab, remove all relays that are not used.

You do not need to change the presetting on the ➢*Error Levels* tab.

5. To control the Fisons GC connect one of the **Fis8000A**, **Fis8000B**, or **Fis8000C** control panels in the client of your Dionex Chromatography Management System to the corresponding timebase.

Application

The Fisons 8000 Gas Chromatograph ➢*Device Driver* allows controlling the oven temperature of the Fisons 8000 gas chromatograph and the Mega 2 GCs.

In addition, you can record the signals of two channels (GC_1, GC_2) and address up to seven valves. Controlling the temperature of up to three so-called "heating zones" (additional temperature-controlled modules that are externally controlled) is possible as well.

If the Fisons 8000 is supplied with the **Digital Flow and Pressure Controller (DFPC)**, the **Flow** and **Pressure** can be controlled as well.

Further Information

For an overview on the Fisons Gas Chromatograph, see **Fisons: Gas Chromatograph 8000 - Overview**.

For an overview on the Fisons instruments for which Dionex device drivers are available, see **Fisons**.

Also, see:

Fisons Autosamplers AS800 and AS200S (the latter corresponds to the CTC A200S, see **CTC ANALYTICS**)

FISONS: AS800 GC Autosampler- Overview

Device Type:	GC Autosampler
Device Driver:	**FisonsAS800_Sampler**
Supported Hardware Options:	

What is required?

License:	Device Control
Connection:	RS232 cable (for details, see **Fisons AS: Cable 8914.0127 / 8914.0143** in the appendix of these Installation Instructions)
Hardware Prerequisites:	Data acquisition requires an A/D converter, e.g. a ➢*UCI-100 Interface* with the corresponding signal cables Free RS232 port
Software Prerequisites:	• FisCfg.cdc configuration module • Message.dll
Control Panel:	FISAS800.pan

Further Information

For information on how to install the Fisons AS800 GC Autosampler, see **Fisons: Autosampler - Installation**.

For an overview on the different Fisons instruments for which Dionex device drivers are available, see **Fisons**.

FISONS: AS800 GC Autosampler- Installation

Hardware Installation

Device Connection:

The Fisons GC autosamplers are connected to the Fisons 8000 gas chromatograph via a 37-pin connecting cable. When the injection is completed, the GC sampler sends the signal to the GC, which in turn sends it to the Dionex Chromatography Management System via a relay. The pins 12 and 24 of the GC AUX connector are used. Connect the signal and GND lines of a remote input to these.

GC Fisons 8000 AUX Connector		Remote Input (e.g. A/D Board)
(25-pin; Sub-D, female)		(9-pin, Sub-D, male)
12	----------	Signal
24	----------	GND (0V)

In the **Server Configuration**, specify the remote input that is used by the Fisons AS800 sampler under **Inject Port** on the **Sampler** tab!

Device Settings:

The following communications parameters must be used: 9600 Baud, 8 Data Bits, No Parity, 1 Stop Bit, Rts/Cts handshake.

Some Fisons AS800 GC samplers are set by the manufacturer to a baud rate that is not suitable for the ➢*Device Drivers* of the Dionex Chromatography Management System.

When switching on the sampler, press the **Meth** and **Seq** keys simultaneously to check the baud rate setting. The following information will be displayed:

```
AS800 SET UP: b9600
ACT INJ SMP SYR MAN
```

The value given to the top right is the baud rate setting. This information may not be available in previous firmware versions. If so, press **EXIT** to leave the setup menu.

Device Settings: (Cont'd) If the baud rate is not set to 9600, move the cursor to the baud rate field using the key **<** (arrow to the left). Set the new baud rate with the up and down arrow keys and leave the setup menu by pressing **EXIT**.

Restrictions: Not known.

Software Installation

Install the **Fisons AS800 Sampler** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System
3. Add the **FisonsAS800_Sampler** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *FisonsAS800_Sampler* tab, have the Demo Mode switched off.

   On the *Sampler* tab, select a free inject port.

   You do not need to change the presetting on the ➢*Error Levels* tab.
5. To control the Fisons autosampler connect the **FISAS800** control panel in the client of your Dionex Chromatography Management System to the corresponding timebase.

Application

The Online Help offers information on *Commands and Parameters of the Fisons AS800*.

After the **Connect** command, the parameter values are initially unknown to the Dionex Chromatography Management System (blank fields in the AS800 control panel). You should enter meaningful values before injection. Use one of the **Method A/B/C/D** buttons on the control panel or specify them in the sample program (also, see **How to ...: Actions in the PGM Editor Creating a Program)**.

A sensible starting point might be this:

```
; Assuming a standard 10 µl syringe.
; Injection Volume should be 1.0 µL.
PreInjCleanVol = 10.0
PreInjCleanCycA = 3
CleanCycles = 1
PostInjCleanCycC = 0
; PostInjCleanVol = 10.0
PullUpCount = 6
PullUpDelayTime = 2.0
AirVolume = 3.0
FillingVolume = 5.0
AspirationSpeed = 100
InjectionSpeed = 100
PreInjDelayTime = 1
PostInjDelayTime = 2
```

Troubleshooting

Note: If an error occurs during operation (e.g. excessive sample volume), the error is displayed on the instrument only. To continue the analysis, you must confirm the error message directly at the sampler (by pressing the Enter key). This is possible after unlocking the sampler keyboard in the Dionex Chromatography Management System. Use either the **Disconnect** command or the **KeyboardUnlocked** command. Better yet: **Disconnect** the sampler, turn it off and on again, wait until it is ready, and reconnect.

Error	Description	Remedial Action

Missing vial	The sampler display shows:
	`End Sample`
	`Total Injections 0`
	In addition, the Dionex Chromatography Management System waits forever for an inject response.
		Abort the batch.

Error	Description	Remedial Action

Bad vial	After some retries, the sampler display shows something like this:
	`PLG NDL INJ TUR CNTR`
	`--- BSY --- ---  *`
	This happens quite easily if the vials are not perfectly crimped.
		Disconnect the sampler, press EXIT (on the sampler's keyboard). When prompted whether to pause, continue, or abort the sample, choose Abort. Abort the batch and reconnect.

Illegal parameter (e.g. Volume/ Position > Max or Air + Sample Volume > Max)	The sampler displays an error message.	Disconnect the sampler. Press sampler key, as necessary.
Continuous beep and display cleared	Severe damage may occur (destroyed syringe, vials etc.)!	**Turn off the sampler immediately!**
Strange behavior of any other kind		Disconnect the sampler, turn it off and on again, wait until it is ready, and reconnect.

Further Information

For an overview on the Fisons Autosampler, see **Fisons: AS800 GC Autosampler - Overview**.

The Fisons AS200S Autosampler corresponds to the CTC A200S sampler; see **CTC ANALYTICS**

For information on how to install the Fisons AS800 Autosampler, see **Fisons: Autosampler - Installation**.

For an overview on the different Fisons instruments for which Dionex device drivers are available, see:

Fisons

Fisons 8000 Gas Chromatograph

GILSON

The following Gilson instruments are currently supported:

- **Gilson UV Detectors 116, 117, and 118**
- **Gilson Fraction Collector 201/202 and 206**
- **Gilson Liquid Handler 215**
- **Gilson Autosamplers 235 and 235p**
- **Gilson Autosamplers 231, 232 Bio, and 234**
- **Gilson XL-Series (Autosamplers 221XL, 222XL, 231XL, 232XL, 233XL)**
- **Gilson Pumps 302, 303**
- **Gilson Pumps 305, 306, 307**
- **Gilson Valves**
- **Gilson Autosampler 231XL (Old Device Driver)**

Caution: Under the Dionex Chromatography Management System, the GSIOC bus available from Gilson is used exclusively for combining several pumps in a high-pressure gradient system. All other instruments (e.g. ➢*Autosampler* and Detectors) are controlled individually via separate serial interfaces. All instruments (except those with serial interface) must therefore be connected via an original Gilson cable (GSIOC adapter Model 605) to a PC interface. **The adapter is shipped with the baud rate set to 19200 Baud. For controlling specific instruments via the Dionex Chromatography Management System (i.e., in case of specific drivers (see setting on the tab "General" of the corresponding instrument properties)), it is necessary to set the baud rate to 9600 Baud.** To do this, open the connector housing. Resolder the cable from land A to land B (for details, see the Gilson **605 RS232 Adapter and GSIOC Protocol - USER'S GUIDE**).

Tip: Always connect Gilson instruments requiring a GSIOC cable to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) as communication problems might occur with other RS232 ports (e.g. with the COM ports of the PC or the **Dionex Universal Chromatography Interface (UCI-100)**).

The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the ➢*UCI-100* Universal Chromatography Interface, however, are not designed for this.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

GILSON: UV Detectors 116, 117, and 118 - Overview

Device Type:	UV116 two-channel UV detector or UV117/118 single channel UV detector
Device Driver:	**Gilson 116 UV Detector / Gilson 117 UV Detector** (use the latter one for the UV117 and the UV118 detector, respectively)
Supported Hardware Options:	The only difference between these two detectors is the wavelength range: UV117 up to 380 nm, UV118 up to 700 nm.

What is required?

License:	Device Control
Connection:	GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) The cable is not available from Dionex!
Hardware Prerequisites:	Multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM board, Dionex part no. 5906.2095) Free RS232 port
Control Panel:	UVD170-2.pan

Further Information

For information on how to install the Gilson UV detectors 116, 117, and 118, see **Gilson: UV Detectors 116, 117, and 118 - Installation**.

For on overview on the different Gilson instruments for which Dionex device drivers are available **Gilson**.

GILSON: UV Detectors 116, 117, and 118 - Installation

Hardware Installation

Device Connection:

Caution:

Controlling the Gilson 116, 117, and 118 UV detectors via the RS232 interfaces of the PC (COM ports) or the ➢*UCI-100* Universal Chromatography Interface is not supported. The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this. Connect the adapter to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) instead.

Caution:

The GSIOC adapter 605 is shipped with the baud rate set to 19200 Baud. For controlling the Gilson 116, 117, and 118 detectors via the Dionex Chromatography Management System, it is necessary to set the baud rate to 9600 Baud. To do this, open the connector housing. Resolder the cable from land A to land B (for details see the Gilson 605 RS232 Adapter and GSIOC Protocol - USER'S GUIDE).

Device Settings:

Data transfer is performed at 9600 baud. Please check the baud rate setting on the detector. If necessary, change it to 9600.

This is possible in the **Setup editing mode** of the instrument. Press the <prep> key until **Set Baud Rate** appears in the display. Enter the correct value.

The GSIOC address is also set in this mode. Press the <prep> key until **unit id code** is displayed. Enter the GSIOC address. The default value is 16. The value entered here must correspond to the value in the **Server Configuration** (configuration of the Gilson UV Detector).

Restrictions:

Not known.

Software Installation

Install the **Gilson 116 UV Detector** (or Gilson 117 UV Detector) ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 116 UV Detector** (or Gilson 117 UV Detector, respectively) under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address. (The address is given on the rear panel. It can be changed as described above - see **Device Settings**.)

   Open the **Signal Configuration** dialog box by double-clicking the respective channel on the *Signals* tab. Assign a channel to the signal and name the signal in the **Signal Name** field according to the selected detector type.

   You do not need to change the presetting on the *Error Levels* tab.
5. To control the Gilson UV detectors connect the **UVD170-2** control panel in the client of your Dionex Chromatography Management System to the corresponding timebase (if necessary, remove those components that are not required from the control panel).

Application

Note: For consistency reasons, the UV-detector parameters **Peak Width** and **Sensitivity** are called **Response** and **Range** in the Dionex Chromatography Management System.

Further Information

For an overview on the Gilson UV detectors, see **Gilson: UV Detectors 116, 117, and 118 - Overview**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Fraction Collectors 201/202 and 206 - Overview

Device Type:	Fraction collector with up to 120 positions
Device Driver:	**Gilson 201/202 Fraction Collector** or **Gilson 206 Fraction Collector**
Supported Hardware Options:	With the Fraction Collector 206: • 3 relays • 2 inputs

What is required?

License:	Device Control
Connection:	GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) The cable is not available from Dionex!
Hardware Prerequisites:	Multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM board, Dionex part no. 5906.2095) Free RS232 port
Control Panel:	GIL201.pan

Further Information

For information on how to install the Gilson fraction collectors, see

Gilson: Fraction Collectors 201/202 - Installation

Gilson Fraction Collector 206 - Installation

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Fraction Collectors 201/202 - Installation

Hardware Installation

Device Connection:

GSIOC RS232 adapter cable 605 (see **Gilson: GSIOC Cable**)

The cable is not available from Dionex!

Caution:

Controlling the Gilson 201/202 fraction collectors via the RS232 interfaces of the PC (COM ports) or the ➢*UCI-100* Universal Chromatography Interface is not supported. The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this. Connect the adapter to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) instead.

Caution:

The GSIOC adapter 605 is shipped with the baud rate set to 19200 Baud. For controlling the Gilson 201/202 faction collectors via the Dionex Chromatography Management System, it is necessary to set the baud rate to 9600 Baud. To do this, open the connector housing. Resolder the cable from land A to land B (for details see the Gilson 605 RS232 Adapter and GSIOC Protocol - USER'S GUIDE).

Device Settings:

Setting the Manual Mode and Defining the Rack Code

Perform the following steps to define the program with the file number **1**.

Display		Press Key
		RESET
FILE NUMBER	....	DELETE
WHICH NUMBER		1
		ENTER

Device Settings: (Cont'd)

Any existing program with the file number 1 will be deleted. This may take a few seconds. If this program does not exist, the screen will show **DOES NOT EXIST**.

In both cases, pressing the following keys allows creating the new program 1. As the Rack Code, select the currently used type (e.g. 10).

Display		Press Key
FILE NUMBER		1
		ENTER
SELECT MODE		MAN.
MANUAL MODE		ENTER
RACK CODE		10
RACK CODE	10	ENTER
DELAY	0.00	ENTER
READY-HIT ADV.		

The **READY-HIT ADV**. display and the lit **MAN**. LED indicate that the instrument is in manual mode and is ready to operate.

Enter the **File Number** just defined on the instrument (here: 1) and the Rack Code under *Rack Type and Program File* (link available in the Online Help only) in the **Server Configuration** of the Dionex Chromatography Management System.

Restrictions:

Not known.

Software Installation

Install the **Gilson 201/202 Fraction Collector** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 201/202 Fraction Collector** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

On the *General* tab, select a free COM port and enter the GSIOC address. (The address is given on the rear panel. It can be changed as described above - see **Device Settings**.)

On the *Rack Type and Program File* tab, enter the numbers of the desired rack types and files.

You do not need to change the presetting on the *Error Levels* tab.

To control the Gilson 201/202 fraction collectors connect the **GIL201** control panel in the client of your Dionex Chromatography Management System to the corresponding timebase.

Application

After switching the instrument on, the model name and then the number of the current program is displayed on the instrument screen (e.g. **FILE NUMBER 3**).

Caution: The **Connect** command can only be performed in the Dionex Chromatography Management System if the instrument is set to the **Manual** mode. The **READY-HIT ADV**. display and the active **MAN**. LED indicate that the instrument is currently in the **Manual** mode and ready to operate. If this is not the case, the error message **Gilson 201/202 program ... is not a manual program** is entered in the Audit Trail. Connecting the instrument to the Dionex Chromatography Management System is not possible then!

The following rack types are available

Rack Code 0	80 vials
Rack Code 1	80 test tubes (13 x 100 mm; 9 ml)
Rack Code 2	119 test tubes (6 x 50 mm; 1 ml)
Rack Code 4	80 test tubes (12 x 100 mm; 8 ml)
Rack Code 7	Holder for micro titer boards
Rack Code 8	120 vials (6 x 32 mm; 0,6 ml)
Rack Code 9	120 vials (7 x 40 mm; 1,4 ml)
Rack Code 10	27 funnels with outlet tube

Rack Code 20	108 test tubes (10 x 100 mm)
Rack Code 21	60 test tubes (13 x 100 mm; 9 ml)
Rack Code 22	44 test tubes (18 x 180 mm)
Rack Code 23	44 mini vials (17 x 65 mm; 8ml)
Rack Code 24	14 scintilution vials (28 x 60 mm; 20ml)
Rack Code 28	108 test tubes (10 x 75 mm; 3,5 ml)
Rack Code 29	60 test tubes (13 x 75 mm; 5 ml)

Further Information

For an overview on the Gilson fraction collectors, see **Gilson: Fraction Collectors 201/202 and 206 - Overview**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Fraction Collector 206 - Installation

Hardware Installation

Device Connection:

GSIOC RS232 adapter cable 605 (see **Gilson: GSIOC Cable**)

The cable is not available from Dionex!

Caution:

Controlling the Gilson 206 fraction collector via the RS232 interfaces of the PC (COM ports) or the ➢*UCI-100* Universal Chromatography Interface is not supported. The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this. Connect the adapter to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) instead.

Device Connection: (Cont'd)

Note:

Contrary to the Fraction Collectors 201 and 202, the Gilson Fraction Collector 206 uses a baud rate of 19200 Baud. Therefore, do not modify the 605 cable!

Device Settings:

Restrictions: Not known.

Software Installation

Install the **Gilson 206 Fraction Collector** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 206 Fraction Collector** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address. (The address is given on the rear panel.)

   On the *Rack* tab, enter the number of the installed rack type.

   On the *Relays* tab, remove all relays that are not used.

   On the *Inputs* tab, remove all inputs that are not available.

   You do not need to change the presetting on the ➢*Error Levels* tab.

To control the Gilson 206 fraction collector connect the **GIL201** control panel in the client of your Dionex Chromatography Management System to the corresponding time

Application

After switching the instrument on, the model name and then the number of the current program is displayed on the instrument screen (e.g. **FILE NUMBER 3**).

Caution: The **Connect** command can be performed in the Dionex Chromatography Management System only if the instrument is set to the **Manual** mode. The **READY-HIT ADV**. display and the active **MAN**. LED indicate that the instrument is currently in the **Manual** mode and ready to operate. If this is not the case, the error message **Gilson 201/202 program ... is not a manual program** is entered in the Audit Trail. Connecting the instrument to the Dionex Chromatography Management System is not possible then!

Further Information

For an overview on the Gilson fraction collectors, see **Gilson: Fraction Collectors 201/202 and 206 - Overview**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Liquid Handler 215 - Overview

Device Type:	Liquid handler with x positions
Device Driver:	**Gilson Liquid Handler 215**
Supported Hardware Options:	• 2 Gilson 819 inject ports • 3 relays • 2 inputs

What is required?

License:	Extended Device Control Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	**Modem Cable (1:1 RS Cable): 8914.0128 or 8914.0144** (for details, see the appendix of these Installation Instructions)
Hardware Prerequisites:	Free RS232 port (COM1 or COM2, because the included Gilson configuration software supports COM1 and COM2 only)

Further Information

For an overview on how to install the Gilson liquid handler, see **Gilson: Liquid Handler 215 - Installation**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Liquid Handler 215 - Installation

Hardware Installation

Device Connection:	Connection to the PC is via a **Modem Cable (1:1 RS Cable): 8914.0128 or 8914.0144** (for details, see the appendix of these Installation Instructions) The Gilson 819 inject port is connected to the liquid handler via a GSIOC cable from Gilson (see **Gilson: GSIOC Cable**). If there is a second Gilson 819, use another GSIOC cable on the corresponding free connector of the first GSIOC cable.
Device Settings:	The SW-2 (baud rate/mode selector) switch on the instrument's rear panel must be set to position 6 (19200 Baud, GSIOC Master).
Restrictions:	Not known.

Software Installation

Install the **Gilson 215 Liquid Handler** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 215 Liquid Handler** under the desired timebase (via the **Add Device** command of the context menu).

4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address. (The address is given on the rear panel. It can be changed as described above - see **Device Settings**. When selecting the COM ports, please note that the included Gilson configuration software supports COM1 and COM2 only.)

   On the *Sampler* tab, enter the name of the installed tray, the syringe volume, and the maximum syringe speed. The driver checks the last two entries that are based on the configuration and corrects them, if necessary.

   On the ➢*Inject Port* tab, enter the GSIOC address of the respective inject port, the loop volume, and the home coordinates of the injection needle. (Ensure correct input of the loop volume and the coordinates!)

   On the ➢*Relays* tab, remove all relays that are not used. On the ➢*Inputs* tab, remove all inputs that are not available.

   You do not need to change the presetting on the ➢*Error Levels* tab.

Application

Configuring the Liquid Handler

Use the Gilson **709** software to configure the Liquid Handler.

Caution: The Gilson software (except the Tray editor) is currently supported under Windows 98 only, and not under Windows NT/Windows 2000! The Gilson software removes the used COM port from the system, so that the Dionex Chromatography Management System cannot access the port!

These problems can be solved as follows:

- Switch to another COM port after completing the configuration.
- Uninstall the Gilson software after the configuration.
- Install both, Windows 98 and NT/2000 on the PC (caution: install Windows 98 first!). Then, install the Gilson software under Windows 98 (only), and install the Dionex Chromatography Management System under Windows NT/2000.
- Gilson supplies a GSIOC.SYS driver for Windows NT/2000. However, this driver must be installed manually. With this driver, the Gilson software runs

under Windows NT/Windows 2000 as well. After uninstalling this driver and booting the PC, the Dionex Chromatography Management System can be started.

Configure the Liquid Handler with the **215Setup** program. Check especially the coordinates of the wash station and write down the coordinates of the injection port.

Use the **TrayEdit** program to define the tray layout. Specify the zone names and the vial numbering. The vials from which to inject should be located in the first zone. Assign a zone name, e.g. **Samples**.

You can define further zones, e.g. for fraction collection or sample preparation. Please note that the driver for zone names supports the letters A-Z (no special characters), numbers, and the characters **%,** and **_**, only. If you enter other characters in the tray editor, these will be replaced by **_**.

The file name should not exceed nine characters (+ .**gty**). Save the resulting file in the folder **Chromel\bin**, **e.g., \Chromel\bin\gil215.gty**.

Further Information

For an overview on the Gilson liquid handler, see **Gilson: Liquid Handler 215 - Overview**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Autosamplers 235 and 235p - Overview

Device Type:	Autosampler with up to 384 positions
Device Driver:	**Gilson 235 Autoinjector**
Supported Hardware Options:	• 5 relays • 4 inputs

What is required?

License:	Extended Device Control Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	**Modem Cable (1:1 RS Cable): 8914.0128 or 8914.0144** (for details, see the appendix of these Installation Instructions)
Hardware Prerequisites:	Free RS232 port

Further Information

For an overview on how to install the Gilson autosamplers 235 and 235p, see **Gilson: Autosamplers 235 and 235p - Installation**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Autosamplers 235 and 235p - Installation

Hardware Installation

Device Connection: Connection to the PC is via a **Modem Cable (1:1 RS Cable): 8914.0128 or 8914.0144** (for details, see the appendix of these Installation Instructions)

Normally, the Peltier cooling of the 235p sampler is connected to relay 3 so that it can be switched on and off via the software. We recommend keeping this setting and naming relay 3 in the Dionex Chromatography Management System accordingly.

Device Settings: The SW-2 (baud rate/mode selector) switch on the instrument's rear panel must be set to position 6 (19200 Baud, GSIOC Master).

Restrictions: Not known.

Software Installation

Install the **Gilson 235 Autoinjector** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 235 Autoinjector** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address. (The address is given on the rear panel. It can be changed as described above - see **Device Settings**. When selecting the COM ports, please note that it may be possible that the Gilson tray editor, which is required for configuring special sample trays, and the included Gilson sampler configuration software blocks COM1 and COM2.)

   On the *Sampler* tab, enter the name of the installed tray file. The pull down box lists all tray files (max. 9 characters) that are available in the **Chromel\Bin** directory. If the tray file is located in a different directory,

enter the whole path. In addition, you can specify the syringe volume, the maximum syringe speed, and the loop volume. Selecting the syringe volume from the selection list automatically sets the corresponding maximum syringe speed.

On the *Relays* tab, remove all relays that are not used.

On the *Inputs* tab, remove all inputs that are not available.

You do not need to change the presetting on the *Error Levels* tab.

Application

Configuring the Sample Tray

As the sampler can access any coordinates almost every sample tray including **homemade** trays can be used. To ensure this flexibility, the driver takes the dimensions and coordinates of the vials from the **tray file**.

Dionex supplies some tray files for the most commonly used sample racks:

Tray File	Rack Code	Vial Type
235_350	350	96-hole micro titer, flat
235_350s	350	384-hole micro titer, flat
235_351	351	96-hole micro titer, deep
235_352	352	2 ml
235_353	353	0.7 ml
235_354	354	96-hole micro titer, cooled, flat (235p)
235_354s	354	384-hole micro titer, cooled, flat (235p)

If you use a different rack or if special requirements must be fulfilled, you must generate a tray file yourself. For this purpose, use the Tray Editor from the Gilson Software 709. You can also use the editor to modify existing tray files, if you wish to number the vials in a different order or reserve special vial positions, e.g. for specific applications, by assigning separate zone names.

The program allows you to define the layout of the sample rack and to determine zone names and vial numbering. The vials to be used for injection should be placed in the first zone. Name this zone e.g. **samples**.

☞ ***Tip***: With the **Inject** command, the samples always have to be in the first zone. (The zone number does not influence their actual position.)

Additional zones, e.g. for fractionating or sample preparation, can be defined. Please note that the driver only admits the characters A-Z (no umlaut, accents,

ß ...), %, _, and numbers to be used in zone names. Other characters entered in the tray editor will be replaced by _.

Save the result, e.g. under **\Chromel\bin\MyTray.gty**.

Tray Files

For this device driver, various standard tray files are already available (see below). Insert your rack into the sampler so that the first sample is at the front left. If the corresponding Gilson program is available on your computer, you can freely program different sample distributions by yourself.

235_350.gty, 235_351.gty, 235_353.gty and **235_354.gty :**

(The table lines of the track files indicate the position numbers in the respective rack line).

373 374 ... 384
... ...
301 302 ... 312
289 290 ... 300

277 278 ... 288
... ...
205 206 ... 216
193 194 ... 204

181 182 ... 192
... ...
109 110 ... 120
97 98 ... 108

85 86 ... 96
... ...
13 14 ... 24
1 2 ... 12

235_352.gty:

185 186 ... 192
... ...
9 10 ... 16
1 2 ... 8

☞ ***Tip:*** If you change the syringe, communicate the new syringe volume

to the sampler. You can do this in the **Server Configuration**.

In addition, the coordinates for waste, rinse station, and injection port can be changed for specific applications.

Caution: Usually, the default values should be used. Re-adjust the sampler, if these positions are not hit exactly.

Further Information

For an overview on the Gilson autosamplers 235 and 235p, see **Gilson Autosampler 235 - Overview**.

For an overview on the different Gilson instruments for which device drivers are available, see **Gilson**.

GILSON: Autosamplers 231, 232 Bio, and 234 - Overview

Device Type:	Autosampler with up to x positions
Device Driver:	**Gilson 231 Autosampler**, **Gilson 232 Bio Autosampler**, and **Gilson 234 Autoinjector**, respectively
Supported Hardware Options:	

What is required?

License:	Device Control Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) The cable is not available from Dionex!

Hardware Prerequisites:	Free RS232 port
Control Panels:	GIL231.pan GIL232.pan

Further Information

For an overview on how to install the Gilson autosamplers 235 and 235p, see **Gilson: Autosamplers 231/ 232 Bio, and 234 - Installation**.

For an overview on the different Gilson instruments for which device drivers are available, see **Gilson**.

GILSON: Autosamplers 231, 232 Bio, and 234 - Installation

Hardware Installation

Device Connection: GSIOC RS232 adapter cable 605 (see **Gilson: GSIOC Cable**)

The cable is not available from Dionex!

Caution:

Controlling the Gilson autosamplers 231, 232 Bio, and 234 via the RS232 interfaces of the PC (COM ports) or the ➢*UCI-100* Universal Chromatography Interface is not supported. The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this. Connect the adapter to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) instead.

Caution:

The GSIOC adapter 605 is shipped with the baud rate set to 19200 Baud. For controlling the Gilson autosamplers 231 and 232 via the Dionex

Device Connection: (Cont'd)

Chromatography Management System, it is necessary to set the baud rate to 9600 Baud. To do this, open the connector housing. Resolder the cable from land A to land B (for details see the Gilson 605 RS232 Adapter and GSIOC Protocol - USER'S GUIDE).

Note:

Contrary to the autosamplers 231 and 232 Bio, the Gilson Autosampler 234 uses a baud rate of 19200 Baud. Therefore, do not modify the 605 cable!

Device Settings:

Restrictions: Not known.

Software Installation

Install the **Gilson 231 Autosampler** (or Gilson 232 Bio Autosampler or Gilson 234 Autoinjector) ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 231 Autosampler** (or Gilson 232 Bio Autosampler or Gilson 234 Autoinjector) under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address.

   For the 231/232 Bio autosamplers:

   On the respective rack tab (➢*Rack* for the 231 autosampler, *Rack* tab for the 232 Bio autosampler), select the code number of the installed default rack. Select **None of these** to specify the maximum number of samples first. Manually enter the number in the *INI-File* that is selected on the **INI File** tab.

For the 234 autosampler:

On the *Sampler* tab, enter the name of the installed tray file. The pull down box lists all tray files (max. 9 characters) that are available in the **Chromel\Bin** directory. If the tray file is located in a different directory, enter the whole path. In addition, you can specify the syringe volume, the maximum syringe speed, and the loop volume. Selecting the syringe volume from the selection list automatically sets the corresponding maximum syringe speed.

On the *Relays* tab, remove all relays that are not used.

On the *Inputs* tab, remove all inputs that are not available.

You do not need to change the presetting on the *Error Levels* tab.

5. To control the installed Gilson autosampler connect the **GIL231** or **GIL232** control panel in the client of your Dionex Chromatography Management System to the corresponding time

Application

Before controlling these ➢*Autosamplers* via the Dionex Chromatography Management System, some information must be transferred to the instruments. As usual with Gilson instruments, this is by downloading a basic (INI) file. Please note the instructions in your Autosampler Manual. The name of the INI File must be included in the device configuration (**INI** tab) in the **Server Configuration** of the Dionex Chromatography Management System.

For the Gilson 231, the rack types 0, 2, 7, 8, and 10 are supported. For the Gilson 232 Bio, the rack types 30, 31, 32, 33, and 34 are supported. For both instruments, any other rack type can be defined. In this case, the correct rack must be entered manually in the INI File.

For an example INI File similar to a BASIC program, see **Installing and Controlling Third-Party Instruments** **Gilson INI File**.

In addition, the autosampler's GSIOC address must be entered in the **Server Configuration** (**General** tab dialog box). The default address is 10. This value must correspond to the value set on the instrument.

Tray Files

For these Gilson device drivers, various standard tray files are already available. Insert your rack into the sampler so that the first sample is at the front left. If the corresponding Gilson program is available on your computer, you can freely program different sample distributions by yourself.

234_036.gty:

(The table lines of the track files indicate the position numbers in the respective rack line).

C		...	1	8	…	107
		...	2	9	…	108
B	B	...	3	10	…	109
B	B	...	4	11	…	110
B	B	...	...	...	...	...
B	B	...	7	14	…	113

C		...	A	A	A	…
		...	A	A	A	…
1	5	...	A	A	A	…
2	6	...	A	A	A	…
3	7	...	...	...	...	...
4	8	...	A	A	A	…

For example, "normal" samples may be given under A, standard samples under B, and the wash solution under C.

Further Information

For an overview on the Gilson autosamplers 231, 232 Bio, and 234, see **Gilson: Autosamplers 231/ 232 Bio, and 234 - Overview**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Autosamplers XL Series (221XL, 222XL, 231XL, 232XL, 233XL) - Overview

Device Type:	Autosampler with up to x positions
Device Driver:	**Gilson XL Series (Extended)** (Do not confuse with the **Gilson 231 Autosampler** and the **Gilson 231 XL Autosampler** device drivers!)
Supported Hardware Options:	• Syringe module (dilutor) 402 • Inject port • Switching valve • 8 relays • 5 inputs

What is required?

License:	Extended Device Control Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	Connection to the PC is via a **Modem Cable (1:1 RS Cable): 8914.0128 or 8914.0144** (for details, see the appendix of these Installation Instructions) For the Gilson 402 syringe module (syringe pump, dilutor): GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions - the cable is not available from Dionex).
Hardware Prerequisites:	Free RS232 port
Control Panel:	GIL231XL.pan

Further Information

For an overview on how to install the Gilson autosamplers of the XL series, see **Gilson: Autosamplers XL Series - Installation**.

For an overview on the different Gilson instruments for which Dionex Chromatography Management System are available, see **Gilson**.

GILSON: Autosamplers XL Series (221XL, 222XL, 231XL, 232XL, 233XL) - Installation

Hardware Installation

Device Connection:

Caution:

Before connecting the autosampler to the PC, remove the supplied keypad. Do not connect the autosampler with the keypad and the PC at the same time!

Connection to the PC is via a **Modem Cable (1:1 RS Cable): 8914.0128 or 8914.0144** (for details, see the appendix of these Installation Instructions)

Using a simple 9-pin Gilson RS232 cable as 1:1 RS cable is possible as well. The Gilson 402 syringe module (**Syringe Pump**, **Dilutor**) is connected to the autosampler via a GSIOC cable from Gilson (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions - the cable is not available from Dionex).

Device Settings:

The DIP-switches should show the factory-set presetting:

Autosampler:

Dip-Switch	1	2	3	4	5	6	7	8
Top	x	x	x		x		x	
Bottom				x		x		x

Dilutor 402:

Dip-Switch	left	right
1		x
2	x	
3		x
4	x	
5	x	
6	x	
7	x	
8	x	

Restrictions:

Not known.

Software Installation

Install the **Gilson XL Series (Extended)** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson XL Series (Extended)** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address.

   On the *Geometry* tab, select the tray file according to your tray. You can modify the file at the desired position by selecting the **Custom** option via the arrow under **Drain**, **Rinse,** or **Work Area Size**.

   On the *Dilutor 402* tab, enter the desired parameters for the 402 syringe module.

   On the *Inject Port / Switching Valve* tab, specify the settings of the respective motorized switching valve.

   On the *Relays* tab, remove all relays that are not used.

   On the *Inputs* tab, remove all inputs that are not available.

   You do not need to change the presetting on the *Error Levels* tab.
5. To control the installed Gilson autosampler connect the **GIL231XL** control panel or any especially developed control panel in the client of your Dionex Chromatography Management System to the corresponding time

Application

Tray Files

For this device driver, various standard tray files are already available. Insert your rack into the sampler so that the first sample is at the front left. If the corresponding Gilson program is available on your computer, you can freely program different sample distributions by yourself.

231XL00.gty:

(The table lines of the track files indicate the position numbers in the respective rack line).

1 6 ... 76
2 7 ... 77
... ...
5 10 ... 80

231XL07.gty:

1 9 ... 89
2 10 ... 90
... ...
8 16 ... 96

231XL08.gty:

1 6 ... 115
2 7 ... 116
... ...
5 10 ... 120

231XL10.gty:

1 2 ... 13

27 26 ... 15 14

Differences from Gilson 215

Due to the differing wash principle, the XL series offers the two parameters **InnerWashVolume** and **OuterWashVolume** instead of the **WashVolume** parameters. In addition, the **MoveToRinse** command offers the **MoveToDrain** option.

If two syringes are installed, the additional **Syringe**, **RightSuckedVolume**, and **RightDilutorValve** are available.

Caution: The Z-axis of the XL-series points down, the Z-axis of the 215 points up. To position the needle 2 cm above the vial floor, enter **Z = TubeBottom - 20** (instead of **Z = TubeBottom + 20** as with the 215), otherwise the needle is driven into the vial floor!

To allow lifting the needle via the same command, both systems support the **NeedleUp** command.

Differences from the Device Driver Gil231XL.CDD

The "old" device driver Gil231XL.CDD required additional hardware and software (Gilson 606 RS converter, Gilson software GYNK_231.EXE). Its capabilities are mainly limited to the sample position and sample number input. The actual injection must be defined via the Gilson software on the keypad. For compatibility, this device driver is still included.

The "new" device driver GilXLExt.CDD requires no additional hardware or software. (Exception: for defining special sample trays, the Gilson Tray editor is used). All capabilities of the autosampler are supported directly by the device driver.

To update an existing installation of the Dionex Chromatography Management System to the new device driver, proceed as follows:

- Ensure that the **Extended Device Control** license is available for your system.
- Uninstall the previous device driver.
- Remove the control unit (keypad), the RS232 converter 606, and the null modem cable to the PC.
- Connect the autosampler directly to the PC using a 1:1 RS cable (not a null modem cable).
- Install the new device driver as described above.
- Convert the injection methods of the Gilson software into the ➢*Program* of the Dionex Chromatography Management System (must be performed manually).

Further Information

For an overview the Gilson autosamplers of the XL series, see **Gilson: Autosamplers XL Series - Overview**.

We do not recommend using the old device driver, however, it is possible. For details, see **Gilson Autosampler 231XL, 232XL, 233XL (Old Device Driver)**

For an overview on the different Gilson instruments for Dionex device drivers are available, see **Gilson**.

GILSON: Autosamplers 231XL, 232XL, 233XL (Old Device Driver) - Overview

We recommend operating these ➢*Autosamplers* with the new **Gilson Autosamplers XL-Series (221XL, 222XL, 231XL, 232XL, 233XL** device driver (**Gilson XL Series (Extended)**). Their capabilities are mainly limited to the sample position and sample number input. The actual injection must be defined via the Gilson software on the keypad. For compatibility, this device driver is still included.

Device Type:	Autosampler
Device Driver:	**Gilson 231 XL Autosampler** (Do not confuse with the **Gilson 231 Autosampler** and the **Gilson XL Series (Extended)** device drivers!)
Supported Hardware Options:	

What is required?

License:	Device Control Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	Gilson GSIOC bus cable (**no** Gilson GSIOC RS232 adapter cable 605!) - The cable is not available from Dionex. **Null Modem Cable (RS232-Kabel)**: **8914.0129 or 8914.0103A** (for details, see the appendix of these Installation Instructions)
Hardware Prerequisites:	RS232 converter box 606 Free RS232 port
Software Prerequisites:	Gilson software GYNK_231.EXE
Control Panel:	GIL231XL.pan

Further Information

For an overview on how to install the Gilson 231 XL, 232XL, and 233XL autosamplers (old device driver), see **Gilson: Autosamplers 231XL, 232XL, 233, XL (Old Device Driver) - Installation**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Autosamplers 231XL, 232XL, 233XL (Old Device Driver) - Installation

Hardware Installation

Device Connection:	Connecting the autosampler to the converter box is via the Gilson RS232 cable. The PC connection of the box is via the **Null Modem Cable (RS232 Cable -** Dionex part nos. 8914.0129 or 8914.0103A - for details, see the appendix of these Installation Instructions).
Device Settings:	As soon as the individual components are connected via the corresponding cables, the software of the system can be configured. Use the control unit to load the program GYNK_231.EXE (version 3.15 or higher) and then perform the programming.
Restrictions:	Not known.

Software Installation

Install the **Gilson 231 XL Autosampler** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 231 XL Autosampler** under the desired timebase (via the **Add Device** command of the context menu).

4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address.

   You do not need to change the presetting on the *Error Levels* tab.

5. To control the installed Gilson autosampler connect the **GIL231XL** control panel or any especially developed control panel in the client of your Dionex Chromatography Management System to the corresponding time

Further Information

For an overview on Gilson autosamplers of the XL series with the new device driver, see **Gilson: Autosamplers XL Series (221XL, 222XL, 231XL, 232XL, 233XL) - Overview**.

For an overview on the Gilson 231 XL, 232XL, and 233XL autosamplers with the old device driver, see **Gilson: Autosampler 231XL, 232XL, 233XL (Old Device Driver) - Overview**. However, using the old device driver is not recommended.

For further details, see **Gilson: Sample Preparation Systems**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Pumps 302, 303 - Overview

Device Type:	Pumps
Device Driver:	**Gilson 302 Pump**
Supported Hardware Options:	Up to three Gilson 302/303 pumps

What is required?

License:	Device Control Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) The cable is not available from Dionex!
Hardware Prerequisites:	Multi-serial, 8-fold PCI interface board (Equinox 8-RS232 Multi-Com board, Dionex part no. 5906.2095) Free RS232 port
Control Panel:	GIL306Gradient.pan

Further Information

For an overview on how to install the Gilson 302/303 pumps, see **Gilson: Pumps 302/303 - Installation**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Pumps 302, 303 - Installation

Hardware Installation

Device Connection: The device driver supports up to 3 Gilson pumps of the type 302/303. If several Gilson pumps are combined in a high-pressure gradient system, connection is via the GSIOC bus. The bus cable is connected via the original Gilson GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) with a serial PC interface. The bus cable can connect up to four pumps.

Caution:

Controlling the Gilson pumps 302/303 via the RS232 interfaces of the PC (COM ports) or the ➢*UCI-100* Universal Chromatography Interface is not supported. The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this. Connect the adapter to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) instead.

Device Settings: Each pump has its own GSIOC address (0 to 63). The address is set via a DIP-switch. This switch is located inside the pump on the back of the front panel.

Restrictions: Not known.

Software Installation

Install the **Gilson 302 Pump** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 302 Pump** under the desired timebase (via the **Add Device** command of the context menu).

4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address.

   The *GSIOC and Head Types* tab allows defining the GSIOC addresses for the Gilson pump as well as the pump head types that are used.

   You do not need to change the presetting on the *Error Levels* tab.

5. To control the installed Gilson pump connect the **GIL306Gradient** control panel or any especially developed control panel in the client of your Dionex Chromatography Management System to the corresponding time

Further Information

For an overview on Gilson pumps 302/303, see **Gilson Pumps 302/303 - Overview**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Pumps 305, 306, 307 - Overview

Device Type:	Pumps
Device Driver:	**Gilson 305/306/307 Pump**
Supported Hardware Options:	Up to three Gilson 305/306/307 pumps

What is required?

License:	Device Control Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) The cable is not available from Dionex!
Hardware Prerequisites:	Multi-serial, 8-fold PCI interface board (Equinox 8-RS232 Multi-Com board, Dionex part no. 5906.2095)

Free RS232 port

Control Panel: GIL306Gradient.pan

Further Information

For an overview on how to install the Gilson 305/306/307 pumps, see **Gilson: Pumps 305/306/307 - Installation**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Pumps 305, 306, 307 - Installation

Hardware Installation

Device Connection: The device driver supports up to 3 Gilson pumps of the type 305/306/307. The pumps are connected to the GSIOC bus via the **GSIOC from Controller** connector. The bus is connected to the serial PC port via the original GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) with a serial PC interface.

Caution:

Controlling the Gilson pumps 3057306/307 via the RS232 interfaces of the PC (COM ports) or the ➢*UCI-100* Universal Chromatography Interface is not supported. The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this. Connect the adapter to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) instead.

Device Settings: Each pump must have a unique GSIOC address assigned. This address must be entered on the

instrument and in the **Server Configuration** of the Dionex Chromatography Management System. For the models 305 and 307, the following procedure is required:

- Press <Menu>.
- Press <I/O>.
- Press <Next> until **GSIOC Unit ID:** appears.
- Enter the ID and press <Enter>.
- Press <Quit>.

For the model 306, the ID is set via a DIP-switch on the rear of the instrument (the switches 1-6 correspond to 1-bit 0, 2-bit 1, etc.). Use switches 7 and 8 to set the baud rate (9600 Baud = 7/off and 8/on; 19200 Baud = 7/on and 8/off).

Restrictions: Not known.

Software Installation

Install the **Gilson 305/306/307 Pump** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson 305/306/307 Pump** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address.

   The *GSIOC and Head Types* tab allows defining the GSIOC addresses for the Gilson pump as well as the pump head types that are used.

   You do not need to change the presetting on the *Error Levels* tab.
5. To control the installed Gilson pump connect the **GIL306Gradient** control panel or any especially developed control panel in the client of your Dionex Chromatography Management System to the corresponding time

Application

Set the following communications parameters: 9600 Baud, 8 Bit, 2 Stop, Even Parity, and no Handshake. Use the same cabling for gradients and for operating two or three pumps. All pumps must be connected to the same GSIOC bus. A master/slave connection via the **GSIOC to Slave Pump** connector (model 305) is not possible!

The Dionex Chromatography Management System performs pressure monitoring. Therefore, do not enter pressure limits on these pumps! If the pressure is below the lower limit, the pump will stop after 60 seconds. The **Refill Time** and **Compressibility** pump parameters are supported as well.

Further Information

For an overview on the Gilson 305/306/307 pumps, see **Gilson: Pumps 305/306/307 - Overview**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Valves (817, 819, UVSM) - Overview

Device Type:	Valves
Device Driver:	**Gilson Valve Module**
Supported Hardware Options:	• Gilson 817: up to 8 valve positions • Gilson 819: up to 2 valve positions • UVSM: up to 8 valve positions • ValveMate: up to 8 valve positions

What is required?

License:	Device Control Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	**817, 819, and UVSM:** GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) The cable is not available from Dionex! **ValveMate:** **Modem Cable (1:1 RS Cable): 8914.0128 or 8914.0144** (for details, see the appendix of these Installation Instructions)
Hardware Prerequisites:	Multi-serial, 8-fold PCI interface board (Equinox 8-RS232 Multi-Com board, Dionex part no. 5906.2095) Free RS232 port
Control Panel:	GIL231XL.pan

Further Information

For an overview on how to install the Gilson valves, **GILSON: Valves - Installation**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON: Valves (817, 819, UVSM) - Installation

Hardware Installation

Device Connection:

The ValveMate can be connected with ➢*Modem Cable* (Dionex part no. 8914.0128 for a 25-pin port or Dionex part no. 8914.0144 for a 9-pin port, no null modem cable!). The Gilson 817, 819, and UVSM valves are connected from the GSIOC port to the PC via a Gilson adapter cable 605.

Caution:

Controlling the Gilson valves via the RS232 interfaces of the PC (COM ports) or the ➢*UCI-100* Universal Chromatography Interface is not supported. The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this. Connect the adapter to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) instead.

Note:

Contrary to most other Gilson devices, the Gilson valves use a baud rate of 19200 Baud. Therefore, do not modify the 605 cable!

Restrictions:

Not known.

Software Installation

Install the **Gilson Valve Module** ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Gilson Valve Module** under the desired timebase (via the **Add Device** command of the context menu).

4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address.

   On the *Valve* tab, determine the options of the installed Gilson valve. Four different naming schemes are available for identifying the valve positions. The **Custom** setting is intended for the Dionex Service (for defining their own scheme).

   You do not need to change the presetting on the ➢*Error Levels* tab.

5. To control the installed Gilson valve connect the **GIL231XL** control panel or any especially developed control panel in the client of your Dionex Chromatography Management System to the corresponding timebase.

Application

The valve type 819 is an injection valve that is usually used with the Gilson 215 Liquid Handler only. In this case, the GilValve.CCD driver is not required, as the Gilson 215 driver supports up to two 819-injection valves.

While the valve type 819 supports two valve positions only, the other types support two to eight valve positions.

Further Information

For an overview on the Gilson valves, see **Gilson valves - Overview**.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON Sample Preparation Systems (Old Device Driver)

We recommend to operate the Gilson Sample Preparation Systems with the new **Gilson Autosampler 231XL, 232XL, 233XL** device driver (**Gilson XL Series (Extended)**. If using the old **Gilson 231 XL Autosampler** ➢*Device Driver* nevertheless, note the following requirements:

System Requirements

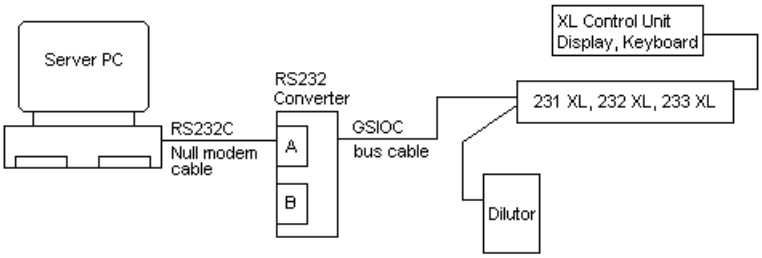
Gilson

- ➢*Autosampler* 231 XL, 232 XL or 233 XL
- Dilutor 402, ...
- XL control unit (display and keyboard)
- Gilson RS232 converter box 606
- Gilson GSIOC connecting cable
- Null modem connecting cable
- Gilson interface software GYNK_231.EXE version 3.15 or higher

Dionex

- PC with COMx
- CHROMELEON from version 3.10
- Gilson 231 XL Autosampler device driver

Connecting the Sample Preparation System



Connection Cable Converter Box (channel A) - COMx

GSIOC Converter (25-pin MinD, female)		COMx (25-pin MinD, female)	COMx (9-pin MinD, female)
3	----------	2	3

2	----------	3	2
7	----------	7	5
		Internal: 4 - 5	Internal: 7 - 8

Starting the Sample Preparation System

As soon as the sample preparation system has been connected as shown above, the software configuration of the system must be defined. To be on the safe side, you should make a backup copy of the Gilson system diskette to your PC, using the DISKCOPY command.

Then insert the copied diskette into the drive on the side of the control unit. Switch on all Gilson system components! The control unit loads the operating system and the device driver software GYNK_231 from the diskette. After the usual prompts for the date and time, the program is in the main menu shown below.

```
----GILSON GYNK_231 3.15—Default.XCP----
 231XL: 10/1230    RACKS:0   ZONES:0
 DIL :
 MP3 :
 HPP :
 M506:            M606 :
---------NO PROGRAM------MEM:83416-------
  FILE   CONFIG  EDITOR   RUN    MANUAL
```

In the title line, the name of the control software (GYNK_231) and the version number appears (version 3.15 or higher). The name of the current method file is also specified. This file contains all parameters. Below that, the screen lists all system components with their GSIOC addresses. In addition, you can see the number of the currently installed racks and zones.

Configuring the Sample Preparation System

Pressing the function key <CONFIG> allows you to change from the main menu to the configuration menu.

```
----UNIT----Gynk_231/CONFIG--------------
  XYZ-ROBOT   231B V1.11       to ID: 10




---------ADD-/DEL-UNIT = <ENTER> --------
 ZDRIVE   RINSE    TRAY    VALVES    QUIT
```

For the operation via the Dionex Chromatography Management System, the system component **IFACE 606** must be set up.

```
----CONFIG/=====UNIT====================
               HPPUMP      < free >
               IFACE 506   < free >
               IFACE 606   < free >
               M819-Nr.1   < free >
               M819-Nr.2   < free >
----ENTER================================
                INIT     REMOVE    QUIT
```

After pressing ENTER and selecting IFACE 606 with the arrow keys, the component is set up with INIT. Choose the preset Unit-Id 61 by pressing OK. Now the following menu appears:

```
----CONFIG/UNITA/IFACE 606==============




========================================
   CONFIG-A  CONFIG-B  CHAR        QUIT
```

As the channel A is the default in many communications routines, the communication should be configured via the channel A. Via CONF-A, choose the configuration screen for channel A. Enter the values listed below:

```
----CONFIG/UNITA/IFACE 606/CONFIG-A=====
Baudrate    : < 9600 >
Parity      :   NONE
Data bits   :      8
Stop bits   :      1
Handshake   :   NONE
===========INPUT: CURSOR <- / ->========
   RESET                      OK    ABORT
```

Finally, you should check the presetting of the communications protocol under the menu CHAR in CONFIG/UNITS/IFACE 606. It should appear as follows:

```
----CONFIG/UNITA/IFACE 606/CHAR=========
CH.A Char START   :   /
     Char END     : BSlsh

CH.B Char START   :   /
     Char END     : BSlsh
========SELECTION: CURSOR <- / ->========
   RESET                      OK    ABORT
```

This completes the configuration of the IFACE 606. Quit the menu via QUIT. Choose QUIT again to terminate the component configuration. You will be prompted to save the changes.

The following screen will appear:

```
----ABIMED GYNK_231  3.15==DEFAULT.XCP==
231XL: 10/1230   RACKS: 0    ZONES: 0
DIL  :  0/1000
MP3  :
HPP  :
M506 :           M606: 61
=========NO PROGRAM===MEM: 80872========
  FILE   CONFIG   EDITOR   RUN   MANUAL
```

Now, the sample tray types and the sample zones must be set up. By pressing CONFIG again, you will return to the selection of the components previously set up.

```
----UNIT----Gynk_231/CONFIG--------------
  XYZ-ROBOT   231B V1.11      to ID: 10
  DILUTOR 1   402S V2.21      to ID:  0
  INTERFACE   606  V1.0       to ID: 61


---------ADD-/DEL-UNIT = <ENTER> --------
 ZDRIVE   RINSE    TRAY    VALVES    QUIT
```

After selecting XYZ-ROBOT, further configuration is via TRAY.

```
----Gynk_231/CONFIG/XYZ-ROBOT/TRAY------




=========================MEM: 79280 ====
          RACKS  ZONES  CHECK       QUIT
```

After the sample rack has been specified under the menu item RACKS, you can divide the rack in several ZONES. For a rack of the type 0 with a capacity of 80 samples, the division could be as follows:

```
=T  ZoneName    ===Vials=== ? SUM  Rack==
    SAMPLE_A       1-40     P 40   1-1
    RESULT_A  41    -80     P 40   1-1



===Racks:1===Vials:80===================
 APPEND   INSERT  DELETE  RUN-?    QUIT
```

The Dionex device driver supports two standard zone names, SAMPLE_A, and RESULT_A. Other source zones cannot be used for the sample extraction! This means that all inject samples of a batch run must be placed in one of the two sample zones!

The zones each contain 40 sample positions, numbered from 1 to 40 in a **Sample** file. In the above example, the sample 1 of the zone RESULT_A has the position 41. Of course, it is possible to set up and assign more zones on the rack (see selection list under the menu item APPEND or INSERT) to meet to individual requirements.

Caution: Samples to inject must always be located in SAMPLE_A or RESULT_A. The parameter **?** (see top line of display) must be set to **P**. This is achieved by repeatedly pressing RUN-? until **P** appears on the display.

Which source zone is used for the injection, is stated in the corresponding Gilson method file, the contents and significance of which is described below.

Caution: Under the Dionex Chromatography Management System the selected source zone must also be specified. This is by setting the corresponding properties. The default setting is SAMPLE_A.

The configuration settings required for the operation via the Dionex Chromatography Management System are now completed. After repeatedly pressing QUIT and saving the operation, the main screen appears again.

```
----ABIMED GYNK_231  3.15==DEFAULT.XCP==
231XL: 10/1230   RACKS: 1    ZONES: 2
DIL  :  0/1000
MP3  :
HPP  :
M506 :           M606: 61
=======NO PROGRAM=====MEM: 78824========
  FILE   CONFIG   EDITOR   RUN   MANUAL
```

Creating the Standard Task for Operating the Gilson Sample Preparation System with the Dionex Chromatography Management System

The two required minimum tasks for operating the **Gilson 231 XL Autosampler** device driver are described below.

Program for Method Selection

To access various injection methods (sub programs) from the Dionex Chromatography Management System, the following main program must be

created (for notes on using the editor refer to the Gilson user manual for the **Xtray** software!).

```
=========GYNK_231-EDITOR================
1 DoMethod606
< PRG-End >



======================MEM: 77072========
  CLIP    INSERT    DELETE    PARAM    QUIT
```

When inserting **DoMethod606**, only the communications channel must be set in the 606 Interface. Press CONFIG and set the 606-Channel parameter to **A**.

The main program is responsible for starting one of a maximum of 10 possible injection methods. The Dionex Chromatography Management System sends the name of a sub program to the main program. DoMethod606 loads the sub program that then controls sample processing. The sub program is active as long as the user explicitly selects another sample preparation method (sub program). Thus, the active sub program is interrupted. The sample preparation program returns to the DoMethod606 task and receives the name of the sample preparation method from the Dionex Chromatography Management System. DoMethod606 is quit only after choosing the **Disconnect** command of the Dionex Chromatography Management System.

The main program consists of a **DoMethod606** call. It is up to the user to start other tasks before and after DoMethod606. Ensure that DoMethod606 is running while the Dionex Chromatography Management System controls the sample preparation system.

The main program can be saved under any file name (extension **XCP**). Proceed as follows:

From the main menu, choose the FILE menu item. In the subsequently appearing selection menu, choose SAVE.

```
============FILE:DEFAULT.XCP==========
for DoMethod-Tasks (.XSP-File)
Tasklist without configuration:
LOAD=<1>  SAVE=<2>  LIST=<3>


======================MEM: 78768========
  LOAD    SAVE    LIST    LOCK    QUIT
```

Caution: For saving a main program (XCP files), use the function SAVE (F3). Via SAVE = <2> (key **2**), "sub programs" are generated with the extension **XSP**! See below for further information.

Injection Methods (Sub Programs)

In the Dionex Chromatography Management System, the injection method is selected via a property. As soon as this property is set in a PGM File or in the **Online**, DoMethod606 (in the main program) starts the corresponding sub program, the name of which must be **1.XSP**, **2.XCP** ... **10.XSP** in the file directory of the sample preparation system!

The minimum sub program appears as follows:

```
=========GYNK_231-EDITOR================
1 SendConf606
2 BeginLoop
3 InjectK606 RESULT_A
4 EndLoop
< PRG-End >
======================MEM: 76536========
  CLIP    INSERT    DELETE    PARAM    QUIT
```

It consists of two further tasks:

The task **SendConfig606** sends the parameter limits for the current sample preparation system to the Dionex Chromatography Management System at the beginning of the sub program. Thus, the Dionex Chromatography Management System can check the limits for the sample position and the injection volume.

The InjectK606 task within the loop <BeginLoop 1> ..... <EndLoop>. It receives the sample position and the injection volume from the Dionex Chromatography Management System. The loop is passed until the user replaces the old sub program by loading the new injection method.

The following steps are required for creating a **sub-program**:

- Start the editor.
- Delete the existing program.
- Insert the task **SendConf606**. Set the **606-Channel** parameter to **A**.
- Insert **BeginLoop**.
- Insert the task **InjectK606**. Set the parameters of this task via the following screen.

```
=========Task-3/InjectK606/PARAM========
```

```
=======================================
  TCONF   INJPAR1   INJPAR2   ->PAR2    QUIT
```

The following parameters must be set:

TCONF 'Sourcezone' to		'SAMPLE_A'	or
		'RESULT_A'	
INJPAR1	'606-Channel' to	'A'	
'Command - Echo' to		'AN'	

Configure the other parameters as described in the documentation for the Gilson Sample Preparation System Software.

- Insert **EndLoop**

Before InjectK606, the user can insert any tasks for sample preparation in the Begin... End loop. The InjectK606 task can be included only once in the loop.

When closing the editor the user is prompted whether changes should be saved immediately. It is important to select **Do not save** here. Otherwise, the "main program" will be overwritten. The "sub-program" must be saved via the **File** menu.

```
============FILE:DEFAULT.XCP==========
```

```
for DoMethod-Tasks (.XSP-File)
Task list without configuration:
LOAD=<1>  SAVE=<2>  LIST=<3>


======================MEM: 78768========
  LOAD    SAVE    LIST    LOCK    QUIT
```

After selecting the key <2>, choose **New** to save the "sub-program" under a new name (1.XSP to 10.XSP).

For information on the different loading and saving functions of the main and sub tasks, see the following paragraph.

Notes on Using the Editor of the Sample Preparation System

Before its extension for the Dionex Chromatography Management System, the sample preparation system recognized only task files with the extension **XCP**. With the introduction of sub programs, there are now XSP files the names of which are not correctly displayed in the title lines of the menu displays. After loading an **XSP2 File** in the **File** menu (function **1**), it is no longer possible to determine the name of the file currently in the editor, as the name of the last loaded XCP file is displayed. It is therefore necessary to consider the file type of the last opened file. Otherwise, saving a file may generate (not serious) or overwrite (serious) a file of another type!

Notes on the Operation via the Dionex Chromatography Management System

Before the Dionex Chromatography Management System is started, the main task must be activated on the Sample Preparation System.

Starting the Main Task

Perform the following steps:

- Use the **Load** function to load the main task in the **File** menu.
- Return to the main menu with **Quit** and press **Run**.
- Confirm all following prompts by <ENTER>.

- Press **Ok**. The program should now be ready to start. Decide whether to activate the audit of the sample preparation system or not.
- Then activate the program by pressing **Start**. In the display, the prompt of the method file name appears through the Method606 task.

Now, the sample preparation system is ready to receive the method name and other commands via RS232 from the PC of the Dionex Chromatography Management System.

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

GILSON INI File (Example)

The following example describes the structure of an INI File typical for Gilson ➢*Autosampler*. Select the INI File on the *INI File* tab (link available in the Online Help only). See the **Comment** section for a description of the individual lines.

Section		Comment
[Gilson-231]		
SamplerID = 10		GSIOC sampler address
DilutorID = 0		GSIOC address
Syringe = 500		Dilutor syringe volume
RackCode = 0		Rack code (to identify rack)
TriggerInject = 1		Determines which change from load to inject position will be interpreted as inject response
[Inject]		
1	INJECT 1	Rheodyne in inject position
2	RACK CODE 0	Rack code = 0
3	C0 = 1	Number of samples = 1
4	INPUT C1/1	Start position enquiry
5	IF C0 + C1 > 81	Safety condition
6	GOTO 3	
7	INPUT C2/31	Get inject volume
8	B3 = 1	B3 = variable for y coordinate

Section		Comment
9	FOR A = 1/5	Calculus of Y-(B3) and
10	B = C1 - 16	X-(C1) coordinates of sample position
11	IF B < 1	
12	GO TO 16	
13	C1 = C1 - 16	
14	B3 = B3 + 1	
15	NEXT A	
16	C9 =1	Variable for program start
17	C = 0	Set sample counter to 0
18	RINSE	Wash syringe needle outside
19	DISP. 0/500/9	
20	TUBE 0/0	Wash needle inside
21	DISP. 0/500/4	Wash inject port
22	FOR B = B3/5	Y- direction on rack
23	FOR A = C1/16	X- direction on rack
24	C = C + 1	Increment sample counter
25	PRINT C/1	Display sample number
26	IF C > C0	Reset condition
27	HOME	
28	TUBE A/B	Go to position A/B
29	HEIGHT	Move needle to maximum elevation
30	WAIT 2	Wait 2/100 min.
31	IF C9 = 1	Variable for program start
32	GO TO 34	
33	WAIT /3/0	Wait for address 3 to reach state 0
34	ASPIR 0/5/1	Draw 5 µl air
35	HEIGHT 0	Move needle to lowest position
36	ASPIR 0/C2 + 15/1	Draw inject volume + 15 µl
37	WAIT 2	Wait 2/100 min.
38	TUBE 0/0	Inject position
39	DISP 0/15/1	Wash dead volume with 15 µl sample solvent
40	WAIT 2	Wait 2/100 min.
41	INJECT 0	Move Rheodyne valve to load position
42	DISP 0/C2/1	Load sample volume to loop
43	WAIT 2	Wait 2/100 min.
44	INJECT 1	Rheodyne to inject position

Section	Comment
45 AUXIL 7/1	Start integrator
; 45 AUXIL 1/1	Command for device no. 203 994 and 203 995
46 WAIT 5	5/100 min. waiting time
47 AUXIL 7/0	Reset integrator start signal
; 47 AUXIL 1/1	Command for device No. 203 994 and 203 995
48 C9 = 2	Program continuation variable
49 DISP 0/500/9	Wash
50 RINSE	
51 DISP 0/500/9	
52 NEXT A	Next sample in X- direction
53 C1 = 1	Set X coordinate for next sample row
54 NEXT B	Next row
56 HOME	
*** END OF INJECT PROGRAM	

[Prog-0]
[Prog-1]
[Prog-2]
[Prog-3]
[Prog-4]
[Prog-5]
[Prog-6]
[Prog-7]
[Prog-8]
[Prog-9]

For an overview on the different Gilson instruments for which Dionex device drivers are available, see **Gilson**.

ISCO

FoxiJr Fraction Collector

Connecting the **ISCO FoxiJr Fraction Collector** to the Dionex Chromatography Management System is via a serial ➢*Modem Cable* (Dionex part no. 8914.0128 for a 25-pin port or Dionex part no. 8914.0144 for a 9-pin port) that must connect the following pins:

ISCO FoxiJr		PC	
25-pin (male)		25-pin (female)	9-pin (female)
		8 (cable shield)	1 (cable shield)
3	----------	3	2
2	----------	2	3
7	----------	7	5

As soon as a physical connection is established, the instrument and software installation can be started in the **Server Configuration**.

- Switch the instrument on and press the soft-key button B (**Config**) until the mode **Serial control = Off** appears in the display.
- Use the **Select** keys (**C** / **D**) to switch the mode on.
- Press the Enter key (**E**).
- Then set the baud rate via the **Select** keys (**C** / **D**) to 9600 baud. Press **Enter**.

Perform the software installation of the instrument in the **Server Configuration** of the Dionex Chromatography Management System by using the **ISCO_Foxi_Jr_Fraction_Collector** ➢*Device Driver*.

You now have the possibility to control the instrument via the ⇒*Connect/Disconnect*, Tube (= position of the collection container) and Valve (= switching between **Collect** and **Waste**) commands.

ISCO Foxi200 (Fraction Collector)

Controlling the ISCO **Foxi 200 Fraction Collector** under the Dionex Chromatography Management System requires the **ISCO Foxi 200 Fraction Collector** ➢*Device Driver*.

Connecting the fraction collector is via a standard ➢*Modem Cable* (Dionex part no. 8914.0128 for a 25-pin port or Dionex part no. 8914.0144 for a 9-pin port, no null modem cable!).

Please ensure that the baud rate is set to 9600. For information on setting the baud rate, see your Foxi200 manual.

Each Foxi200 has a unit ID (1 .. 7). Each ID can be controlled with the Dionex Chromatography Management System. The Dionex Chromatography Management System scans for all unit Ids during connect.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

JASCO

The following JASCO instruments can be controlled:

JASCO Autosamplers 950 and 1555

JASCO Detectors 970/975 (UV) and 920 (Fluorescence)

JASCO Pump 980 (LPG/HPG)

☞ ***Tip***: Controlling JASCO instruments requires the **Extended Device Control Option**. Select *About CHROMELEON* (link available in the Online Help only) in the Help menu of the Dionex Chromatography Management System client to check whether this option is available.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

JASCO Autosamplers 950 and 1555

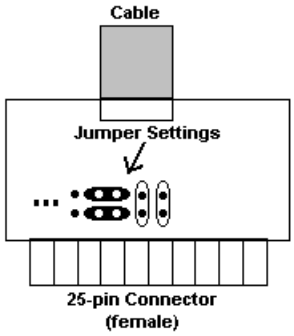
JASCO 950 and 1555 (Autosamplers)

Controlling the JASCO 950 and JASCO 1555 Autosamplers requires the **Jasco 950/1555_Sampler** ➢*Device Driver* to be installed in the **Server Configuration**.

The ➢*Autosamplers* are controlled via a serial interface cable (Dionex part no. 8914.0113 for a 25-pin port or Dionex part no. 8914.0134 for a 9-pin port) with the following pin assignment:

JASCO		PC	
		25-pin (female)	9-pin (female
2	----------	3	2
3	----------	2	3
7	----------	7	4
Internal:		Internal	Internal:
4 --- 5		4 --- 5	7 --- 8
6 --- 20			

Set the jumpers on the control board of the serial interface of the JASCO device (directly at the 25-pin serial female connector) as follows (very often the factory default setting is different!):



Otherwise, serial control will not be possible. As soon as there is a physical connection, the instrument and the software can be installed in the **Server Configuration**. Interface parameters: 4800 baud; 8 data bits; no parity; 2 stop bits; handshake XON.

For an overview on the different JASCO instruments for which Dionex device drivers are available, see **JASCO**.

JASCO Detectors 970/975 (UV) and 920 (Fluorescence)

Data Acquisition via the UCI-100 Universal Chromatography Interface

Data acquisition via an UCI-100 Universal Chromatography Interface additionally requires connecting the green wire (digital GND) of the UCI-100 analog cable to the REC/GND terminal of the JASCO UV detectors (or the REG/G terminal of the fluorescence detector, respectively.) In addition, the ground the UCI-100 analog cable to the detector housing (do not confuse with the REG/GND terminal - the shield ground, i.e. the knurled nut at the housing, is called GND as well.)

JASCO 970/975 (UV Detectors)

Controlling the JASCO 970 and 975 UV detectors under the Dionex Chromatography Management System requires the **Jasco970_UV_VIS_Detector** or **Jasco975_UV_VIS_Detector** device driver, respectively.

The required cable is a Dionex cable (Dionex part no. 8914.0113 for the 25-pin connection or Dionex part no. 8914.0134 for the 9-pin connection - for information on the pin assignment see **JASCO Autosamplers 950 and 1555**)

For information on the interface parameters, see the JASCO 950 Autosampler

JASCO 920 (Fluorescence Detector)

Controlling the JASCO 920 Fluorescence Detector under the Dionex Chromatography Management System requires the **Jasco920_Fluorescence_Detector** device driver.

For information on the serial interface cable and the interface parameters, see the JASCO Autosampler 950.

For an overview on the different JASCO instruments for which Dionex device drivers are available, see **JASCO**.

JASCO Pump 980

Controlling the JASCO 980 pump under the Dionex Chromatography Management System requires the **Jasco980 Pump** device driver.

Tip: Controlling the pump requires firmware version 2.60 or higher.

Connection of the Jasco 980 pump to the Dionex Chromatography Management System is via an RS 232 cable. That is why installation of an RS 232 module in the pump is required. A Dionex cable (Dionex part no. 8914.0113 for a 25-pin port or 8914.0134 for a 9-pin port) is used for the connection. For details on the pin assignment, see **JASCO Autosamplers 950 and 1555**.

The JASCO 980 pump is suitable for both, Low Pressure Gradients (LPG) and High Pressure Gradients (HPG):

LPG: Controlling a pump with the Dionex Chromatography Management System. The pump controls the solvent mixer, which is connected to the pump's **Low Pressure Grad**. output.

HPG: Controlling pump 1 with the Dionex Chromatography Management System. The pump controls additional pumps via LC-Net connections.

Tip: The setting whether the pump is operated as high pressure or low-pressure gradient pump has to be made directly at the pump (SHIFT 5 on the keypad).

Note: Due to the extremely slow communication between the Dionex Chromatography Management System and the pump, the execution of the flow command is delayed for several seconds. This can be compensated only by a correspondingly programmed method.

When the lower pressure limit is fallen below, the pump is switched off only after approx. two minutes as the tolerance time of the pump is correspondingly long.

For an overview on the different JASCO instruments for which Dionex device drivers are available, see **JASCO**.

KNAUER

The **Knauer UV Detector 2600** is connected via a standard RS232 cable (➢*Null Modem Cable* with 9-pin male connector on the instrument's side; Dionex part no. 8914.0103A for a 25-pin port or 8914.0129 for a 9-pin port). From the 2 RS232 ports on the instrument's rear panel use port 1.

Configure the instrument within the setup as described below:

1. Place the cursor in the Setup Menu using the "arrow keys."
2. Press the "arrow down" key seven times.
3. The Control Menu is displayed.
4. Press the "arrow right" key once and then the "arrow down" key until **RS232** is displayed. Further options are **KNAUER**.**NET**, **RS-485** and **analog**.
5. Press the "arrow right" key again to set the baud rate.
6. Press the "arrow down" key until 9600 baud is displayed.
7. Pressing the "arrow right" key once again and then the "arrow left" key returns you finally to the main status menu.

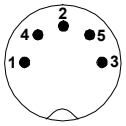
Install the detector in the **Server Configuration** using the **Knauer_UV_Detector_2600** ➢*Device Driver*.

***Note**:* The detector has two analog outputs for two wavelengths to be acquired simultaneously. As with the **KONTRON Detector 430**, an oscillating grating is used. The wavelength is 190 - 740 nm. By entering a wavelength of 0 nm, channels can be switched off. Thus, the oscillation of the grating is eliminated and the signal quality considerably enhanced. To enable an entry of 0 nm, the wavelength range offered by the Dionex device driver is between 0 nm to 740 nm. When values between 1 nm and 189 nm are entered, an error message is indicated in the audit trail. The message is displayed only at the running time and not yet during the Ready Check.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

KONTRON

Kontron instruments are connected via a special RS connecting cable (Dionex part no. 8914.0112 for a 25-pin connection or Dionex part no. 8914.0133 for a 9-pin connection). The pins of the Kontron diode connector (5-pin) must be connected to the pins of the 25-pin Sub-D-connector or 9-pin Sub-D connector as shown below:



1. CTS
2. GND
3. RxD
4. RTS
5. TxD

Kontron diode connector

KONTRON		PC (25-pin)
1	----------	4
2	----------	7
3	----------	2
5	----------	3
		Internal:
		5 --- 6 --- 20

KONTRON		PC (9-pin)
1	----------	7
2	----------	5
3	----------	3
5	----------	2
		Internal:
		4 --- 6 --- 8

The baud rate set on the unit must correspond to the baud rate specified in the Dionex device driver. Normally, the baud rate is 4800 bit/sec.

Caution: Upon power-up of the PC it may happen that incorrect characters are generated which the KONTRON instruments cannot handle. An error message is displayed and must be reset. Proceed as follows:

1. First, start your PC.
2. Wait until the booting is finished.
3. Start your instruments after booting.
4. Finally, start the server application.

If you are using the KONTRON ➢*Autosampler* 360, it may happen that due to those incorrect characters the sample position from the previous sample is taken as position for the current sample etc.

KONTRON Autosamplers 360/560 and 460

A separate ➢*Device Driver* is supplied for each instrument type (driver name: **Kontron 360/560 Autosampler** or **Kontron 460 Autosampler**).

Caution: If you are using the KONTRON Autosampler 360/560, it may happen that due to those incorrect characters described above the sample position from the previous sample is taken as position for the current sample etc. Therefore, proceed as described above when switching on your PC and your instruments.

Note: Some functions of the Autosampler 460 require the **Extended Device Control Option**. Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.

The Online Help assists you in establishing the *Syringe Type Kontron360* and the *Syringe Type Kontron460* in the **Server Configuration**. In addition, the Online Help describes the general settings (*General*) as well as the *Error Levels*.

KONTRON Autosampler 465

The Dionex Chromatography Management System supports the following additional commands of the Kontron Autosampler 465 enabling pre-column derivatization:

Command	Comment
StartPosition	Return to the start position
GetReagent	Draw a reagent from a defined position
Mix	Mixing
AddReagentAndMix	Add reagent and mix with sample
AirSegment	Draw air segment

Tip: Using these commands requires the **Extended Device Control Option**. Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.

Parameter	Comment
Position	Sample position
ReagentPosition	Reagent position
ReagentVolume	Reagent volume to be used
AirVolume	Air volume drawn after the syringe needle has been raised from the vial
MixingVolume	Mixing volume

KONTRON Pumps 322/325 (52X) and 420/422

There is a common device driver (**Kontron Pumps 32X and 52X**) for the Kontron gradient pumps 322 (high-pressure) and 325 (low-pressure). For the pump type 322, the number of solvents must be reduced from three (default) to two.

KONTRON Gradient Former 425

Controlling the KONTRON Gradient Former 425 requires the **Kontron 425 Gradient Former** device driver.

The Online Help supports you in setting the **Solvents** and the **Heads** in **Server Configuration**: *Solvents* and *Pump Heads*. In addition, the Online Help describes the general settings (*General*) as well as the *Error Levels*.

KONTRON Detectors 430/535 and 432 (332)

A separate device driver (**Kontron Detector 430**, **Kontron Detector 432**, and **Kontron Detector 535**) is available for each detector type. The models 430 and 535 differ only in the **Filter** property, which the type 535 additionally offers. Via the settings **Passive**, **Active** and **Automatic** the signal can be filtered. Controlling the detector type 332 requires the same device driver as the detector 432.

KONTRON Fluorescence Detector SFM 25

The SFM 25 is connected via a special RS232C cable (Dionex part no. 8914.0125 for a 25-pin connection or Dionex part no. 8914.0141 for a 9-pin connection) with the following pin assignment:

KONTRON SFM25 (25-pin)		PC (9-pin)
2	----------	2
3	----------	3
4	----------	1
5	----------	
6	----------	7
7	----------	5
8	----------	4
20	----------	6
Internal 4 --- 5		Internal: 7 --- 8

The **Autoblank** (zero value) and **Calibrate** (maximum value) commands of the Kontron SFM25 allow adjusting the range factor in the Dionex Chromatography Management System.

Install the instrument in the installation program (= **Server Configuration**) via the **Kontron_SFM25_Fluorescence_Detector** device driver.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

KRATOS

Controlling the Kratos UV Detector Spectroflow 783 under the Dionex Chromatography Management System requires the **Kratos Spectroflow 783 UV Detector** ➢*Device Driver*.

The instrument is connected to the server PC via a special RS connecting cable (Dionex part no. 8914.0116 for a 25-pin connection or Dionex part no. 8914.0136 for a 9-pin connection).

The pin assignment is as follows:

KRATOS Spectroflow		PC	
(9-pin SUB-D connector)		(25-pin)	(9-pin)
1	----------	7	5
3	----------	2	3
4	----------	3	2
		Internal:	Internal:
		4 --- 5	7 --- 8

For connecting the instrument, use the 9-pin port labeled **SERIAL A** on the rear of the instrument.

For optimum operation via the RS232 port, the **Baud Rate** (9600 baud) and **Response Delay** (4/60 sec) parameters must be set on the instrument (see Detector manual).

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

MERCK HITACHI

Various Merck HPLC pumps and several Merck ➢*Autosamplers* can be controlled:

1. **MERCK HITACHI Pumps**

L6200/L6210 (Device Driver: Merck Hitachi L6200/L6210 Pump)

(Also, see **MERCK HITACHI: Pumps - Program Example**)

L6250 (Device Driver: Merck Hitachi L6250 Pump

L7100 (Device Driver: Merck Hitachi L7100 Pump)

2. MERCK HITACHI Autosamplers

AS2000 (Device Driver: Merck Hitachi AS2000 Autosampler)

AS4000 (Device Driver: Merck Hitachi AS4000 Autosampler)

L7250 (Device Driver: Merck Hitachi L7250 Autosampler (controlled via RS232) and Merck Hitachi L7200/L7250 AS (D-Line) (controlled via D-Line))

L7200 (Device Driver: Merck Hitachi L7200/L7250 AS (D-Line))

Settings and Commands for the Different Autosamplers

3. MERCK HITACHI UV-VIS Detector

L4250 (Device Driver: Merck Hitachi L4250 Detector)

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

MERCK HITACHI: Pumps L6200/L6210 and L6250

MERCK HITACHI L6200 and L6210 (HPLC Pumps)

The Dionex Chromatography Management System provides the **Merck Hitachi L6200/L6210 Pump** ➢*Device Driver* as common driver with all-important functions for the MERCK HITACHI L6200 and L6210 pumps. Please note the following:

- The connection is via a special serial RS232 cable (Dionex part no. 8914.0111 for a 25-pin connection or Dionex part no. 8914.0132 for a 9-pin connection) that must connect the following pins (➢*Null Modem Cable*):

MERCK HITACHI L62xx Pumps		PC (25-pin)	PC (9-pin)
2	----------	3	3
3	----------	2	2
7	---------	7	7
Internal:		Internal:	Internal:
4 connected to 5		5 connected to 4	7 connected to 8

- In addition, the switch on the back of the unit must be switched to the **Remote** position. Switch 1 on the horizontal board inside must have the following settings:

Switch 1	1	2	3	4	5	6
	Off	On	On	On	Off	Off

- Switching from high-pressure to low-pressure gradient is performed on the instrument itself. For the high-pressure gradient, a L6000 pump (slave pump) must be connected to the Hitachi I/O-bus. The Dionex Chromatography Management System is not capable of checking this!
- For the pump type L6210 (inert pump), a pressure limit of 145bar must be entered in the **Server Configuration**. Otherwise, the pump ignores all flow commands. The maximum pressure of the L6200 pump is 400bar.

In addition, the Online Help offers support for setting the **Limits** and **Solvents** in the ➢*Server Configuration* program: *Pump Heads and Limits* and *Solvents*. Besides, the Online Help describes the general settings (*General*) as well as the *Error Levels*.

MERCK HITACHI HPLC Pump L6250

Controlling the MERCK HITACHI HPLC Pump L6250 under the Dionex Chromatography Management System requires the **Merck Hitachi L6250 Pump** device driver. To start the pump, please note the following:

The connection is established via the same pin assignment, which is valid for the L6200 pump. In addition, the settings of switch 1 are the same as for the L6200 pump.

For optimum performance, set the upper pressure limit to 147 bar.

In addition, the Online Help offers support for setting the **Limits** and **Solvents** in the **Server Configuration**: *Pump Heads and Limits* and *Solvents*. Besides, the Online Help describes the general settings (*General*) as well as the *Error Levels*.

For a program example for Merck Hitachi pumps, see **MERCK HITACHI: Pumps - Program Example**

For information on installing the Merck Hitachi Pump L7100, see:

MERCK HITACHI Pumps: L7100

For information on installing the Merck Hitachi Autosamplers, see:

MERCK HITACHI Autosampler: AS2000/AS4000

MERCK HITACHI Autosampler: L7250

MERCK HITACHI Autosampler: L7200.

For information on how to install the UV-VIS detector L4250, see **MERCK HITACHI UV-VIS Detector L4250**

For an overview on Merck Hitachi instruments for which Dionex device drivers are available, see:

MERCK HITACHI

MERCK HITACHI: Pumps - Program Example

To avoid overloading the Merck pumps with too fast a sequence of commands, allow for at least 0.1 min between the individual commands. For a program example for the L6200 pump, see below:

```
-0.100   Pressure.LowerLimit =   0
   Pressure.UpperLimit =   400
   %A.Equate =    "%A"
   %B.Equate =    "%B"
   %C.Equate =    "%C"
;******* Detector commands: ****************
   UV_VIS_1.Mode =   UV
   UV_VIS_1.Range =  0.200
   UV_VIS_1.Response =  1.0
   UV_VIS_1.Step =   Auto
   UV_VIS_1.Average =   On
   UV_VIS_1.Wavelength =   260

 0.000   UV_VIS_1.Autozero
   Flow =   1.000
   %B =  10
   %C =  0
   Inject
   UV_VIS_1.AcqOn
   Flow =   1.000
   %B =  10
   %C =  0

;The gradient starts after 0.1 minutes to avoid overload the pump with
too fast a sequence of commands:
```

```
0.100 %B =  10

10.000   %B =  90

15.000   %B =  90

16.000   %B =  10

30.000   UV_VIS_1.AcqOff
   Flow =   1.000
   %B =  10
   %C =  0

   End
```

For information on installing the Merck Hitachi pumps (L6200/L6210 and L6250), see **MERCK HITACHI Pumps.**

MERCK HITACHI: Pump L7100

Controlling the MERCK HITACHI L7100 pump under the Dionex Chromatography Management System requires the **Merck Hitachi L7100 Pump (D-Line)** ➢*Device Driver*.

☞ ***Tip***: Controlling this instrument requires the **Extended Device Control Option**. Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.

In addition, please note the following:

The HPLC pump L7100 must be connected to a D-line converter via a D-line cable. Use the upper D-line socket of the L7100 (label **RELAY BOX**), only this socket of the D-line converter has current supply. The D-line converter itself is connected via a conventional null modem cable (for the Dionex part nos., see ➢*Null Modem Cable*) with a free COM port of the controlling PC.

D-Line Converter		PC (25-pin)	PC (9-pin)
2	----------	2	3
3	----------	3	2
5	----------	7	5

The driver uses the default settings of the D-line converter for the serial communication: 4800 Baud, 8N1. To check: this setting is currently used if the DIP-switch settings on the board inside the D-line converter are as follows:

Switch 1	1	2	3	4	5	6
	Off	Off	On	On	On	Off

Notes:

- To operate the pump L7100 in stand-alone mode, without D-line connection: Press the **Utility** key while switching the pump on. Use the displayed menus to remove D-line operation from the configuration. See also the manual for the L7100.
- The D-line converter does not support the **Disconnect** command. After successfully connecting the pump (the display changes from **D-LINE SYSTEM IS NOT READY** to the flow display), the D-line system cannot be de-initialized. **Pump.Disconnect** only stops the pump and sets the status of **Pump.Connected** to **disconnected**.
- The pump L7100 does not support locking the keyboard. Even during control via the D-line and the Dionex Chromatography Management System, it would be possible to perform all actions directly via the pump. However, this is not recommended during controlled operation. If the driver detects keyboard operation, a corresponding warning is included in the Audit Trail.
- Occasionally, there are deviations between the values indicated on the display of the pump and the values of the corresponding properties of the Dionex Chromatography Management System. These deviations are due to the pump's firmware. Sometimes, the firmware does not supply the displayed value for status requests via D-line. However, the deviations are negligible rounding errors.

- The **Extended Device Control** feature is required for the L7100 device driver.

In addition, the Online Help offers support for setting the **Limits** and **Solvents** in the **Server Configuration**: *Pump Heads and Limits* and *Solvents*. Besides, the Online Help describes the general settings (*General*) as well as the *Error Levels*.

For information on installing other Merck Hitachi pumps (L6200/L6210 and L6250), see:

MERCK HITACHI Pumps: L6200/L6210 and L6250).

For information on installing the MERCK HITACHI Autosamplers, see:

MERCK HITACHI Autosampler AS2000/AS4000

MERCK HITACHI Autosampler 7250

MERCK HITACHI Autosampler L7200

For information on how to install the UV-VIS detector L4250, see **MERCK HITACHI UV-VIS Detector 4250**

For an overview on the different MERCK HITACHI instruments for which Dionex device drivers are available, see:

MERCK HITACHI

MERCK HITACHI: Autosamplers AS4000 and AS2000

Controlling the Merck Hitachi ➢*Autosamplers* AS4000 and AS2000 requires the **Merck Hitachi AS4000 Autosampler** or **Merck Hitachi AS2000 Autosampler** ➢*Device Driver*.

Control is via the special serial RS232 interface cable (Dionex part no. 8914.0111 for the 25-pin port or Dionex part no. 8914.0132 for the 9-pin port) which is described in detail under **MERCK HITACHI Pumps: L6200/L6210 and L6250**).

Caution: For information on the communication via serial interface, see the appropriate Autosampler Manual. Especially note the settings of the 6-fold communications DIP-switch on the rear of the instrument.

The following settings are required for the AS4000/AS2000 for the **COM** mode (serial communication):

Switch	1	2	3	4	5	6
	Off	On	On	Off	Off	Off

Communication is enabled with the following parameters: 4800 baud, 7 data bits, even parity bit, and 2 stop bits.

Differences between AS 4000 and AS2000

The two autosamplers AS4000 and AS2000 only differ in three parameters:

Parameter	AS2000	AS4000
Sample number	100	200
Dilutor number	2	1
Syringe size (µl)	500	5000

The Online Help illustrates the two **Server Configuration** pages on these autosamplers: *General* and *Error Levels*.

For information on installing other Merck Hitachi autosamplers, see:

MERCK HITACHI: Autosampler L7250

MERCK HITACHI: Autosampler L7200.

For information on installing Merck Hitachi pumps, see:

MERCK HITACHI: Pumps L6200/L6210 and L6250

MERCK HITACHI: Pump L7100

For information on how to install the UV-VIS detector L4250, see **MERCK HITACHI UV-VIS Detector L4250**

For an overview on the different MERCK HITACHI instruments for which Dionex device drivers are available, see **MERCK HITACHI**.

MERCK HITACHI: AS4000 - Program Example

To avoid stressing the Merck ➢*Autosamplers* with a fast succession of commands, allow at least for 0.1 min between the individual commands. A program example for the AS4000 could look as follows:

```
;******* Pump Commands: ***************
        Pressure.LowerLimit = 2
   Pressure.UpperLimit =   200
   %A.Equate =    "Water"
   %A.Type =   Automatic

;******* Detector Commands: ***************
   UV_VIS_1.Wavelength =   254
   UV_VIS_1.Bandwidth =    1
   UV_VIS_1.Step =   0.20
   UV_VIS_1.Average =   On
   UV_VIS_1.RefWavelength =   600
   UV_VIS_1.RefBandwidth =    1

   Flow =   0.300

;******* Autosampler Commands: ***************
;(Allow for at least 0.1 min between the individual commands to avoid
stressing the autosampler with a rapid succession of commands)
-2.100   Home
   Wash


-1.600   LeadVolume = 30.0
-1.550   RearVolume = 30.0

-1.500   Height Z = 0.0, NeedleSpeed = Fast
        Aspirate  DilutorNumber = 1, SyringePos = 5.0, PlungerSpeed =
        VeryFast
;Aspirate 5 µl air

   GotoTube RackCode = 1, TubeNumber = Position
;Go to the sample vial
        Aspirate  DilutorNumber = 1, SyringePos = LeadVolume + Volume +
        RearVolume, PlungerSpeed = VeryFast
;Aspirate sample from sample vial
```

```
Height Z = 0.0, NeedleSpeed = Fast
       Aspirate  DilutorNumber = 1, SyringePos = 5.0, PlungerSpeed =
       VeryFast
;Aspirate 5 µl air

-1.000   GotoWashPort
;Wash outside of needle

-0.500   GotoInjectPort
       Dispense  DilutorNumber = 1, SyringePos = 5.0 + LeadVolume +
       14.9, PlungerSpeed = VeryFast
;Dispense air + leadVolume + dead volume
   GotoValvePos   ValvePos = Load
       Dispense  DilutorNumber = 1, SyringePos = Volume, PlungerSpeed =
       VeryFast
;Dispense injection volume

   Syringe = -1

0.000 UV.Autozero
   Inject
   UV_VIS_1.AcqOn
;do not execute another program, Inject switches the valve only
   GotoWashPort
   Home

8.000 UV_VIS_1.AcqOff

   End
```

MERCK HITACHI: Autosampler L7250

Controlling the Merck Hitachi ➢*Autosampler* L7250 requires the **Merck Hitachi L7250 Autosampler** ➢*Device Driver*.

Tip: Some functions of this instrument require the **Extended Device Control Option**. Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.

Instrument connection is via a special serial RS232 cable (Dionex part no. 8914.0111 for the 25-pin port or Dionex part no. 8914.0132 for the 9-pin port).

The following pins must be connected:

MERCK HITACHI L 7250		PC	
(9-pin Sub-D female)		(25-pin, Sub-D female)	(9-pin, Sub-D female)
2	----------	2	3
3	----------	3	2
5	----------	7	5
Internal:		Internal:	Internal:
7 - 8		4 - 5	7 - 8

Choose the following communications settings, as described in the **Instruction Manual, Advanced Operation**:

- Switch the instrument off.
- Press UTILITY and simultaneously switch the instrument on.
- Set the following parameters:

Baud rate:	4800
Data bits:	7
Parity:	Even
Stop bits:	2
Termination:	CR

- Switch the instrument off.

Caution: In contrast to the AS 4000, only dilutor 1 is supported. For the **Move Needle** command, there are different maximum values (x = 156, y = 156, z = 57).

The Online Help provides information on the two **Server Configuration** pages for these autosamplers: *General* and *Error Levels*.

For information on installing other Merck Hitachi autosamplers, see:

MERCK HITACHI: Autosampler AS2000/AS4000

MERCK HITACHI: Autosampler L7200.

For information on installing Merck Hitachi pumps, see:

MERCK HITACHI: Pumps L6200/L6210 and L6250

MERCK HITACHI: Pumps L7100

For information on how to install the UV-VIS detector L4250, see **MERCK HITACHI UV-VIS Detector L4250**

For an overview on the different MERCK HITACHI instruments for which Dionex device drivers are available, see **MERCK HITACHI**.

MERCK HITACHI: Autosampler L7200

Controlling the Merck Hitachi ➢*Autosampler* L7200 requires the **Merck Hitachi L7200/L7250 AS (D-Line)** ➢*Device Driver*.

Tip: Controlling this instrument requires the **Extended Device Control Option**. Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.

Instrument connection is via a special serial RS232 cable (Dionex part no. 8914.0111 for the 25-pin port or Dionex part no. 8914.0132 for the 9-pin port) and a D-Line converter (for details about D-Line cabling and communication setup please see **MERCK HITACHI: Pumps L7100**

Due to limitations in the D-Line command set, only the following basic operations are supported:

- **Connect** (see: ⇒*Connect/Disconnect*)
- **Disconnect** (disconnects sampler from the Dionex Chromatography Management System but does not disconnect sampler from D-Line control)
- ⇒*Inject* (with the **Vial Number** and **Sample Volume** parameters)
- **Sampler busy**

Note: The Merck Hitachi L7200/L7250 AS(D-Line) device driver can also be used to control a L7250 Autosampler that is connected to a D-Line system. However, controlling L7250 autosamplers via RS232 (see above) is preferred.

In addition, the Online Help offers support regarding the two **Server Configuration** pages: *Rack* and *Syringe*. Besides, the Online Help describes the general settings (*General* tab) as well as the *Error Levels*.

For information on installing other Merck Hitachi autosamplers, see:

MERCK HITACHI Autosampler AS2000/AS4000

MERCK HITACHI Autosampler: L7250.

For information on installing Merck Hitachi pumps, see:

MERCK HITACHI: Pumps L6200/L6210 and L6250

MERCK HITACHI: Pumps L7100

For information on how to install the UV-VIS detector L4250, see **MERCK HITACHI UV-VIS Detector L4250**

For an overview on the different MERCK HITACHI instruments for which Dionex device drivers are available, see **MERCK HITACHI**.

MERCK HITACHI: Settings and Commands for the Different Autosamplers

Supported Autosampler

For ➢Autosampler …	…controlled via…	…use device driver
AS2000	RS232	Merck Hitachi AS2000 Autosampler
AS4000	RS232	Merck Hitachi AS4000 Autosampler
L7250	RS232	Merck Hitachi L7250 Autosampler
L7250	D-Line	Merck Hitachi L7200/L7250 AS (D-Line)*
L7200	D-Line	Merck Hitachi L7200/L7250 AS (D-Line)

* The Merck Hitachi L7200/L7250 AS (D-Line) device driver requires the **Extended Device Control Option**.

Supported Device Properties

	AS2000	AS4000	L7250	L7200
InjectPortWashs	0-20	0-20	0-20	0-20³
InjectPortWashSpeed	1 (Low) ... 5 (High)	1 (Low) ... 5 (High)	1 (Low) ... 5 (High)	1 (Low) ... 5 (High)3
NeedleWashs	1-20	1-20	1-20	1-20³
NeedleWashSpeed	1 (Low) ... 5 (High)	1 (Low) ... 5 (High)	1 (Low) ... 5 (High)	1 (Low) ... 5 (High)³
WasteVolume	Not supported	Not supported	0-4000.0 µl	0-4000.0 µl²
WashVolume	10.0-100.0 µl	10.0-1000.0 µl	10.0-1000.0 µl	
LeadVolume	0-100.0 µl	0-1000.0 µl	0-1000.0 µl	0-500.0 µl²
RearVolume	0-100.0 µl	0-1000.0 µl	0-1000.0 µl	0-500.0 µl²
FeedVolume	0-100.0 µl	0-1000.0 µl	0-1000.0 µl	0-500.0 µl²
DeadVolume	0-100.0 µl	0-1000.0 µl	0-1000.0 µl	
Syringe	0-100.0 µl	0-1000.0 µl	0-1000.0 µl	
InjectionMethod	0 (Compatibility) 1 (Cut) 2 (All)	0 (Compatibil.) 1 (Cut) 2 (All)	0 (Compatibil.) 1 (Cut) 3 (FullLoop)	1 (Cut) ... 3 (FullLoop)²
SyringeSpeed	1 (Low) ... 5 (High)	1 (Low) ... 5 (High)	1 (Low) ... 5 (High)	
NeedleDownSpeed	1 (Slow) ... 2 (Fast)	1 (Slow) ... 2 (Fast)	1 (Slow) ... 2 (Fast)	1 (Slow) ... 2 (Fast)
VolSyringe	1 (100µl) - 2 (500 µl)	1 (100 µl) - 5 (5000 µl)	1 (100 µl) - 5 (5000 µl)	Not supported
PumpPlungerWash	Not supported	Not supported	0 (No) or 1 (Yes)	0 (No) or 1 (Yes)³
VolOptionalSyringe	Not supported	1 (100 µl) - 5 (5000 µl)	Not supported	Not supported
NumberOfDilutors	Not supported	1 or 2	Not supported	Not supported
Dilutor	Not supported	1 or 2	Not supported	Not supported
RackCode	1 - 16	1 - 16	1 - 16	Not supported
⇒*Volume*	1 - 500.0 µl	1 - 5000.0 µl	1 - 5000.0 µl	1 - 500.0 µl
⇒*Position*	1 - 100	1 - 200	1 - 200	1 - 200

² If one of these properties is set, all other settings that are marked with ² are set, too. Check the parameters sent to the autosampler with extra care.

³ If one of these properties is set, all other settings that are marked with ³ are set, too. Check the parameters sent to the autosampler with extra care.

Supported Device Commands

	AS2000	AS4000	L7250	L7200

⇒Connect (/Disc.)	Supported	Supported	Supported	Supported
Disconnect	Supported	Supported	Supported	Not supported
Aspirate (see ⇒Draw)	0 - 500.0 µl, Speed	Dilutor, 0 - 5000.0 µl, Speed	0 - 5000.0 µl, Speed	Not supported
⇒Dispense	0 - 500.0 µl, Speed	Dilutor, 0-5000.0 µl, Speed	0-5000.0 µl, Speed	Not supported
GotoTube	1 - 100, RackCode	1 - 200, RackCode	1 - 200, RackCode	Not supported
GotoWashPort	Supported	Supported	Supported	Not supported
GotoInjectPort	Supported	Supported	Supported	Not supported
MoveNeedle	X:0-163.0 mm	X:0-244.0 mm	X:0-156.0 mm	Not supported
	Y:0-68.0 mm	Y:0-163.0 mm	Y:0-156.0 mm	
	Z:0-38.0 mm	Z:0-57.0 mm	Z:0-57.0 mm	
Height	Z:0-38.0 mm	Z:0-57.0 mm	Z:0-57.0 mm	Not supported
GotoSyringePos	0 - 500.0 µl, Speed	Dilutor, 0-5000.0 µl, Speed	0 - 5000.0 µl, Speed	Not supported
GotoSValvePos	0 (Bottle) or 1 (Needle)	Dilutor, 0 (Bottle) or 1 (Needle)	0 (Bottle) or 1 (Needle)	Not supported
GotoValvePos	0 (Inject) or 1 (Load)	0 (Inject) or 1 (Load)	0 (Inject) or 1 (Load)	Not supported
Home	Supported	Supported	Supported	Not supported
Reset	Supported	Supported	Supported	Supported
Wash	Supported	Supported	Supported	Not supported
WashPumpPlunger	Not supported	Not supported	Supported*	Not supported
Inject	Supported - see below	Supported - see below	Supported - see below	Supported
Wash_X	Supported - see below	Not supported	Supported - see below	Not supported
WashDil_X	Not supported	Supported - see below	Not supported	Not supported
GotoOpValvePos	Not supported	Not supported	0 (Inject) or 1 (Load)*	Not supported

* Executing these properties requires the **Extended Device Control**  **Option**.

Inject Programs:

AS2000
AS4000
L7250

Depending on the current value of the **Syringe** device property, three different programs are internally executed during processing an ⇒*Inject* command. For AS2000 and L7250 the dilutor property always equals 1.

Syringe>0
- GotoSyringePos SyringePos=0
  - Speed=<*current value of property* ***Speed***>
  - Dilutor=<*current value of property* ***Dilutor***>
- GotoSValvePosSValvePos=Bottle
  - Dilutor=<*current value of property* ***Dilutor***>
- GotoSyringePos SyringePos=<*current value of property* ***Syringe***>
  - Speed=<*current value of property* ***Speed***>
  - Dilutor=<*current value of property* ***Dilutor***>
- GotoTube TubeNumber=<*current value of property* ***Position***>
  - RackCode=<*current value of property* ***RackCode***>
- Aspirate AspirateVol=<*current value of property* ***Volume***>
  - Speed=<*current value of property* ***Speed***>
  - Dilutor=<*current value of property* ***Dilutor***>
- GotoInjectPort
- GotoValvePos ValvePos=Load
- GotoSyringePos SyringePos=0
  - Speed=<*current value of property* ***Speed***>
  - Dilutor=<*current value of property* ***Dilutor***>
- GotoValvePos ValvePos=Inject

Syringe=0
- GotoTube TubeNumber=<*current value of property* ***Position***>
  - RackCode=<*current value of property* ***RackCode***>
- Aspirate AspirateVol=<*current value of property* ***Volume***>
  - Speed=<*current value of property* ***Speed***>
  - Dilutor=<*current value of property* ***Dilutor***>
- GotoInjectPort
- GotoValvePos ValvePos=Load
- GotoSyringePos SyringePos=0
  - Speed=<*current value of property* ***Speed***>
  - Dilutor=<*current value of property* ***Dilutor***>
- GotoValvePos ValvePos=Inject

Syringe<0
- GotoValvePos ValvePos=Inject

L7200

Based on the current parameter settings, the autosampler performs an injection. The **Inject** command transmits the vial number and the sample volume only.

Wash Programs:

AS2000
AS4000
L7250

This is the program that is run when the extended wash command (Wash_X resp. WashDil_X) is executed. For AS2000 and L7250 the dilutor property always equals 1.

GotoWashPort
GotoSValvePosSValvePos=Bottle
  Dilutor=<*current value of property* ***Dilutor***>
GotoSyringePos SyringePos=<*current value of property* ***Syringe***>
  Speed=<*current value of property* ***Speed***>
  Dilutor=<*current value of property* ***Dilutor***>
GotoSValvePosSValvePos=Needle
  Dilutor=<*current value of property* ***Dilutor***>
GotoSyringePos SyringePos=0
  Speed=<*current value of property* ***Speed***>
  Dilutor=<*current value of property* ***Dilutor***>
GotoInjectPort
GotoSValvePosSvalvePos=Bottle
  Dilutor=<*current value of property* ***Dilutor***>
GotoSyringePos SyringePos=<*current value of property* ***Syringe***>
  Speed=<*current value of property* ***Speed***>
  Dilutor=<*current value of property* ***Dilutor***>
GotoSValvePosSValvePos=Needle
  Dilutor=<*current value of property* ***Dilutor***>
GotoSyringePos SyringePos=0
  Speed=<*current value of property* ***Speed***>
  Dilutor=<*current value of property* ***Dilutor***>

L7200

not supported

For details on how to install the different autosampler types, see the following topics:

AS2000

AS4000

L7250

L7200

MERCK HITACHI: UV-VIS Detector L4250

Controlling the Merck Hitachi UV-VIS Detector L4250 requires the **Merck Hitachi L4250 Detector** ➢*Device Driver*.

Instrument connection is via a special serial RS232 cable (Dionex part no. 8914.0111 for the 25-pin port or Dionex part no. 8914.0132 for the 9-pin port) that must connect the following pins:

MERCK HITACHI L4250		PC	
(25-pin male)		(25-pin female)	(9-polig female)
2	----------	3	3
3	----------	2	2
5	----------	5	5
internal		internal:	internal:
4 connected to 5		5 connected to 4	7 connected to 8

The PAN-RS232C switch on the back of the unit must be switched to the **RS232C** position. DIP-switch 2 (labeled **Mode**) must have the following settings:

Switch 1	1	2	3	4	5	6
	Off (down)	On (up)	On	On	Off	Off

For further information on the **Server Configuration**, see *General*, *UV_VIS_X*, and *Error Levels* in the Online Help.

For information on installing other Merck Hitachi autosamplers, see:

MERCK HITACHI Autosampler AS2000/AS4000

MERCK HITACHI Autosampler: L7250.

For information on installing Merck Hitachi pumps, see:

MERCK HITACHI: Pumps L6200/L6210 and L6250

MERCK HITACHI: Pumps L7100

For an overview on the different MERCK HITACHI instruments for which Dionex device drivers are available, see **MERCK HITACHI**.

NELSON Interfaces

The Dionex Chromatography Management System offers two ➢*Device Drivers* to control different Nelson boxes:

The **Nelson 941 Interfaces** driver supports the PE Nelson Interfaces Type 941 and 901 or 902 (NCI 900).

The **Nelson 950/960/970** driver supports the PE Nelson Interfaces Types 950, 960, and 970.

Caution: At present, no drivers are available for the type 940 and all previous types (with 700 or 800 numbers). In addition, no driver is available for the **Perkin Elmer Analytical Interface**. (For the exact type name, see the instrument's rear panel.)

For details on the Nelson device drivers, see the following topics:

NELSON Interfaces: Pin Assignment

NELSON Interfaces: Device Driver Configuration

NELSON Interfaces: Properties

NELSON Interfaces: Data Acquisition Restrictions

NELSON Interfaces: Differences from Conventional Nelson Box Installations

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

NELSON Interfaces: Pin Assignment

RS Cable

The pin assignment of the serial cable varies for the different types.

The type 941 is fitted with a 25-pin male connector:

PC		Nelson 941
25-pin connector	**9-pin connector (Alternative)**	**25-pin connector**
1	Ground	1
3	2	2
2	3	3
7	5	7

This is a standard null modem cable (for the Dionex part nos. see: ➢*Null Modem Cable*).

The types 950, 960, and 970 are fitted with a 25-pin female connector.

The cable must connect the pins 1, 2, 3, 4, 5, and 7 of this connector with the same pins of the 25-pin male connector on the PC (i.e. not crossed, with hardware handshake).

PC		Nelson 950 - 970
25-pin connector	**9-pin connector (Alternative)**	**25-pin connector**
1	Ground	1
2	3	2
3	2	3
4	7	4
5	8	5
7	5	7

This is a modem cable (for the Dionex part nos., see ➢*Modem Cable*).

For the serial interface, the **type 901** is fitted with an RJ45 connector:

PC		Nelson 941
25-pin connector	**9-pin connector (Alternative)**	**RJ45 connector**
2	3	6
3	2	3
7	5	4-5

Set the **DIP-switches** 6 and 7 to ON, all other DIP-switches to OFF.

The Nelson Box 901 is a one-channel version. Therefore, do not install the second channel, which is provided by the driver. As standard, the Nelson Box 901 has two relays only (Ready and Relay #1) but the 941 driver also knows relays 2-7, which, however, are optionally available only.

Start, Stop, Ready

The start input is intended for the sampler start signal (inject response). Normally, the assignment of the previous installation (e.g. ACCESS*CHROM) can be used.

The stop input is intended for the stop signal to terminate the data acquisition. As the Dionex Chromatography Management System does not support this option, any connected cable should be removed.

The Ready output informs the instruments that the box and the data system are ready for injection and for data acquisition. Under the Dionex Chromatography Management System, this signal is activated with the **Inject** command and is deactivated as soon as the inject response is returned. If possible, this cable should be connected. Exception: If a separate Dionex device driver controls the sampler, the sampler should not be connected to the **Ready** output. The reason for this is that the sampler may not inject, since the **Ready** line is not cleared.

Channels A-B and Relays 1-7

Normally, the assignment of the previous installation can be used.

Rack/Vial Port

The Dionex Chromatography Management System uses this port to read the sample position. For the assignment, see the manual for the box. Please note that the pin assignment is as follows. Left row from top to bottom: 1 to 8; right row: 9 to 15. Normally, the assignment of the previous installation can be used.

For the Nelson Box 901, the rack/vial port is optionally available, only.

For further information on the Nelson Interfaces, see:

- **NELSON Interfaces**
- **NELSON Interfaces: Device Driver Configuration**
- **NELSON Interfaces: Properties**
- **NELSON Interfaces: Data Acquisition Restrictions**
- **NELSON Interfaces: Differences from Conventional Nelson Box Installations**

NELSON Interfaces: Device Driver Configuration

In the default configuration (set only the COM port, use all other presetting), the device driver supplies all functions for a non-controlled timebase. The **Remote Inject** and the **Integrator** are virtually integrated. Installing a serial sampler or detector device driver is also possible. In this case, the included device drivers must be deactivated to clear the corresponding ports for the other device drivers.

Integrated "Remote Inject"

The integrated **Remote Inject** device driver is configured on the **Remote Inject** tab.

If **Read Sample Position from Rack & Vial Port** is selected, the sample position is read from the port (RVP) immediately after injection. The following options are available:

- Select **Invert Inputs** if the meaning of **True** and **False** is inverted (e.g., if position 1 is read as 4094 (= 3FFEh)).
- **Mask** should only be changed if further signals not related to the sampler position are connected to the RVP (this is a Hex number that is linked via **and** to the value read by the RVP).
- Set **Encoding** to **binary** if the sampler performs binary coding of the sampler position (This is not common, otherwise position 16 is read as 10).

Using a Different Sampler Device Driver

If a different sampler device driver is used, the integrated **Remote Inject** driver should be deactivated. In this case, the start input of the box is available as **RemoteStart** port for other drivers using a digital **Inject Response**. This port should then be used instead of an AD board input. The **Inject** command of the sampler activates the ready line of the box, as with the integrated **Remote Inject**.

For device drivers using a serial **Inject Response** (no **Inject Response** port can be set here - this applies to most sampler device drivers), the **Inject** command of the sampler does not activate the ready line.

Integrated Channels

When configuring the integrated channels (on the **Signals** tab), the **Server Configuration** of the Dionex Chromatography Management System theoretically allows assigning different ports to these channels. However, this is not possible: there is a fixed connection between the channels and the corresponding ports of the Nelson box.

Using a different Detector Device Driver

If a different detector device driver should be used for one or both channels, the integrated channel must be deactivated (**Signals** tab). The Nelson driver supplies the channel as the port **Channel_A** or **Channnel_B**. For the detector driver, this port can be used instead of an AD board port.

For further information on the Nelson Interfaces, see:

- **NELSON Interfaces**
- **NELSON Interfaces: Pin Assignment**
- **NELSON Interfaces: Properties**
- **NELSON Interfaces: Data Acquisition Restrictions**
- **NELSON Interfaces: Differences from Conventional Nelson Box Installations**

NELSON Interfaces: Properties

VoltageRange

This value specifies the voltage range of the A/D converter (maximum signal). Any voltage exceeding this value is cut (by the box). The lamp **Over Range** of the box will light up.

This parameter directly affects the signal resolution.

Channels

Indicates on which channels the box records data. Usually, the channels are set automatically; this setting should not be changed.

SamplingStep

This is the actual interval the box uses for data recording. If possible, this interval is set automatically to correspond to the STEP of the channels. This setting will produce the best results.

With the setting SamplingStep < 0.1 s, the signal resolution will decrease.

For further information on the Nelson Interfaces, please also refer to:

- **NELSON Interfaces**
- **NELSON Interfaces: Pin Assignment**
- **NELSON Interfaces: Device Driver Configuration**
- **NELSON Interfaces: Data Acquisition Restrictions**
- **NELSON Interfaces: Differences from Conventional Nelson Box Installations**

NELSON Interfaces: Data Acquisition Restrictions

General

It is not possible to change the data acquisition parameters of the box during data acquisition.

For optimum synchronization of the **Inject Response** and the data acquisition start, the data acquisition should be started immediately after injection (the digital **Inject Response** should be used).

Data Acquisition on two Channels

Although the type 941 offers two channels, data acquisition is possible only on one channel. Simultaneous data acquisition on both channels is not possible.

With the types 950-970, simultaneous data acquisition is possible on both channels.

It is not possible to independently control data acquisition on the two channels, as the box has only one A/D converter that is alternately switched to the two channels (**Multiplexing**).

This is why both channels can only be switched on and off simultaneously. Both channels are recorded with the same **VoltageRange** and **SamplingStep**. As the maximum sampling rate of the A/D converter is only 100 Hz, the **SamplingStep** must be set to multiples of 0.02s.

Releasing the Start/Stop Keys and Inputs

Caution: By pressing the Start key while holding down the Stop key, it is possible to release the Start/Stop keys on the instrument. However, this will lead to errors the device driver is unable to prevent.

For further information on the Nelson Interfaces, see:

NELSON Interfaces

NELSON Interfaces: Pin Assignment

NELSON Interfaces: Device Driver Configuration

NELSON Interfaces: Properties

NELSON Interfaces: Differences from Conventional Nelson Box Installations

NELSON Interfaces: Differences from Conventional NELSON Box Installations

Sequence Processing and Buffer Action

Conventional Nelson data systems (e.g. ACCESS*CHROM) allow recording entire sequences with the box as long as there is sufficient buffer space. Then the data is transferred to the data system.

The Dionex Chromatography Management System reads the data immediately, so that virtually no buffer action is required. The buffer only temporarily stores data during delays in data transfer (usually less than one second).

In the Dionex Chromatography Management System, it is necessary to first define the sequences, i.e. the number and run time of the samples. Recording data is only possible if the Dionex Chromatography Management System is ready. The Dionex Chromatography Management System uses the ready relay to indicate the ready status.

Using the Stop Input

Operators working with conventional Nelson Box Installations are used to define the end of data acquisition via the stop input of the box. The Dionex Chromatography Management System does not support this. The end time must be explicitly defined in the ➢*Program*.

Why is the Box not "Ready"?

As mentioned above, the Dionex Chromatography Management System uses the ready relay to indicate the ready status. The ready relay is switched on during the **Inject** command. Otherwise, it is switched off.

How can you prevent loss of data when the Dionex Chromatography Management System does not use the buffers as no data because the program does not expect any data?

Use the **Ready** output of the box. Most samplers are fitted with a suitable input (**Ready**, **Remote Start**, etc.).

For further information on the Nelson Interfaces, see:

NELSON Interfaces

NELSON Interfaces: Pin Assignment

NELSON Interfaces: Device Driver Configuration

NELSON Interfaces: Properties

NELSON Interfaces: Data Acquisition Restrictions

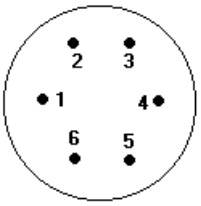
PHARMACIA

PHARMACIA LKB2150 HPLC Pump

The **LKB2150 Pump** ➢*Device Driver* of the Dionex Chromatography Management System supports controlling up to three pumps. Each pump must be connected to a separate serial port and is addressed using the following (fixed) communications parameters.

Baudrate:	9600
Data bits:	8
Stop bits:	2
Parity:	Odd
Handshake:	None

The upper 6-pin socket **Remote** on the back of the instrument is connected as follows with the 9-pin / 25-pin serial connector.



Back of instrument		**25-pin Serial port**	**9-pin Serial port**
Pin 1: GND	----------	7	5
Pin 2: not used			
Pin 3: Flow pulse out			
Pin 4: Stop in/out			
Pin 5: Remote in			
Pin 6: Serial in	----------	2	3
Internal: 1---5			

By connecting the pins 1 - 5 on the pump connector, the pump is immediately switched to **Remote** operation after it is switched on!

PHARMACIA Fraction Collector LKB2211 SuperRac

These instructions describe the required steps to operate the LKB Superray 2211 Fraction Collector under the Dionex Chromatography Management System.

The following requirements must be fulfilled:

- The Dionex Chromatography Management System computer must have 6 free relay channels, e.g. on the ➢*Dionex 16 Relays Card*. In the **Server Configuration**, these relays are installed under ➢*Sharable Devices*.
- The connecting cable must connect the relay contacts and 25-pin Sub-D-connector 'Ext. Input - Output' on the rear of the instruments (see example for details).
- Before the installation in the Dionex Chromatography Management System, the user must correctly initialize the fraction collector.

Initialization

To initialize the fraction collector, the following steps must be performed after switching the instrument on or after a **Reset**:

- Select type of the used sample rack (type A to E).
- Determine the fraction size. For operation under the Dionex Chromatography Management System, time control must be selected.
- Determine the time interval. Normally, the time interval determines the duration for which the fraction collector stays above a container. When using with the Dionex Chromatography Management System, the data system determines the switching time to the next container. ***The user must therefore ensure that the entered time interval is larger than the total analysis time.***
- Enter the number of fractions. Define the minimum number of collector containers belonging to one fraction loop. ***The user must ensure that a sufficient number of containers is reserved for a sample.***

For further details, see the **Instruction Manual LKB 2211-010 SuperRac**.

Assigning Control Functions

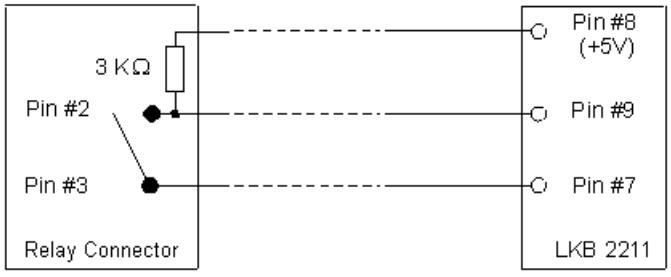
Control functions are assigned to specific relays via **Server Configuration** of the Dionex Chromatography Management System using the **Relays** tab dialog box of the LKB2211 driver. The following functions are available:

Function:	Description:
Start_Loop	Starts a sample loop. If a fraction collector moves to the first collecting container (Tube 1) in the sample loop. The status of the fraction collector changes from **Rdy** to **RUN**.
Step	Moves the fraction collector to the next container within the sample loop.
Return_Loop	Moves the fraction collector to the start position of the sample loop. The status of the fraction collector is **Rdy**.
Return	Moves the fraction collector to the start position of the sample loop 0. The status of the fraction collector is **Rdy**.
New_Loop	Moves the fraction collector to the next sample loop. The status of the fraction collector is **Rdy**.
Waste_Valve	With this relay, the flow can be diverted from the collection containers to the waste container.

Dionex Connecting Cable

The cable connects the **Ext.Input-Output** output of the LKB2211 with the output of the Dionex 16 relays board. The cable has a 25-pin Sub-D-connector and a 37-pin Sub-D-connector (see the pin assignment below).

To actuate a control function, the respective control input is connected with the ground output (Pin #7) for duration of approx. 1s. The only exception to this is the valve control input. Here, the solvent is directed to the waste container as long as the valve control input is connected with the ground, i.e. the valve has the status **On**. To avoid interferences, all TTL control inputs of the instrument must be connected with the +5V output using 3KOhm **Pull Up** resistors.



The connection illustrated here for pin 9 must also be installed for the pins 10, 11, 12, 13, and 24 of the LKB connector.

***Note**:* It is recommended to control the fraction collector LKB2211 only via a completely assembled and tested connecting cable. The

entire connection for the 16-relay board is available from Dionex as a kit.

Example: Pin Assignment when using a Dionex 16 Relays Board

The relays 1 to 6 of the Dionex 16 relays board are used with the function assignment described below. The following pins of the relay board connector (37pin Sub-D-connector) must be connected with the pins of the LKB connector (25pin Sub-D-connector). For a description of the LKB connector, refer to the **Instruction Manual LKB 2211-010 SuperRac**.

Relay #	Function	Pin # Relay Board Connector	Pin # LKB-Connector
1	Return	2	9
2	Step	4	10
3	Return_Loop	6	11
4	Start_Loop	8	12
5	New_Loop	10	13
6	Waste_Valve	12	24
		3	7
		5	7
		7	7
		9	7
		11	7
		13	7

In addition, the Online Help offers support regarding the special **Server Configuration** page on LKB SuperRacs: *Relays*.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

RAININ / VARIAN Pumps: SD-1, SD-200/SD-300, and ProStar 215 - Overview

Device Type:	Pumps
Device Driver:	**Rainin/Varian SD-1-Pump** or. **Rainin/Varian SD-200/SD-300-Pump** (use the latter one for the ProStar 215 pump)
Supported Hardware Options:	Up to three Gilson 302/303 pumps

What is required?

License:	Device Control
	Select *About CHROMELEON* (link available in the Online Help only) in the **Help** menu of the Dionex Chromatography Management System client to check whether this option is available.
Connection:	GSIOC RS232 adapter cable 605 (for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions)
	The cable is not available from Dionex!
Hardware Prerequisites:	Multi-serial, 8-fold PCI interface board (Equinox 8-RS232 Multi-Com board, Dionex part no. 5906.2095)
	Free RS232 port
Control Panel:	GIL306Gradient.pan

Further Information

For an overview on how to install the Rainin/Varian pumps, see **Rainin/Varian Pumps: SD-1, SD-200/SD-300, and ProStar 215 - Installation**.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

RAININ / VARIAN Pumps: SD-1, SD-200/SD-300, and ProStar 215 - Installation

Hardware Installation

Device Connection:

The device driver supports up to 3 pumps of the type SD-1, SD-200/300, or ProStar 215. The Rainin pumps use the same kind of SIOC bus as the **Gilson: Pumps 302/303 - Overview**. Therefore, a RS232/SIOC adapter is required (e.g. the Gilson GSIOC RS232 adapter cable 605 - for details, see **Gilson: GSIOC Cable** in the appendix of these Installation Instructions) to connect the PC to the first pump.

Caution:

As the adapter is shipped with a default baud rate of 19200 Baud, the baud rate must be set to 9600 baud to operate the **SD-200/SD-300** or **ProStar** (see settings on the **General** page) pumps under the Dionex Chromatography Management System. Open the connector housing and resolder the cable from land A to land B (for details **see 605 RS232 Adapter and GSIOC Protocol - USER's GUIDE**).

Contrary to the other Rainin/Varian pumps the **SD-1** driver communicates at a baud rate of 19200 Baud. Therefore, do not modify 605 cable when using the SD-1 pump!

Caution:

Controlling the pumps via the RS232 interfaces of the PC (COM ports) or the ➢*UCI-100* Universal Chromatography Interface is not supported. The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this. Connect the adapter to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) instead.

Device Connection: (Cont'd)	If several pumps are used in a high-pressure gradient system, the second pump can be connected to the first one with a GSIOC cable and the third pump can be connected to the second.
Device Settings:	Each pump has its own SIOC address (0 to 63). The address is set via a DIP-switch. This switch is located inside the pump on the back of the front panel.
Restrictions:	Not known.

Software Installation

Install the **Rainin/Varian SD-1-Pump** (**Rainin/Varian SD-200/SD-300-Pump**, respectively) ➢*Device Driver* in the **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Rainin/Varian SD-1-Pump** or the **Rainin/Varian SD-200/SD-300-Pump** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *General* tab, select a free COM port and enter the GSIOC address.

   The *GSIOC and Head Types* tab allows defining the SIOC addresses for the pump as well as the pump head types that are used.

   You do not need to change the presetting on the *Error Levels* tab.
5. To control the installed Gilson pump connect the **GIL306Gradient** control panel or any especially developed control panel in the client of your Dionex Chromatography Management System to the corresponding time

Further Information

For an overview on the Rainin/Varian pumps, see **Rainin/Varian Pumps: SD-1, SD-200/SD-300, and ProStar 215 - Overview**.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

SOMA

Soma 3710

For controlling the UV Detector Soma 3710, please note the following pin assignment for the RS232 cable:

Soma 3710		PC
25-pin Sub-D (female)		9-pin Sub-D (male)
2 (RXD)	----------	2
3 (TXD)	----------	3
7 (GND)	----------	5

(➢*Null Modem Cable* without handshake plus GenderChanger)

The communication parameters must be as follows: 9600 baud, 8 data bits, no parity, 1 stop bit, and no handshake.

Before connecting, set the device manually into the Remote state. Press the key **Remote** until the green lamp **Remote** lights up at the detector. The detector will remember this state when being switched off.

For devices with firmware version up to 1.78 use the driver **Soma_UV-VIS_Detector_S-3710_178** ➢*Device Driver*. For devices with firmware version 1.79 and higher, the **Soma_UV-VIS_Detector_S-3710_New** driver will be available.

In addition, the Online Help offers support regarding the special **Server Configuration** page on the Soma UVD: *UV*.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

THERMOQUEST

The following ThermoQuest instruments can be controlled:

THERMOQUEST: Trace GC

THERMOQUEST: AS2000 GC Autosampler

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

THERMOQUEST: Trace GC - Overview

Device Type	Gas chromatograph
Device Driver:	**Thermoquest Trace Gas Chromatograph**
Supported Hardware Options:	• Up to 2 **Inlets** Options: - Purged Packed Column Injector (PPKD) - Split/Splitless Injector (SSL) • **Column Oven** **-** High-temperature column oven - Nitrogen cooling - Carbon dioxide cooling • Up to 2 **Detectors** (optionally with oven): - Flame Ionization Detector (FID) - Thermal Conductivity Detector (TCD) • **Electronic pressure/flow control** **-** Column and inlet: DPFC (Digital Pressure Flow Control) - Detector: DGFC (Digital Gas Flow Control)

What is required?

License:	Extended Device Control
Connection:	**ThermoQuest Trace GC: Cable 8914.0148 / 8914.0149** **ThermoQuest AS2000 / Trace GC: Cable** (for details, see the appendix of these Installation Instructions) A/D cable for data transmission (depending on the A/D converter used).
Hardware Prerequisites:	Data acquisition requires an A/D converter, e.g. a ➢*UCI-100 Interface*, a Dionex UI20 (Dionex part no. 46017) or any other A/D converter which is supported by the Dionex Chromatography Management System, e.g. PE Nelson Boxes including the corresponding signal cables. **Serial Interface Board** Multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM board, Dionex part no. 5906.2095)
Software Prerequisites:	• FisCfg.cdc configuration module • Message.dll
Control Panel:	TraceGC_AS.pan

Further Information

For information on how to install the ThermoQuest Trace GC, see **THERMOQUEST: Trace GC - Installation**.

For an overview on the different ThermoQuest instruments for which Dionex device drivers are available, see **THERMOQUEST**.

THERMOQUEST: Trace GC - Installation

Hardware Installation

Device Connection:

THERMOQUEST Trace GC: Cable 8914.0148 / 8914.0149 / 8914.0149 (for details, see the appendix of these Installation Instructions)

A special cable (**THERMOQUEST AS2000 / Trace GC: Cable** - for details, see the appendix of these Installation Instructions) is used to connect the ThermoQuest Trace GC with the ThermoQuest AS2000 autosampler.

In addition, an A/D cable is required for data acquisition (depending on the A/D converter used - e.g. ➢*UCI-100 Interface*).

Device Settings:

(Also, see the Installation Instructions supplied with the instrument.)

The communication settings must be as follows:

Baud rate	38400
Handshake	Rts/Cts
Parity	None
Data bits	8
Stop bits	1

PrepRun Timeout

Since the GC can only be started when it is in **Ready To Inject** mode it is recommended to set the **PrepRun Timeout** long enough to ensure that the injection takes place within this time. The PrepRun Timeout can be set at the GC keyboard [Config] [Oven] [PR Timeout].

Setting Property Values to 'Infinite'

The properties **StopPurgeTime**, **PurgeTime**, **SecCoolingTime**, **SVEDuration**, and **StopAuxPurgeTime** can be set to infinite. This is done manually via the GC keypad. Proceed as follows:

Device Settings: (Cont'd)

- Disconnect the Dionex Chromatography Management System from the GC.
- Make the desired settings.
- Reconnect the Dionex Chromatography Management System to the GC.

Restrictions: Not known.

Software Installation

Install the **THERMOQUEST Trace Gas Chromatograph** ➢*Device Driver* in the **Server Configuration** of the Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **ThermoQuest Trace Gas Chromatograph** under the desired timebase (via the Add Device command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the General tab, select a free COM port.

   On the *Options* tab, specify the limits for the controllable temperature range of the column oven. In addition, select the cooling system used. If installed, also select the electronic flow/pressure control for the column/inlet and/or the high-temperature oven option.

   The *Right/Left Inlet* tab allows you to set up the type and the temperature control for the **Inlet**.

   On the *Right/Left Detector* tab, specify the installed detector(s) and its/their temperature and gas controls.

   Open the **Signal Configuration** dialog box from the *Signals* tab by double-clicking the respective channel. Assign a channel to the signal and name the signal in the **Signal Name** field according to the selected detector type.

   You do not need to change the presetting on the ➢*Error Levels* tab.

5. To control the ThermoQuest Trace GC use the **TraceGC_AS** control panel in the client of your Dionex Chromatography Management System, modify the control panel according to your needs, and connect it to the corresponding timebase.

Application

Notes on the Device Driver:

General

The ThermoQuest Trace GC uses a packet oriented, binary data format to communicate with the PC via the RS-232 interface. When the GC receives a command, it switches into the remote mode and locks the keypad. If no further communication takes place, the GC switches back into the local mode after 30 seconds

The GC will not start the communication by itself; it will only respond to commands and requests sent by the Dionex Chromatography Management System.

Experienced users should be able to control the instrument without any problems. In the Dionex Chromatography Management System, short descriptions of the GC commands are available in the corresponding Command dialog box or the Properties/Link box.

In the Dionex Chromatography Management System, pressure is always stated in bar. Selecting a different pressure unit is not supported. For further information, please contact the Dionex Service.

Sampler

Using the AS2000 autosampler with the GC: If a sample vial is missing at the position specified in the sequence, the sampler treats this as a ➢*Blank Run Sample* (refer to the AS2000 manual page 118). However, the sequence will not be stopped.

If the GC is waiting for an inject response from the autosampler and suddenly becomes **Not Ready** due to gas supply or flow problems, an error message is issued and the sequence is stopped.

Entering a Temperature Gradient

Entering a temperature gradient is via a ➢*Program*.

For the ThermoQuest Trace GC, a temperature profile can be entered with a maximum of six ascents or descents. The maximum temperature change (ascent) is up to 120°C per minute, depending on the oven type.

Gradients are entered in the Program Wizard in the typical format for GC applications (the starting and end temperatures are entered as well as the modification rate). In the program, however, the so-called "base point philosophy" is used (similar to entering a flow or percent gradient in HPLC). Each **temperature** command serves as base point of the gradient program. The Wizard automatically converts the entered rates into the base point representation.

An Inject command is indispensable. No gradient is executed before the Inject command. Thus, temperature gradients can only begin after the Inject command

Temperature Setting

Reaching the nominal temperature on the instrument can take some time. Please note that the oven heats faster than the injector and the detector system. As soon as the nominal temperature is reached, the GC sends a **Ready** signal. Only after this, injection is possible via the autosampler.

Example:

The following program waits until the nominal temperature 150°C is reached, before the Inject command is executed:

```
0.000   GC.Temperature = 150
  Wait  GC.Ready
  Inject
......  ..............
```

Caution: After receiving the nominal temperature value from the Dionex Chromatography Management System, the instrument implements the desired value as fast as possible. When the value is "almost" reached, the **Equilibration Time** passes until the instrument sends the confirmation message to the Dionex Chromatography Management System. The duration of this time interval can be set via the **Equilibration Time** parameter in the Dionex Chromatography Management System.

Troubleshooting

Should you have special questions, contact the Dionex Service.

Further Information

For an overview on the ThermoQuest Trace GC, see **THERMOQUEST: Trace Gas GC - Overview**.

For an overview on the different ThermoQuest instruments for which Dionex device drivers are available, see **THERMOQUEST**.

THERMOQUEST: AS2000 GC Autosampler - Overview

Device Type:	GC autosampler
Device Driver:	**Thermoquest_AS2000**
Supported Hardware Options:	

What is required?

License:	Device Control
Connection:	RS232 cable (see **Fisons AS: Cable 8914.0127 / 8914.0143**)
Hardware Prerequisites:	Data Acquisition requires an A/D converter, e.g. an ➢*UCI-100 Interface* with the corresponding signal cables. Free RS232 port
Software Prerequisites:	• FisCfg.cdc configuration module • Message.dll
Control Panel:	FISAS800

Further Information

For information on how to install the ThermoQuest AS2000 GC autosampler, see **THERMOQUEST: AS2000 GC Autosampler - Installation**.

For an overview on the different ThermoQuest instruments for which Dionex device drivers are available, see **THERMOQUEST**.

ThermoQuest: AS2000 GC Autosampler - Installation

Hardware Installation

Device Connection:

The ThermoQuest AS2000 GC autosamplers is connected to the ThermoQuest Trace GC via a special signal cable (for details, see **THERMOQUEST AS2000 / Trace GC: Cable** in the appendix of these Installation Instructions). When the injection is completed, the GC sampler sends the signal to the GC, which in turn sends it to the Dionex Chromatography Management System.

In the **Server Configuration**, specify the remote input (GC_INJECTOR) that is used by the ThermoQuest AS2000 sampler under **Inject Port** on the **Sampler** tab!

Device Settings:

The following communications parameters must be used: 9600 Baud, 8 Data Bits, No Parity, 1 Stop Bit, Rts/Cts handshake.

Some THERMOQUEST AS2000 GC autosamplers are set by the manufacturer to a baud rate that is not suitable for the ➢*Device Drivers* of the Dionex Chromatography Management System.

When switching on the sampler, press the **Meth** and **Seq** keys simultaneously to check the baud rate setting. The following information will be displayed:

```
AS2000 SET UP: b9600
ACT INJ SMP SYR MAN
```

Device Settings: (Cont'd)

The value given to the top right is the baud rate setting. This information may not be available in previous firmware versions. If so, press **EXIT** to leave the setup menu.

If the baud rate is not set to 9600, move the cursor to

the baud rate field using the key **<** (arrow to the left). Set the new baud rate with the up and down arrow keys and leave the setup menu by pressing **EXIT**.

Restrictions: Not known.

Software Installation

Install the **Thermoquest_AS2000** ➢*Device Driver* in the  **Server Configuration** of your Dionex Chromatography Management System.

1. Start the server of the Dionex Chromatography Management System.
2. Start the **Server Configuration** of the Dionex Chromatography Management System.
3. Add the **Thermoquest_AS2000** under the desired timebase (via the **Add Device** command of the context menu).
4. The following settings are required on the different tabs (the links are available in the Online Help only):

   On the *Thermoquest_AS2000* tab, have the Demo Mode switched off.

   On the *Sampler* tab, select a free inject port.

   You do not need to change the presetting on the *Error Levels* tab.
5. To control the ThermoQuest AS2000 GC autosampler connect the **FISAS800** control panel in the client of your Dionex Chromatography Management System to the corresponding timebase.

Application

The Online Help offers information on the *Commands and Parameters of the Fisons AS800/ThermoQuest AS200*.

After the **Connect** command, the parameter values are initially unknown to the Dionex Chromatography Management System (blank fields in the FISAS800 control panel). You should enter meaningful values before injection.

Use one of the **Method A/B/C/D** buttons on the control panel or specify them in the sample program (also, see: **How to ...: Actions in the PGM Editor**  **Creating a Program)**. A reasonable starting point might be this:

```
; Assuming a standard 10 µl syringe.
; Injection Volume should be 1.0 µL.
PreInjCleanVol = 10.0
PreInjCleanCycA = 3
CleanCycles = 1
PostInjCleanCycC = 0
; PostInjCleanVol = 10.0
PullUpCount = 6
PullUpDelayTime = 2.0
AirVolume = 3.0
FillingVolume = 5.0
AspirationSpeed = 100
InjectionSpeed = 100
PreInjDelayTime = 1
PostInjDelayTime = 2
```

Troubleshooting

 ***Note:*** If an error occurs during operation (e.g. excessive sample volume), the error is displayed on the instrument only. To continue the analysis, you must confirm the error message directly at the sampler (by pressing the Enter key). This is possible after unlocking the sampler keyboard in the Dionex Chromatography Management System. Use either the **Disconnect** command or the **KeyboardUnlocked** command. Better yet: **Disconnect** the sampler, turn it off and on again, wait until it is ready, and reconnect.

Error	Description	Remedial Action

Missing vial	The sampler display shows:
	`End Sample`
	`Total Injections 0`
	In addition, the Dionex Chromatography Management System waits forever for an inject response.
		The current sample is treated ➢*Blank Run Sample*.

Error	Description	Remedial Action

Bad vial	After some retries, the sampler display shows something like this:
	`PLG NDL INJ TUR CNTR`
	`--- BSY --- ---  *`
	This happens quite easily if the vials are not perfectly crimped.
		Disconnect the sampler, press EXIT (on the sampler's keyboard). When prompted whether to pause, continue, or abort the sample, choose Abort. Abort the batch and reconnect.

Illegal parameter (e.g. Volume/ Position > Max or Air + Sample Volume > Max)	The sampler displays an error message.	Disconnect the sampler. Press sampler key, as necessary.
Continuous beep and display cleared	Severe damage may occur (destroyed syringe, vials etc.)!	**Turn off the sampler immediately!**
Strange behavior of any other kind		Disconnect the sampler, turn it off and on again, wait until it is ready, and reconnect.

Further Information

For an overview on the ThermoQuest AS2000 GC autosampler, see **THERMOQUEST: AS2000 GC Autosampler - Overview**.

For an overview on the different ThermoQuest instruments for which Dionex device drivers are available, see **THERMOQUEST**.

TSP

The following TSP instruments can be controlled:

- ➢*Autosamplers* **AS3500 / AS3000 - Overview**
- Pumps **P2000 and P4000**
- UV-Detectors:
  - UV1000
  - UV2000/Linear 205
  - UV3000/Linear 206

☞ ***Tip***: Data acquisition with the TSP UV detectors requires a ➢*UCI100 Interface* (or an ➢*A/D Converter* or a Nelson-Interface, respectively) including the respective signal cables.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

TSP: AS3500 / AS3000 Autosamplers - Overview

Device Type:	Autosampler with x positions
Device Driver:	**TSP AS3000/AS3500 Autosamplers**
Supported Hardware Options:	**Cooler** (rack cooling) **Oven** (rack heating) **Prep Kit** (sample preparation option)

What is required?

License:	Device Control
Connection:	RS232 cable (Dionex part no.: 45789 (cable AI450 to AS3500); for details, see **TSP/Linear: Cable 45789 (Cable AI450 to AS3500)** in the appendix of these Installation Instructions.
Hardware Prerequisites:	Free RS232 port

Further Information

For information on how to install the TSP AS3500/AS3000 Autosamplers, see **TSP AS3500 / AS3000 Autosampler- Installation.**

For an overview on the TSP instruments for which Dionex device drivers are available, see **TSP.**

TSP: AS3500 / AS3000 Autosamplers - Installation

Hardware Installation

Device Settings:

a) For menu option **Input Polarity**

Pump Ready Active = **HI**
Inj Hold Active = **LO**

b) For menu option **Output Polarity**

Set all to **LO**.

Note: If **Inj. Hold Active** is set to **HI**, data acquisition cannot be started.

Restrictions: Not known.

Software Installation

Install the **TSP AS3000/AS3500 Autosamplers** ➢*Device Driver* in the **Server Configuration** (the following links are available in the Online Help only):

Select the RS232 port on the *General* tab.

On the *Installed Options* tab, turn on and off the control of the option(s) installed for the AS3500 autosampler.

You do not need to change the presetting on the *Error Levels* tab.

Application

Nothing particular known

Troubleshooting

Why can't you start the data acquisition?

Is **Inj Hold Active** set to **LO**? If not, data acquisition cannot start.

Further Information

For an overview on the TSP AS3500/AS3000 Autosamplers, see **TSP AS3500 / AS3000 Autosamplers - Overview**.

For an overview on the different TSP instruments for which Dionex device drivers are available, see **TSP**.

TSP: P2000 and P4000 Pumps - Overview

Device Types:	P2000: binary low-pressure gradient pump P4000: quaternary low-pressure gradient pump
Device Drivers:	P2000: **TSP P2000 Pump** P4000: **TSP P4000 Pump**
Supported Hardware Options:	Pump head • Type10 (max. 10.00 ml/min) • Type30 (max. 30.00 ml/min) • Type90 (max. 90.00 ml/min)

What is required?

License:	Extended Device Control
Connection:	RS232 cable (Dionex part no.: 45789 (cable AI450 to AS3500); for details, see **TSP/Linear: Cable 45789 (Cable AI450 to AS3500)** in the appendix of these Installation Instructions.
Hardware Prerequisites:	Free RS232 port.

Further Information

For information on how to the TSP P2000 and P4000 pumps, see **TSP: P2000 and P4000 Pumps - Installation.**

For an overview on the different TSP instruments for which Dionex device drivers are available, see **TSP**.

TSP: P2000 and P4000 Pumps - Installation

Hardware Installation

Device Settings None.

Restrictions: Not known.

Software Installation

Install the TSP P2000 Pump or TSP P4000 Pump ➢*Device Driver* in the **Server Configuration** (the following links are available in the Online Help only):

Select the RS232 port on the *General* tab.

On the *Head Types & Limits* sheet, select your pump head:

- Type10 (max. 10.00 ml/min)
- Type30 (max. 30.00 ml/min)
- Type90 (max. 90.00 ml/min)

Specify the flow and pressure limits (max. 414 bar).

On the *Solvents* sheet, specify the number and names of the eluents that are delivered by the pump.

You do not need to change the presetting on the *Error Levels* tab.

Application

The P2000 pump allows programming linear gradients with up to 9 steps. With P4000 pumps, up to 39 steps can be programmed. The driver does not support non-linear gradients.

Commands and Properties

The pump driver supports the following commands and properties:

Properties	Min	Max	Default	Purpose
HeadType	N/a	N/a	N/a	Indicates the installed pump head
PumpStatus	N/a	N/a	N/a	Indicates the pump status
Ready	NotReady	Ready	N/a	Indicates whether the pump is ready

Note: The **Hold** command cannot be performed during program execution. If the command is given nevertheless, a warning is displayed.

Troubleshooting

Nothing particular known.

Further Information

For an overview on the TSP P2000 and P4000 pumps, see **TSP P2000 and P4000 Pumps - Overview**.

For an overview on the different TSP instruments for which Dionex device drivers are available, see **TSP**.

TSP: UV1000 Detector - Overview

Device Type:	Single channel UV detector
Device Driver:	**TSP UV1000 Detector**
Supported Hardware Options:	No special options.

What is required?

License:	Extended Device Control
Connection:	RS232 cable (Dionex part no.: 45789 (cable AI450 to AS3500); for details, see **TSP/Linear: Cable 45789 (Cable AI450 to AS3500)** in the appendix of these Installation Instructions.
Hardware Prerequisites:	For data acquisition: A/D converter, e.g. an ➢*UCI-100-Interface* with the corresponding signal cables. Fee RS232 port
Software Prerequisites:	• TspCfg.cdc configuration module • Message.dll

Further Information

For information on how to install the TSP UV1000 Detector, see **TSP: UV1000 Detector - Installation**.

For an overview on the different TSP instruments for which Dionex device drivers are available, see **TSP**.

TSP: UV1000 Detector - Installation

Hardware Installation

Device Settings: None.

Restrictions: Not known.

Software Installation

Install the **TSP UV1000 Detector** ➢*Device Driver* in the **Server Configuration** (the following links are available in the Online Help only):

On the *General* tab, select the RS232 port.

On the *Installed Lamps* sheet, select the installed lamps.

On the *Signals* sheet, specify the channel for analog signal acquisition.

You do not need to change the presetting on the *Error Levels* tab.

Application

Commands and Properties

The detector driver supports the following commands and properties:

Property	Min	Max	Default	Purpose
ZeroOnLambda Change	Off	On	Off	Select whether the detector performs an autozero every time the wavelength is changed.
AvailableLamps	None	UV & VIS lamp	UV-lamp only	Indicates which lamps are available (read only).
Range	0.0005 AUFS	3.0000 AUFS	1.0000 AUFS	Amplifying factor for the output signal.

Property	Min	Max	Default	Purpose
Wavelength	190 nm	800 nm	254 nm	Wavelength at which the detector measures the signal: UV lamp: 190 - 380 nm VIS lamp: 366 - 800 nm Both lamps: 190 - 800 nm
Response	0.0	5.0	1.0	Time constant. Denotes the time needed by the detector to reach 98% full scale.

Command	Purpose
UV_LampOn	Switches the deuterium lamp on
UV_LampOff	Switches the deuterium lamp off
Visible_LampOn	Switches the tungsten lamp on
Visible_LampOff	Switches the tungsten lamp off

Note: After a **Reset** command it takes 90 s until the detector is ready to execute further commands.

Troubleshooting

Why is a command not executed?

Have 90 s passed since the last reset? Otherwise, the command cannot be executed because the detector is not yet ready.

Why can't you start the data acquisition?

Is an AS3500 or an AS3000 sampler installed for which **Inj Hold Active** has been set to **HI**? Set this option to **LO** as otherwise the data acquisition cannot start.

Further Information

For an overview on the TSP UV10000 detector, see **TSP: UV1000 Detector - Overview**.

For an overview on the TSP instruments for which Dionex device drivers are available, see **TSP**.

TSP: UV2000 / Linear UV205 Detector - Overview

Device Type:	Two-channel UV
Device Driver:	**TSP UV2000/UVIS205 Detector**
Supported Hardware Options:	No special options.

What is required?

License:	Extended Device Control
Connection:	RS232 cable (Dionex part no.: 45789 (cable AI450 to AS3500); for details, see **TSP/Linear: Cable 45789 (Cable AI450 to AS3500)** in the appendix of these Installation Instructions.
Hardware Prerequisites:	For data acquisition: A/D converter, e.g. an ➢*UCI-100 Interface* with the corresponding signal cables. Free RS232 port.
Software Prerequisites:	Nothing particular known.

Further Information

For information on how to install the TSP UV2000 detector (the Linear UV205 Detector, respectively), see **TSP: UV2000 / Linear UV205 Detector - Installation**.

For an overview on the TSP instruments for which Dionex device drivers are available, see **TSP**.

TSP: UV2000 / Linear UV205 Detector - Installation

Hardware Installation

Device Settings: None.

Restrictions: Not known

Software Installation

Install the **TSP UV2000/UVIS205 Detector** ➢*Device Driver* in the **Server Configuration** (the following links are available in the Online Help only):

On the *General* tab, select the RS232 port.

On the *Signals* sheet, specify the channels for analog signal acquisition.

You do not need to change the presetting on the *Error Levels* tab.

Application

Commands and Properties

The detector driver supports the following commands and properties:

Property	Min	Max	Default	Purpose
DetectionMode	-	-	-	Sets the wavelength mode: Single Mode: 190 - 800 nm (only one detector channel is used) Dual1 Mode: 190 ... 450 nm Dual2 Mode: 366 ... 800 nm
Response	0.0	5.0	1.0	Time constant. Indicates the time needed by the detector to reach 98% full scale.

Property	Purpose
UV_LampOn	Switches the deuterium lamp on
UV_LampOff	Switches the deuterium lamp off
Visible_LampOn	Switches the tungsten lamp on
Visible_LampOff	Switches the tungsten lamp off

Channel-specific Commands and Properties

a) Common to both channels

Property	Min	Max	Default	Purpose
Range	0.0005 AUFS	3.0000 AUFS	1.0000 AUFS	Amplifier gain for the output signal
Wavelength	190 nm	800 nm	254 nm	Wavelength at which the detector measures the signal. Legal range: see **DetectionMode**.

Troubleshooting

Why can't you start the data acquisition?

Is an AS3500 or an AS300 sampler installed for which **Inj Hold Active** has been set to **HI**? Set this option to **LO** as otherwise the data acquisition cannot start.

Further Information

For an overview on the TSP UV2000/Linear UV205 detector, see **TSP: UV2000 / Linear UV205 Detector - Overview**.

For an overview on the TSP instruments for which Dionex device drivers are available, see **TSP.**

TSP: UV3000 / Linear UV206 Detector - Overview

Device Type: Four-channel UV detector

Device Driver: **TSP UV3000/UVIS206 Detector**

Supported Hardware Options: No special options.

What is required?

License: Extended Device Control

Connection: **Null Modem Cable (RS232)**: Dionex part no. 8914.0103A -RS cable (9-pin female to 25-pin female)

Adapter: Dionex part no. 8914.0118 - Adapter (25pol. Sub-D, male-male)

Hardware Prerequisites:	For data acquisition: A/D converter, e.g. an ➢*UCI-100 Interface* with the corresponding signal cables.
	Free RS232 port.
Software Prerequisites	Nothing particular known.

Further Information

For information on how to install the TSP UV3000 detector (the Linear 206 detector, respectively), see **TSP: UV3000 / Linear UV206 Detector - Installation**.

For an overview on the TSP instruments for which Dionex device drivers are available, see **TSP**.

TSP: UV3000 / Linear UV206 Detector - Installation

Hardware Installation

Device Connection:	Connection to the PC is via the RS232 connection. The detector is connected to the RS232 connector via a special **Null Modem Cable** (RS232 - for details, see the appendix of these Installation Instructions).
Device Settings:	None.
Restrictions:	Not known.

Software Installation

Install the TSP UV3000/UVIS206 Detector ➢*Device Driver* in the **Server Configuration** (the following links are available in the Online Help only):

On the *General* tab, select the RS232 port.

On the *Signals* sheet, specify the channels for analog signal acquisition.

You do not need to change the presetting on the *Error Levels* tab.

Application

Commands and Properties

The detector driver supports the following commands and properties:

Property	Min	Max	Default	Purpose
Visible_Lamp	Off	On	N/a	Switches the tungsten lamp on and off (λ = 366 - 800 nm)
UV_Lamp	Off	On	N/a	Switches the deuterium lamp on and off (λ = 190 - 365 nm)
Visible_Lamp_ Intensity	Intensity_ low	Intensity_ OK	N/a	Indicates whether the tungsten lamp intensity is too low (read only)
UV_Lamp_ Intensity	Intensity_ low	Intensity_ OK	N/a	Indicates whether the deuterium lamp intensity is too low (read only)
Connected	Discon- nected	Connec- ted	N/a	Indicates whether the detector is connected.

Channel-specific Commands and Properties

Property	Min	Max	Default	Purpose
Range	0.0005 AUFS	5.0000 AUFS	1.0000 AUFS	Amplifying factor for the output signal.
Response	0.0	9.9	1.0	Time constant. Indicates the time needed by the detector to reach 98% full scale..
Wavelength	190 nm	800 nm	254 nm	Wavelength at which the detector measures the signal. Legal range: See **DetectionMode**

Note: Due to the extensive communication during the execution of the **Connect** command it may take up to 1 min until the instrument is finally connected. The corresponding message is logged in the audit trail.

Troubleshooting

Why can't you start the data acquisition?

Is an AS3500 or an AS300 sampler installed for which **Inj Hold Active** has been set to **HI**? Set this option to **LO** as otherwise the data acquisition cannot start.

Why doesn't the UV detector respond?

Due to the extensive communication during connecting the device (following the **Connect** command), it may take up to 1 min until the device finally responds. The respective message is logged in the Audit Trail.

Further Information

For an overview on the TSP UV3000/Linear UV206 detector, see **TSP: UV3000 / Linear UV206 - Overview**.

For an overview on the TSP instruments for which Dionex device drivers are available, see **TSP**.

VARIAN (GC)

Controlling the Varian 3400 Gas Chromatograph requires the **Varian 3400 Gas Chromatograph** ➢*Device Driver* and the VarCfg.cdc device configuration file.

Dionex Chromatography Management System - Option

Operating the Dionex Chromatography Management System requires the **Extended Device Control** Feature (**Options of the Dionex Chromatography Management System**).

Components

The following components can be controlled:

- Column oven
- Gas flow controller
- Gas pressure controller
- Two detectors
- Auxiliary heater
- Varian 8100/8200 autosamplers
- Split / splitless Varian 1077 Injector

The following detectors are supported:

- Flame Ionization Detector (FID)
- Thermal Conductivity Detector (TCD)
- Thermion Specific Detector (TSD)

Connection

The serial computer port is connected to the Varian GC interface cable (Varian part no. 03-919939-00 Rev 3) via a special 9-pin serial cable (Dionex part no. 8914.0145; for details, see **Varian: Cable 8914.0145** in the appendix of these Installation Instructions).

The following communication parameters are used: 9600 baud, 7 data bits, 1 stop bit, even parity, and no protocol.

Setting Properties:

Properties can only be set if the GC is not in **Sample**, **Run**, or **RunEnd** mode. If a property is set nevertheless, its execution will be postponed until the GC is no longer in one of the modes described above. A message will be issued in the audit trail.

☞ ***Tip***: A blank run in a sample sequence can lead to several **Can't set property** error messages at the beginning of the next sample. These messages can be ignored.

After an **Inject** command, column oven temperature gradients, **Acquisition On/Off**, **Delta**, **Average** and **Step** are the only commands and properties that can be set. Therefore, define all properties that are required for the method before the **Inject** command. A **Reset** command can always be sent.

In case of a program with an isocratic column oven temperature, define the desired temperature before and after the **Inject** command and again at the final program time. Otherwise, the runtime calculation will not be correct.

Example:

```
0.000    GC.Temperature =    100
         Wait                GC.Ready
         Inject
         GC.Temperature =    100
30.000   GC.Temperature =    100
         End
```

Entering a Temperature Gradient:

Temperature gradients can be defined for the column oven heater, only.

Entering a temperature gradient is either directly (**Flow** command from the **Control** menu) or via a ➢*Program*.

Under the Dionex Chromatography Management System, a temperature profile is possible with a maximum of four ascents. The maximum temperature change is 50°C per minute. No descending temperature profiles are possible. The GC will return to the initial temperature when the gradient is completed.

For an overview on manufacturers whose instruments can be controlled via the Dionex Chromatography Management System, see **Installing and Controlling Third-Party Instruments**.

GENERIC DEVICE DRIVER 'GENERIC SERIAL DEVICE'

The generic ➢*Device Driver* enables the user to control instruments that are not supported by a separate device driver of the Dionex Chromatography Management System. The generic driver serves to create the required command strings for controlling an instrument. These strings are then integrated as commands in the user interface of the Dionex Chromatography Management System. This procedure only supports limited bi-directional control. The device driver is able to respond to the strings sent by the instrument, but requesting and evaluating instrument status messages is not possible.

Serial control is usually via command strings. In addition to the abbreviations identifying functions, it is possible to include current parameter values and control characters. Control characters are entered in pointed brackets **<>**, as there are no printable characters to represent them. Control characters define text formatting in lengthy command strings. For controlling serial instruments, they are used to introduce and complete command sequences.

A typical example for a command string controlling the UV wavelength in a detector is **WAVELENGTH=254<CR><LF>**. In this example, the abbreviation for the required function is **WAVELENGTH**, the current wavelength value is 254 nm, and the control characters completing the command sequence are <CR><LF>. <CR> represents the control character **Carriage Return** and <LF> represents **Line Feed**. In ASCII code, these characters correspond to the decimal values <CR>=0D and <LF>=0A.

Short Description of the Installation Steps

To send the command string mentioned above with the generic driver to the detector, the following steps are required in **Server Configuration** of the Dionex Chromatography Management System to create the definition file for this detector:

- Choose **Definition files**... from the **Edit** menu to open a dialog box listing all generic device drivers. Press **New**... to define a new generic device driver. The program then generates the basic structure of a generic device driver with the name **New Generic Device**.
- Specify the device name on the **Driver/Definition** dialog box. The name specified here serves to identify the new device driver. No other device driver should have the same name. This new name will be used as the default name during installation.
- Specify a file name on the **Driver/Definition** dialog box. After saving the configuration on the server, a file with this name is generated with the default extension **GEN** (do not enter this extension!). If a file with the same name already exists, the file extension of the older file is automatically changed to **BAK**, and the new file is saved. The **GEN** files store the entire instrument-specific user input.
- Create a new device.
- Set the parameters for the serial communication format on the **Device/Definition** sheet.
- Create all commands and properties.
- Save the definition.

The installation of the newly created device driver is identical to conventional device drivers of the Dionex Chromatography Management System. The user can install the new driver by double-clicking its name. After setting the required values for the instrument on the configuration dialog boxes, the instrument can be controlled according to the user definitions.

Structure of a Generic Device Driver

The task of the device driver is to control one or several devices via one or several serial interfaces. The term "device" does not necessarily refer to a physical instrument (e.g.: a detector), but the logical summary of properties and functions (e.g.: wavelength and bandwidth of a detector channel). As a result, the strings sent to an instrument are composed of device properties.

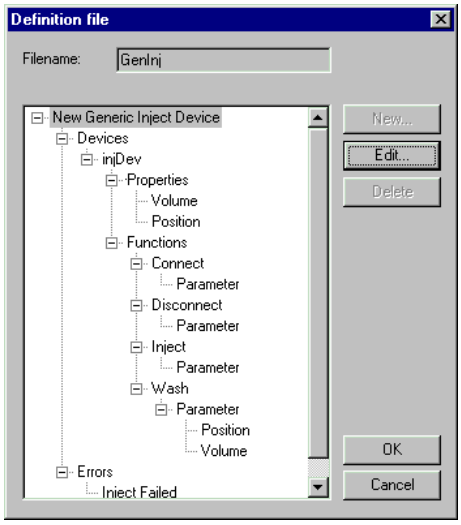
The Dionex Chromatography Management System supports several devices with an additional functionality. Currently, three device types are available for generic device drivers:

- Inject Device (e.g.: for ➢*Autosamplers*),
- Channel Device (e.g.: for the detector channels), and
- Standard Device (no special properties).

Communication via the serial port always requires a device. As instruments generally have one serial port, but are divided in several devices, one of the devices is assigned the serial interface; the other devices have no separate port, but are linked to the special device. Devices without their own serial I/O properly reflect the connect status of the device that performs the serial I/O.

To asynchronously received strings, generic device driver can respond with error messages or other messages. As it is not possible to assign these to a specific device, it is assumed that the device assigned to the serial port is the cause of the error or the message.

The dialog box **Definition file** shows the tree structure of a generic device driver:



The **New**..., **Edit**..., and **Delete** commands can be selected for the items in the tree structure. **New**... creates an appropriate default entry and opens a dialog box for selecting the settings.

Device Driver Settings in the "Driver/Definition" Dialog Box

The device name defined here serves to identify the driver during the installation. This name is used as the default during installation.

Caution: No other device driver should have the same name, otherwise there would be two identical entries in the drivers list.

The definition of the driver is always saved to the **BIN** directory of the installation of the Dionex Chromatography Management System. The device name is used as the file name. The file automatically receives the extension **GEN**. If there is already a file with this name, the extension of the older file is automatically changed to **BAK**, and the new definition is saved. The **GEN** files contain the entire information entered when defining the driver. From this directory, the file can be copied to the **BIN** directory of any other server of the Dionex Chromatography Management System. Device drivers that were generated inadvertently or for test purposes can be removed from the **BIN** directory by deleting the corresponding **GEN** files.

Defining a Device in the "Device/Definition" Dialog Box

Defining a new device driver starts with creating a new device.

- Choose **Devices** or a previously created device from the definition tree structure.
- Click **New**....
- Click the required device type in the dialog box **Select device type**. You can choose between the types **Standard Device**, **Inject Device**, and **Channel Device**. The significance of these types is described further below.

A new device of this type will be created using default settings. The dialog box for editing the properties will be opened.

The device name will appear as entered in the Dionex Chromatography Management System. This name must be unique within the device driver.

This dialog box also serves to define handling and properties of the serial port. The device has no serial interface, uses its own serial interface, or uses the interface of another device. In the first case, the device will not be able to communicate with the instrument - it only serves to define variables in programs. If the device uses its own interfaces, the corresponding properties (baud rate, parity etc.) must be entered. If the device communicates via an interface of another device, the corresponding device name must be entered here.

Defining Commands and Properties

To define new properties and functions within a driver, it is very important to realize the difference between functions and properties. The difference is explained below.

A property is a single numerical value that can be read and written under the Dionex Chromatography Management System. If a property value is modified, the driver sends the corresponding serial command to the instrument. As a variable component, this command usually contains the new numerical value of the property. However, the command can also access the numerical values of other device properties. The property is assigned the new numerical value only if the serial command was performed correctly.

A command can only be activated. During activation, its parameters are set. The parameters cannot be read, but are placeholders for the current numerical values during activation. Activation causes the driver to send a serial command to the instrument. Usually, this command contains the numerical values of the parameters as a variable component. The command can also access the numerical values of the device properties.

Generally, creating functions with parameters should be avoided. It is recommended to use properties or functions without parameters instead. Only these can be represented as controls in the user interface of the Dionex Chromatography Management System. However, if the intention is to explicitly point out that values should only be changed together, it is useful to create a function with several parameters. In addition, generic device drivers cannot read current values from the instrument. Properties that can be changed via the Dionex Chromatography Management System and by the instrument itself should therefore be set via a function with a parameter. This is to prevent that a property can have a different value under the Dionex Chromatography Management System than the actually set value on the instrument.

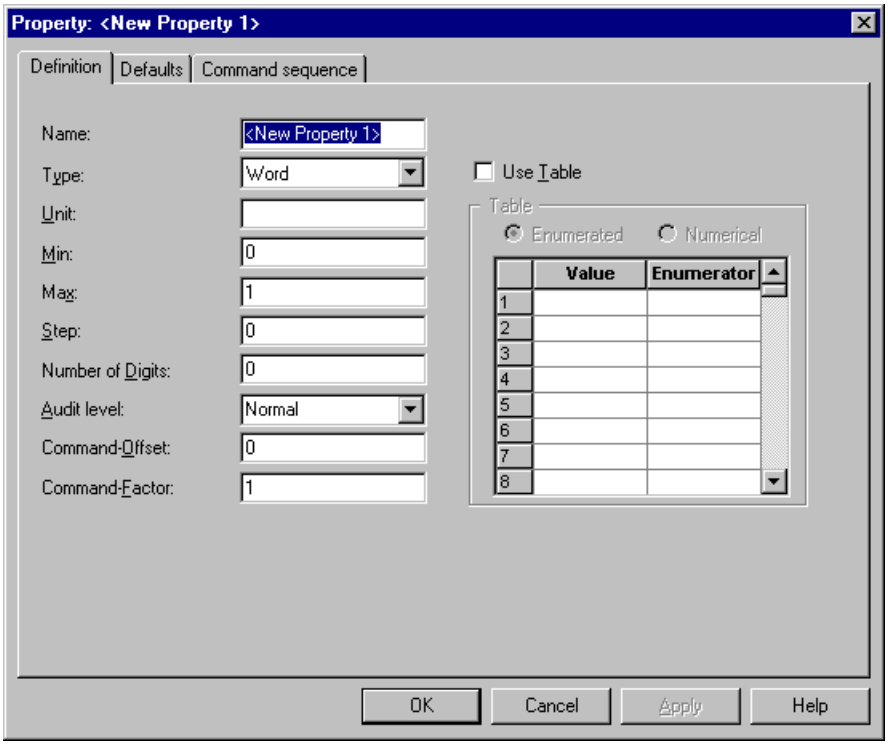
Using the generic serial device, the user can create any number of properties and functions. Each property can be linked with any appropriate control on the

user interface. After each modification of the control contents, a corresponding command is sent to the instrument.

Defining Properties in the "Property/Definition" Dialog Box

It is recommended to create separate properties for values that can be set independently (e.g. **Gain** and **Response**).

- From the **Definition** tree structure, select the item **Properties** or an existing property.
- Click **New**.



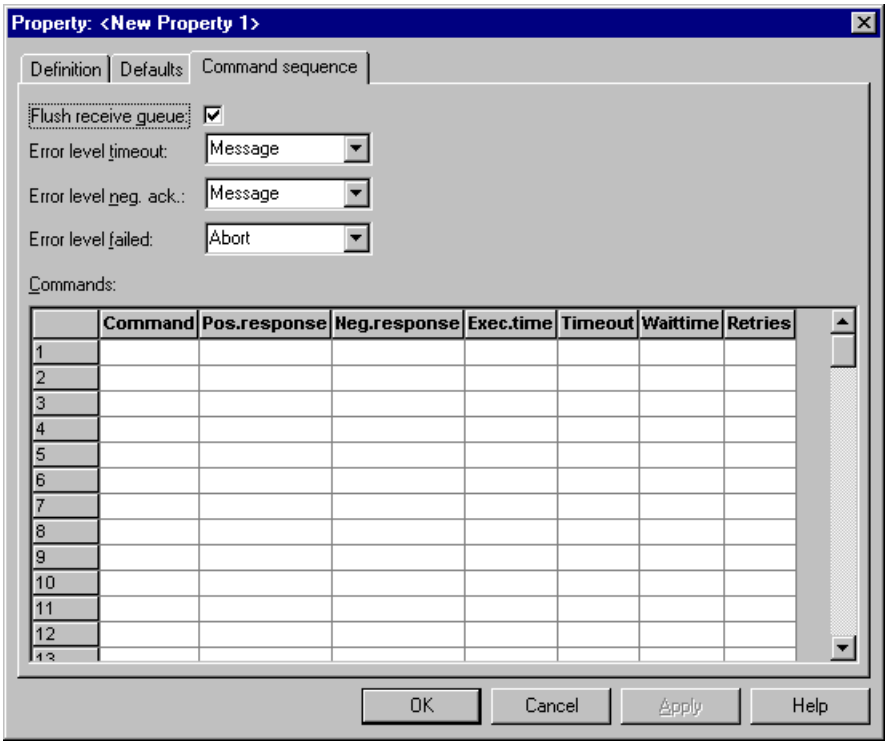
A new property with default settings is created, and the dialog box for editing the property is opened. This dialog box offers various options. The most important one is **Name**.

- Enter the name for the new property (e.g. **Gain**). The name must be unique within the device.

- Determine the format in which the corresponding numerical parameter is displayed on user interface of the Dionex Chromatography Management System.
- Choose an appropriate number format from the **Type** field (an integer in our example).
- Under **Unit**, enter the unit for the number value. **Min** and **Max** determine the available value range. For an amplification factor, the lower limit could be 1 and the upper value could be the corresponding maximum amplification. The Dionex Chromatography Management System does not support any input outside this range.
- The **Step** parameter is not considered for the moment (value = 0) (described below).
- **Number of Digits** should also be 0 for an integer.
- **Audit level** indicates the priority with which messages regarding this property are displayed.
- Via the fields **Command Offset** and **Command Factor**, the sent value can be multiplied by a factor and assigned an offset. With the offset 10 and the factor 2, the value 100 is changed to the value (100 x 2) + 10 = 210.

Defining Serial Commands of Properties in the "Property/Command Sequence" Dialog Box

When changing the current value of a property, the device driver not only sends a serial command, but an entire commands sequence. The value assignment is considered completed only if all commands of the sequence were performed correctly. A serial command is repeated until the maximum number of retries is reached.



- **Flush receive queue** defines whether the driver receive queue should be cleared before sending the first character.
- **Error level timeout** indicates the priority of the error if no positive reply is received within a specified time.
- If the reply is negative, the error level specified under **Error level neg. ack.** will be returned.
- The error level specified under **Error level failed** is used if a command sequence cannot be executed.

The list on the lower part of the dialog box contains the sent command sequence. Each line represents a single command. The commands are sent in the listed order. Each command is composed of the following seven entries:

- **Command**: Enter the format statement for creating the command string to send. The format is described further below.
- **Pos. response**: If the instrument sends a positive response in reply to the command string, the response can be entered here. The driver then waits until the response arrives or shows an error message.
- **Neg. response**: If the instrument sends a negative response in reply to the command string, the response can be entered here. In this case, the driver displays an error message.
- **Exec. time**: The command is considered completed after the time specified here has passed since sending the first character.
- **Timeout**: The positive response must arrive within this period.
- **Waittime**: If a negative response or no positive response was received, the command is repeated after this period.
- **Retries**: The command is repeated as specified here before it is aborted.

Format Instructions for Serial Command Strings

Wherever a command string should be sent or received when defining the driver, the command string must be entered as a valid format instruction. The instruction consists of **ASCII** characters, special characters, and variable references. Variable references can be included only in format instructions that are sent.

ASCII characters are all characters that can be directly displayed in the edit field, i.e. letters and numbers. Special characters include all other characters. To enter special characters, enter **** and two digits with the hexadecimal value of ASCII table (e.g.: \0D is <CR> and \0A is <LF>.

The current value of the property can be included in the format instruction using variable references. These must be entered with the following syntax **@[m][.n]f,<name>@**:

- **@** indicates the start of the variable reference.
- The **m** and **.n** parameter related to the definition of a specific number of digits for the numerical output. The parameters are entered within square brackets **[..]**to indicate that these parameters are optional. (The square brackets are not part of the format instruction and never appear within a valid instruction. They only serve to clearly structure the instruction.)
- The following character (here ‘f’) represents one of the following control characters:

d: Integer variable output as decimal value
u: Unsigned integer variable output as decimal value
o: Integer variable output as octal value
x: Unsigned integer variable output as hexadecimal value with lower case characters
X: Unsigned integer variable output as hexadecimal value with upper case characters
e: Floating-point number in exponential format (3.g. 3000 -> 3e4)
f: Floating-point number
g: Floating-point number in optimum format (e.g. 1.5 -> 1.5 but 2.0 -> 2)
c: Integer variable output as corresponding ASCII character

- ',' is the separation from the variable name.
- 'name' represents the name of a property of the device or a parameter of the current function. If property is referenced, properties of other devices contained within the current generic driver can be accessed by using a fully qualified name: <Device.Property>
- '@' indicates the end of the variable reference.

A simple format instruction with a variable reference for integer variables as the amplification factor could have the following appearance:

GAIN=@d,Gain@\0D\0A

GAIN= is sent to the instrument as fixed text, followed by the result of the reference variable. **@** introduces the variable reference. **d** means that the current value should be returned as an integer decimal value. As no further information is included on the number of digits, the current value determines the number of digits. The current value is extracted from the property **Gain** of the device. The command is completed via <CR><LF>. For further examples for more complex format instructions see below.

Defining Standard Property Settings in the "Property/Defaults" Dialog Box

The device driver initializes all properties with invalid values. If it is possible to establish a connection to an instrument, the field **Connect default** offers two possibilities to re-initialize the properties.

- **Set Value**: The current value of the property is set to the specified value without sending the corresponding command sequence to the instrument.
- **Send Command**: A command sequence is sent to the instrument with the specified value and is set as the new property value after correct performance.

Defining Functions "Function/Definition" Dialog Box

To create a new function, proceed as follows:

- Select the element **Functions** or an existing function in the definition tree.
- Click **New**....

This creates a new function with default settings. The dialog box for editing the function is opened.

- Enter the name of the new function. The name must be unique within the device.
- **Audit level** indicates the priority with which messages regarding this property are displayed in the audit trail.

Defining Serial Commands of Functions in the "Function/Command Sequence" Dialog Box

When a function is selected in the Dionex Chromatography Management System, the device driver sends a command sequence to the instrument. Use the procedure described for properties to define these command sequences (see **Defining Serial Commands of Properties** in the dialog box **Property/Command sequence**).

In the case of functions, format instructions of a command can contain variable references to properties and to function parameters.

Defining Parameters in the "Parameter/Definition" Dialog Box

To extend a function by parameters, proceed as follows:

- Choose the element '**Parameter'** or an existing function parameter from the definition tree structure.
- Click **New**....

A new parameter is then created with default settings. The dialog box for editing the parameter is opened. This dialog box corresponds to the one for defining properties (see **Defining Properties** in the dialog box **Property/Definition**).

The name of the parameter must be unique within the function. All parameters of a function must have different names. Assigning the same name to parameters of different functions is possible. In addition, the same name can be assigned to a property and a parameter. However, in the latter case it is not possible to specify a variable reference to the property, as this type of reference always refers to the parameter by the same name.

Defining Error Messages in the "Error/Definition" Dialog Box

To extend the device driver by an error message, proceed as follows:

- Choose the element **Errors** or an existing error message from the definition tree structure.
- Click **New**....

This creates a new error message with default settings. The dialog box for editing the message is opened. It contains three fields:

- **Error text**: Enter the text to be written to the Audit Trail. Each error message must have its own text.
- **Serial string**: Enter the format instruction (without variable reference) that is received to return an error message.
- **Error level**: Enter the priority of the generated error.

As errors are defined on the driver level, they are valid for all devices of the driver. The error message is linked to the device that is assigned to the serial interface on which the matching command string was received.

Predefined Properties and Functions

The Dionex Chromatography Management System expects drivers and devices to supply certain properties and functions. The type of properties and their names depend from the device type. An inject device must have the function **Inject**, and the properties **Position** and **Volume**. There are also optional properties and functions that the Dionex Chromatography Management System supports only if they actually exist.

Setting these properties and functions is partly predefined and cannot be changed. For the property **Volume**, the type must be set to **Floating Point** and the unit must be **µl**. The function **Inject** cannot be extended by parameters.

When generating a new device, all predefined properties and functions are automatically generated with default settings and must be adapted to the requirements of the driver. Predefined properties and functions that are optional can be deleted.

The following paragraphs offer information on the available device types.

Device Type "Standard Device"

The device type **Standard Device** forms the basis for all other types. All predefined properties and functions are also included with the other types.

As drivers communicate with external instruments, the Dionex Chromatography Management System assumes that the communication with the instrument must be explicitly enabled and disabled. The Dionex Chromatography Management System uses the functions **Connect** and **Disconnect**. In addition, the optional function **Reset** is defined.

- **Connect**: Enter the command string for switching the instrument into the remote mode. When starting the server, the Dionex Chromatography Management System automatically performs the **Connect** function for all serial instruments. This guarantees that user-defined instruments are reset to the serial remote mode after restarting the server and that instruments can be immediately addressed via commands (e.g. after a power failure).

After successfully completing the command sequence of **Connect**, the action specified in the default settings (see **Defining Default Settings of Properties** in the dialog box **Property/Defaults**) is performed for each property.

- **Disconnect**: Here, the command sequence must be entered for switching the instrument to the manual mode. This function is opened when closing the server to make all instruments accessible for the manual mode.
- **Reset**: If the instrument should be set to a defined status in the event of an error, the corresponding command sequence can be entered here.

Device Type "Inject Device"

With the device type **Standard Device**, it is not possible to perform the inject command correctly (as the return signal sent by the sampler after the injection cannot be processed). For this reason, a special device type is required for controlling autosamplers that are not supported by a separate device driver.

In addition to the already described predefined functions of the standard type, the properties **Volume** and **Position** as well as the function **Inject** are required here.

- **Volume**: The Dionex Chromatography Management System always sets this property to the sample volume to be injected.
- **Position**: The Dionex Chromatography Management System always sets this property to the sample position from which to inject.
- **Inject**: This function starts the injection procedure. As this function does not have parameters, the current injection parameters of the properties **Volume** and **Position** must be used.

After the **Inject** command, the Dionex Chromatography Management System waits for the **Inject Response** from the driver, indicating that the injection process is completed. Only then is the time program started.

The device driver offers two possibilities to supply the **Inject Response** to the Dionex Chromatography Management System:

- **Digital inject response**

  If the system has a correctly installed remote input, as e.g. the Dionex UVD 340S, the A/D converter board or the Dionex pump control board, the **Inject Response** can be recorded via the remote input. Choose the value **Digital inject response** when defining the device in the field ‘Inject response’. When installing the driver, the driver must be assigned the remote input to record the signal.

- **Serial inject response**

  Instead of the remote input, the **Inject Response** can be recorded directly via a serial connection. However, it is necessary that the autosampler sends a corresponding string after the injection is completed. If this is the case, and if the command is listed in the manual for the instrument, choose **Serial inject response** in the **Inject response** field. Enter the appropriate format instruction in the field **Serial string**.

Device Type "Channel Device"

For detector drivers, the channels must be connected to analog inputs of the ➢*A/D Converter* during installation. In addition, the Dionex Chromatography Management System supports these devices when automatically generating programs.

The predefined functions of the standard type are usually sufficient. The properties **Wavelength**, **Range**, and **Response** and the function **Autozero** are optional.

- **Wavelength**: This property indicates the wavelength of the analysis.
- **Range**: This property defines the factor, by which the analog output signal is increased or reduced.
- **Response**: This property indicates the time the detector requires for reaching 98% of the full scale.
- **Autozero**: This property resets the output signal to zero.

When installing the driver, the channel must be connected to an analog signal. The signal parameters must be set.

Checking the Control Commands

To check whether the definitions are actually supplying the required command strings for the instrument control, the **Demo** mode is activated. The device driver now sends all formatted command strings of a command to the **Audit** window of the corresponding timebase. Non-printable characters are output as hexadecimal codes following a slash.

The control character <CR> is mapped to **\0d**. The entire output is completed by a period to enable evaluating the total length of the command string. Otherwise, leading or appended blank spaces would not be visible. A typical Audit message has the format:

"{Instrumentname} Send: CommandString."

Caution: In the **Demo** mode, there is no output via the serial port!

If the entire input is interpreted correctly, you can proceed with the following paragraphs. You will find detailed information on format styles and the use of truth tables and lists.

Format Instructions in Detail

The optional parameters **m** and **n** of the general variable reference **@[m][.n]f,<name>@** are especially interesting here.

In the simplest case, **m** is an abstract number for the entire length of the formatted numerical output, including a possibly existing decimal point. Additional information can also be included (e.g. left-align or right-align numerical output in the output field, fill superfluous places with blank spaces ( ) or zero (**0**), etc.). **n** represents the number of decimal places (only sensible for floating point numbers, not available for integer variables).

Example:

The following table contains various format instructions for integer and floating-point numbers. On the right, you can see the corresponding result of the output with these instructions. The quotation marks serve to indicate the orientation of the numbers within the output field that is part of the entire command string!

Number	Type	Format instruction	Result
1234	Integer	@d	‘1234’
1234	Integer	@5d	‘ 1234’
1234	Integer	@05d	‘01234’
1234	Integer	@09d	‘000001234’
1234	Integer	@-7d	‘1234 ’
1234	Integer	@o	‘2332’
1234	Integer	@x	‘4d2’
1234	Integer	@X	‘4D2’
-1234	Integer	@x	‘fffffb2f’
1234.5678	Floating point	@f	‘1234.567800’
1234.5678	Floating point	@.4f	‘1234.5678’
1234.5678	Floating point	@.3f	‘1234.568’
1234.5678	Floating point	@6.2f	‘1234.57’
1234.5678	Floating point	@5.2f	‘1234.57’
1234.5678	Floating point	@-15.2f	‘1234.57 ‘
1234.5678	Floating point	@15.2f	‘ 1234.57’

Discrete Range of Values and Truth Tables

Frequently, specific parameters can only be modified using discrete steps or can only assume certain values. Sometimes, it may be a good idea to assign meaningful terms to specific instrument states that are controlled serially via numerical parameters, e.g. assigning INJECT and LOAD to the motorized switching valve settings instead of **0** and **1**. To enter settings, the parameters **Step** and **Table** are available for numerical values in the edit dialog box.

Discrete Equidistant Value Distributions

The default setting for **Step** is zero. As soon as this integer variable is larger than zero, it determines the number of equidistant steps for the range of values between **Min** and **Max**. The input 1 means that only the values **Min** and **Max** are valid. The input 2 enables **Min**, **Max** and the value (**Min**+**Max**")/2, etc. Thus, **Step** allows selecting a discrete quantity of valid input values from the progressive range of values between **Min** and **Max**. Neighboring values are divided by (**Max**-**Min**)/ **Step**. If the device driver receives numerical input for this parameter that do not correspond exactly to the discrete value, input is automatically replaced by the nearest valid value. A corresponding message is included in the Audit Trail of the timebase.

Frequently, valid values are not equidistant, or the user does not only require numerical values for the instrument status. In this case, use the **Table** (see below).

User-Defined Value Quantities and Lists

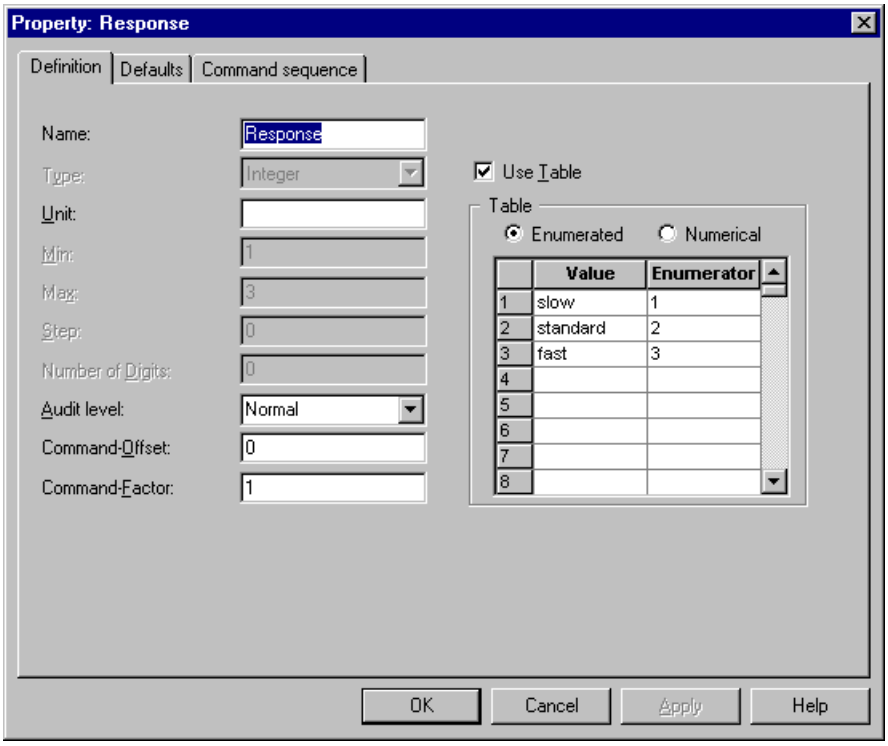
- Activate the table by selecting **Use Table**.

The **Type**, **Min**, **Max**, **Step**, and **Number of Digits** controls for entering the parameter definition are deactivated. The description of the discrete range of values is exclusively via the table. Two different modes are available that can be selected via the **Enumerated** and **Numerical** buttons

Example:

In a detector the time constant **Response** for the output signal is to be controlled via the **CTIME=X<CR><LF>** command string. X can assume the numerical values 1, 2, and 3, which correspond to the instrument presetting **slow**, **standard**, and **fast**. To view the actual settings instead of the numbers, activate the **Table** and choose the **Enumerated** mode.

The column headers of the table are now **Value** and **Enumerator**. Enter the terms for the status description below **Value**, and enter the corresponding numerical values in the **Enumerator** column. For this example, the input should be as follows:



On the screen, the settings **slow**, **standard**, and **fast** appear. These are converted into the command strings: **CTIME=1<CR><LF>**, **CTIME=2<CR><LF>** and **CTIME=3<CR><LF>**.

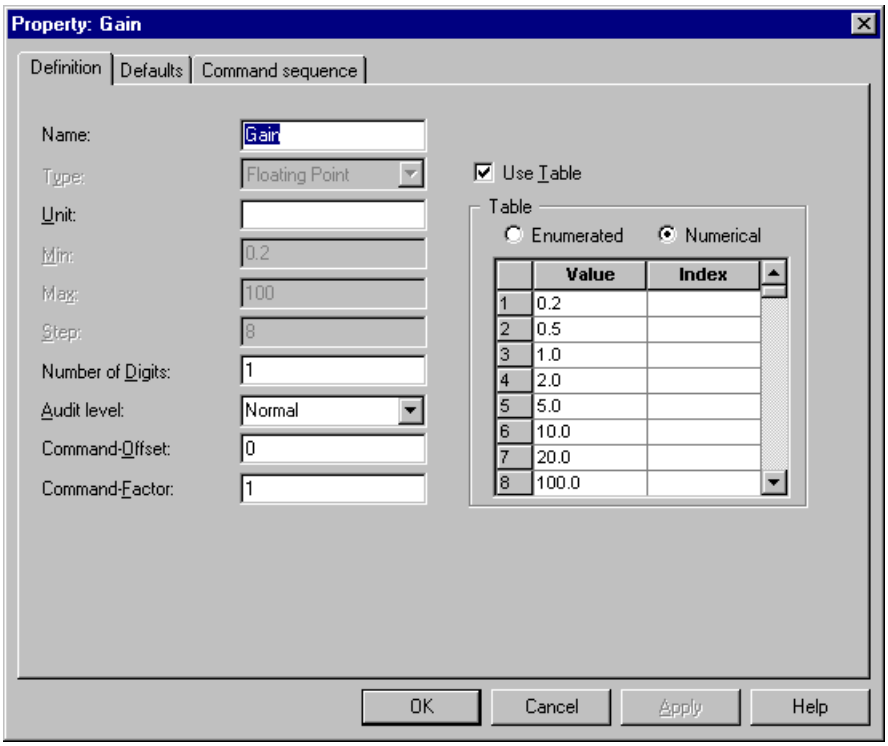
The input mode **Numerical** serves to select discrete, non-equidistant values, or their mapping to the corresponding control indices. This can be used e.g. for specifying amplification factors that are frequently adjustable in the 2,5,10 across several orders.

Example:

For the **Gain** variable, only the values 0.2, 0.5, 1, 2, 5, 10, 20, 100 are valid. They are communicated via the **GAIN=X<CR><LF>** command string to the instrument. **X** represents the current value.

- Choose the **Numerical** mode and enter the values in the **Value** column in an ascending order.
- The **Index** column remains empty.

Now, only discrete values are valid. If the user enters deviating values that are within the **Min** - **Max** range, the device driver changes the value to the nearest valid value. Simultaneously, this correction is documented in the **Audit Trail**.



Indexed Discrete Value Quantities

Frequently, discrete values are indexed in addition, i.e. each value is assigned an integer value. These values are entered in the **Index** column.

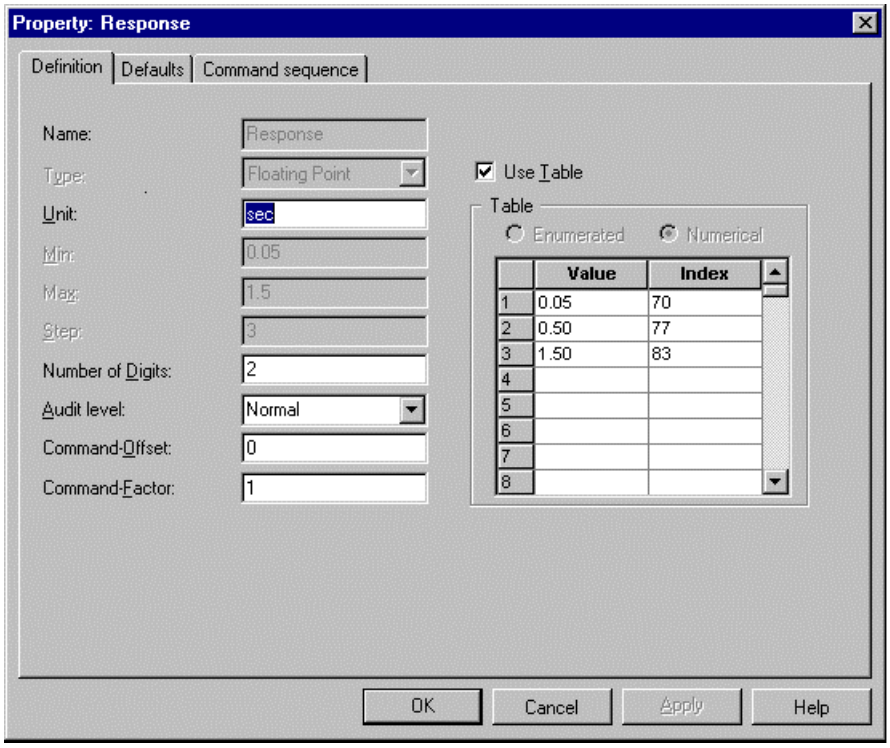
- If you want to index discrete values, each value must receive a corresponding integer value in the **Index** column.

Within the command string, the integer value is used instead of the floating-point number. The device driver converts the values into the indices. These are then sent to the instrument via a format instruction (e.g. **d**).

You can also use this feature to translate enumerated constants into ASCII characters. Enter the corresponding ASCII value as the index and use the format instruction **c**.

Example:

For the **Response** variable, the values 0.05, 0.5, and 1.50 are valid only. They are communicated to the instrument via the **RESPONSE=X<CR><LF>** command string. **X** represents the letter F (ASCII 70), the letter M (ASCII 77) or S (ASCII 83) corresponding to the variable value.



Appendix: Cables and Pin Assignments

Operating the various instruments requires different groups of cables:

- Power cables (refer to the information in the Installation Instructions of the manufacturer that are shipped together with the instrument.)
- Control cables (mainly RS232 cables; most of them are available from Dionex - see below)
- A/D cables (for data acquisition of analog detectors except the Dionex IC detectors, the Dionex UVD160/320, UVD170/340, PDA-100, and HP1100 detectors)

Controlling third-party instruments via the various ➢*Device Drivers* requires different control cables. For further information on these cables, see:

- **Fisons AS: Cable - Dionex P/Ns 8914.0127 / 8914.0143**
- **Fisons GC: Cable - Dionex P/Ns 8914.0126 / 8914.0142**
- **Gilson: GSIOC Cable**
- **HP5890 RS232 Cable**
- **Modem Cable (1:1 RS Cable)**
- **Null Modem Cable (RS232)**
- **THERMOQUEST Trace GC: Cable - Dionex P/Ns 8914.0148 / 8914.0149**
- **THERMOQUEST AS2000 / Trace GC: Cable**
- **TSP/Linear: Cable - Dionex P/N 45789 (Cable AI450 to AS3500)**
- **Varian: Cable - Dionex P/N 8914.0145**

FISONS AS: Cable - Dionex P/Ns 8914.0127 / 8914.0143

Instrument for which the cable is required

Fisons AS800

Pin Assignments

Connecting the Fisons AS800 to the serial interface of the Server PC requires the following cable:

AS800		PC	PC
(9-pin, Sub-D, male)		(25-pin; Sub-D, female)	(9-pin; Sub-D, female)
1			
2	----------	3 (RXD)	2 (RXD)
3	----------	2 (TXD)	3 (TXD)
4	----------	20 (DTR)	4 (DTR)
5	----------	7 (GND)	5 (GND)
6			
7			
8	----------	5 (CTS)	8 (CTS)
9	----------		

Dionex Part Numbers

- **8914.0127** 25-pin - 25-pin; 5m
- **8914.0143** 9-pin - 25-pin; 5m

FISONS GC: Cable - Dionex P/Ns 8914.0126 / 8914.0142

Instrument for which the cable is required

Fisons 8000 GC /Mega 2 GC

Pin Assignment

Connecting the Fisons 8000 to the serial interface of the Server PC requires the following cable:

Fisons GC		PC	PC
(25-pin; male)		(25-pin; female)	(9-pin, female)
4	----------	8	1
2	----------	3	2
3	----------	2	3
5 --- 6	----------	20	4
7	----------	7	5
20	----------	5 --- 6	6 --- 8
8	----------	4	7
22	----------	22	9

Dionex Part Numbers

- **8914.0126** 25-pin - 25-pin; 5m
- **8914.0142** 9-pin - 25-pin; 5m

Gilson: GSIOC Cable

Instruments for which the cable is required

- **Gilson UV Detectors 116, 117, and 118**
- **Gilson Fraction Collector 201/202 and 206**
- **Gilson Autosamplers 231, 232 Bio, and 234**
- **Gilson Pumps 302, 303**
- **Gilson Pumps 305, 306, 307**
- **Gilson Valves (817, 819, and UVSM)**
- **Gilson Autosamplers 231XL, 232XL, 233XL (Old Device Driver)**
- **RAININ/VARIAN Pumps (SD-1, SD-200/SD-300, ProStar 215)**

Caution:

Under the Dionex Chromatography Management System, the GSIOC bus available from Gilson is used exclusively for combining several pumps in a high-pressure gradient system. All other instruments (e.g. ➢*Autosampler* and Detectors) are controlled individually via separate serial interfaces. All instruments (except those with serial interface) must therefore be connected via an original Gilson cable (GSIOC adapter Model 605) to a PC interface. **The adapter is shipped with the baud rate set to 19200 Baud. For controlling specific instruments via the Dionex Chromatography Management System (i.e., in case of specific drivers (see setting on the tab "General" of the corresponding instrument properties)), it is necessary to set the baud rate to 9600 Baud.** To do this, open the connector housing. Resolder the cable from land A to land B (for details, see the Gilson **605 RS232 Adapter and GSIOC Protocol - USER'S GUIDE**).

Tip:

Always connect Gilson instruments requiring a GSIOC cable to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095) as communication problems might occur with other RS232 ports (e.g. with the COM ports of the PC or the **Dionex Universal Chromatography Interface**). The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. However, the RS232 ports of the ➢*UCI-100* Universal Chromatography Interface are not designed for this.

Dionex Part Number

This cable is available from Gilson only.

HP5890: RS232 Cable

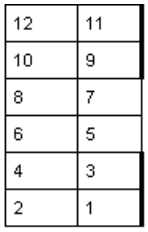
Instrument for which the cable is required

HP5890

Pin Assignment

RS232 Cable

Replace the 25-pin male connector of the Agilent RS232 cable by a 25-pin female connector (Dionex part no. 1282.5021).



12 (not used)	11 (not used)
10 (not used)	9 (not used)
8 (not used)	7 (not used)
6 TXD	5 (not used)
4 GND	3 (not used)
2 RXD	1 (not used)

Pin assignment for the RS232 communication:

HP5890		PC	PC
(12-pin, Sub-D, male)		(25-pin; Sub-D, female)	(9-pin; Sub-D, female)
2	----------	3 (RXD)	2 (RXD)
4	----------	7 (GND)	5 (GND)
6	----------	2 (TXD)	3 (TXD)

Dionex Part Number

The cable is available from Agilent only.

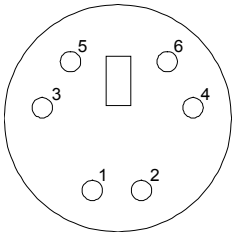
HP6890: A/D Cable

Instrument for which the cable is required

HP6890

Pin Assignment (Front View)

(Please refer to the manufacturer's information in the Installation Instructions that are shipped together with the instrument.)



HP6890 (Agilent analog cable)		A/D Converter
2 (white)	----------	(-)
4 (black)	----------	(+)

Dionex Part Number

The cable is available from Agilent only.

Modem Cable (1:1 RS Cable)

Instruments for which the cable is required:

- **CTC ANALYTICS A200S / Fisons A200S**
- **Gilson: Liquid Handler 215**
- **Gilson: Autosamplers 235 and 235p**
- **Gilson: Autosamplers XL Series (221XL, 222XL, 231XL, 232XL, 233XL)**
- **Gilson: Valves (ValveMate only)**

Pin Assignment

(Also, see ➢*Pin Assignment*):

Instrument			PC	
9-pin male connector	25-pin male connector		25-pin female connector	9-pin female connector
2	3	----------	3	2
3	2	----------	2	3
5	7	----------	7	5
If there is an additional hardware handshake, the following assignments are also required:				
7	4	----------	4	7
8	5	----------	5	8

Modem cables are also called 1:1-RS cables.

Dionex Part Numbers

- **8914.0144** 25-pin - 9-pin, 5m
- **8914.0128** 25-pin - 25-pin, 5m

☞ ***Tip***: Do not confuse non-crossover modem cables (= 1:1 RS cables) with crossover ➢*Null Modem Cables*!

For information on additional or other connections, refer to the installation instructions for the respective instrument for details (also, see **Installing and Controlling Third-Party Instruments**).

Null Modem Cable (RS232)

Instruments for which the cable is required

- **HP1050**
- **HP6890**
- **Gilson: Autosampler 231/232/233XL (Old Device Driver)**
- **TSP: UV3000 / Linear Detector 206**

Pin Assignment

(Also, see ➢*Pin Assignment*)

Instrument			PC	
9-pin female connector	25-pin female connector		25-pin female connector	9-pin female connector
2	3	----------	2	3
3	2	----------	3	2
5	7	----------	7	5
If there is an additional hardware handshake, the following assignments are also required:				
4	7	----------	6	6
6	6	----------	7	4
7	4	----------	5	8
8	5	----------	4	7

☞ ***Tip***: Do not confuse crossover null modem cables with non-crossover ➢*Modem Cables* (1:1 RS cables)!

Dionex Part Numbers

9-pin to 9-pin:

- **8914.0129** for RS cable RU, 2.5m
- **8914.0130** for RS cable RU, 5m
- **8914.0131** for RS cable RU, 10m

25-pin - 9-pin:

- **8914.0103A** for RS cable RU, 2.5m
- **8914.0120** for RS cable RU, 5m
- **8914.0121** for RS cable RU, 10m

If necessary, use an adapter to connect the cable to a 25-pin socket. These null modem cables have been slightly modified to ensure data transmission even with enabled hardware handshake. However, the above hardware handshake is not realized.

For information on additional or other connections, refer to the installation instructions for the respective instrument for details (also, see **Installing and Controlling Third-Party Instruments**).

THERMOQUEST Trace GC: Cable Dionex P/Ns 8914.0148 / 8914.0149

Instrument for which the cable is required:

THERMOQUEST: Trace GC

Pin Assignment

Connecting the ThermoQuest Trace GC to the serial interface of the server PC requires the following cable:

Trace GC		PC	PC
(9-pin, Sub-D, male)		(25-pin; Sub-D, female)	(9-pin; Sub-D, female)
1			
2	----------	3 (RXD)	2 (RXD)
3	----------	2 (TXD)	3 (TXD)
4	----------	20 (DTR)	4 (DTR)
5	----------	7 (GND)	5 (GND)
6			
7			
8	----------	5 (CTS)	8 (CTS)
9	----------		

Dionex Part Number

- **8914.0148** 9-pin to 9-pin
- **8914.0149** 25-pin to 9-pin

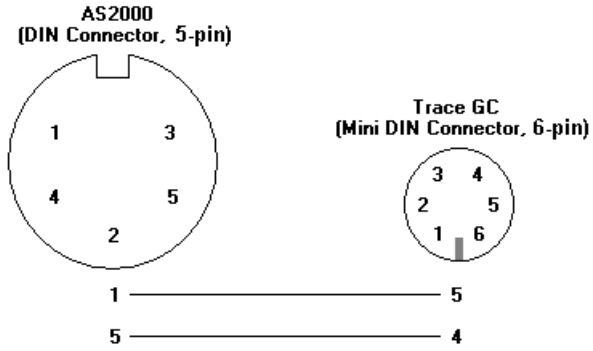
THERMOQUEST AS2000 / Trace GC: Cable

Instruments for which the cable is required:

- **THERMOQUEST: AS2000 GC Autosampler**
- **THERMOQUEST: Trace GC**

Pin Assignments

(Also, refer to the Installation Instructions supplied with the instrument.)



Dionex Part Number

This cable is available from ThermoQuest only.

TSP/Linear: Cable (Cable AI450 to AS3500) - Dionex P/N 45789

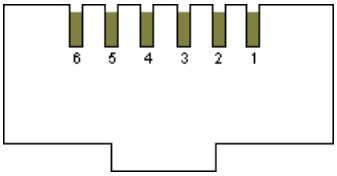
Instruments for which the cable is required:

- **TSP AS3500/AS3000 Autosamplers**
- **TSP P2000 and P4000 Pumps**
- **TSP UV1000 Detector**
- **TSP UV2000 / Linear UV205 Detector**

Pin Assignment

Autosampler (RJ11)		PC (D-Sub 9-pin male)
3	----------	2
4	----------	3
2	----------	5
5	----------	5

The pin assignment at the 6-pin RJ11 connector is as follows:



Dionex Part Number

45789 (Cable AI450 to AS3500)

VARIAN: Cable - Dionex P/N 8914.0145

Instrument for which the cable is required:

VARIAN 3400 GC

Pin Assignment

Varian 3400 (D-Sub 9-pin female)		PC (D-Sub 9-pin female)
6	----------	2
4	----------	3
7	----------	5

Dionex Part Number

8914.0145

Reference Manual

Sequence, Sequence Table, Sample List

A sequence consists of a list of samples to be processed, in which the samples are described (e.g. name, injection volume, dilution, etc.). Details of sample processing are referenced by file names and stored in the respective ➢*PGM Files* in the sequence.

To create a sequence, use the **Sequence Wizard**.

***Tip**:* Do not use special characters (e.g. umlaut) for new directory names or sequences, as this may cause problems in Novell networks!

The new sequence may be reedited afterwards in the ➢*Browser*. Each line of the table represents a sample. Theoretically, the number of samples is not limited, but 100 sample entries should be exceeded only in exceptions. The more sequences are created, i.e., the fewer samples are included in one sequence, and the higher is the access speed to samples. In addition, it is easier to keep track of the samples processed.

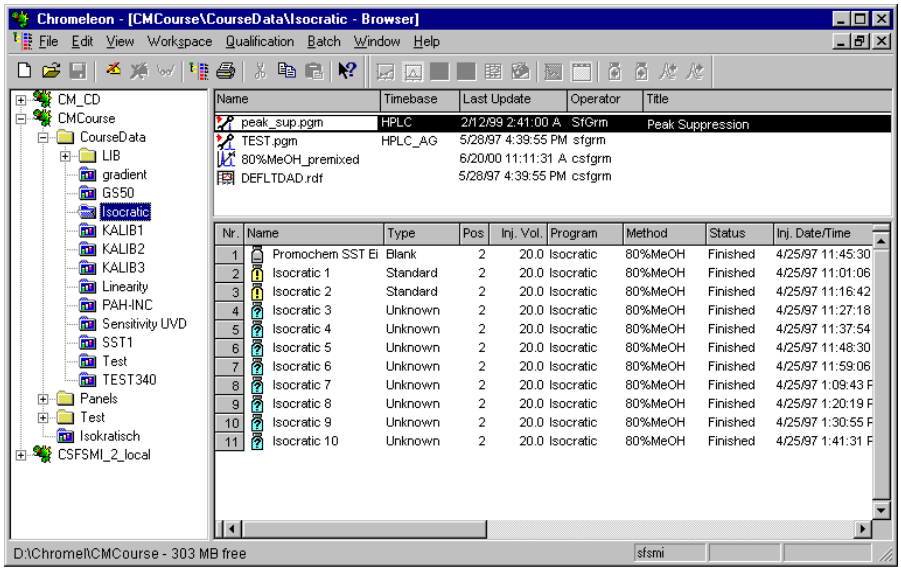
Tip: Injections that are made from the same vial are regarded as separate samples!

The sequence table also defines how to process a sample. This includes information on the sample itself (injection volume, position, weight, dilution factor, etc.) as well as references to chromatographic methods that specify which program (PGM file) to be performed for the analysis and the evaluation parameters to be used (QNT method).

Usually, sequences are started from a ➢*Control Panel*. However, they can be started directly in the Browser as well provided the sequence has already been assigned to the respective ➢*Timebase*. Either press **Start** in the ➢*Batch* menu or choose the corresponding button of the online ➢*Toolbar*.

The entire data collected in connection with creating and processing a sequence, including raw data and protocol data recorded during the analysis, is saved in the sequence directory of a ➢*Datasource* or in the underlying database. Of course, this includes the raw and protocol data recorded during the analysis.

Similar to datasources, sequences can be "locked." In this status, data and results can only be read, not modified or extended. For details on locking datasources, directories, and sequences, see **Data**: **Datasource**.



The screenshot shows the default configuration of the Browser, which can be reconfigured as required. You may add or delete columns or change their order, respectively according to your specific requirements. The layout is saved as well. Therefore, if you reedit the sequence at later date, the representation will correspond to the one of your last access. The samples are entered in the table in the order in which they are to be processed. For information on the parameters that describe the individual samples, see the ⇒*Sample Variables* below.

Sample Variables (Overview)

The variables in the  **Sample List (Sequence Table)** columns are referred to as sample variables. They characterize a sample and are stored in a database as part of the ➢*Sample Data*. For an explanation of the columns, see the following pages:

⇒*Comment* (Sample Comment)

⇒*Dil. Factor* (Dilution Factor)

⇒*Inj. Date/Time*

⇒*Inj. Vol.* (Injection Volume)

⇒*ISTD Amount* (Amount of the ➢*Internal Standard*)

⇒*Method* (QNT Method)

⇒*Name* (Sample Name)

⇒*No.* (Sample Number)

⇒*Pos.* (Sample Position)

⇒*Program* (also, see: ➢*PGM File*)

⇒*Replicate ID*

⇒*Sample ID*

⇒*Status* (Sample Status)

⇒*Type* (Sample Type)

⇒*Weight* (Sample Weight)

Comment *(Sample Comment)*

Type:	**Text**
Dimension:	**---**
Value Range:	**All printable characters**
Default:	**---**
Related Param.:	⇒*Name* (sample name)
Description:	In addition to the sample name, further comments can be entered. Use F8 to open an enlarged edit field.

Dil. Factor *(Dilution Factor)*

Type:	**Floating point value**
Dimension:	**---**
Value Range:	**0000.001 ... 99999999**
Default:	**1.0**
Related Param.:	⇒*Inj. Vol.* (injection volume) ⇒*Weight* (sample weight)
Description:	The ⇒*Sample Variable* **Dilution Factor** is a correction factor for amount calculation formulas. As the injection volume, it can also be used for multi-point calibrations to define the dilution of subsequent calibration samples. For integration samples, it serves to account for any dilution that was made before the injection.
Function:	The calculated values for all peaks of a sample are corrected by the appropriate dilution factor.
***Note**:*	The effect is reciprocal to injection volume, i.e., a larger dilution factor indicates that less component is present.

Inj. Date / Time *(Time of Injection)*

Type:	**Character String**
Dimension:	**Month/Day/Year Hours:Minutes:Seconds**
Value Range:	**---**
Default:	**---**
Related Param.:	**Time**
Description:	This column cannot be edited. The Dionex Chromatography Management System enters the injection time and date of the sample in the corresponding column of the sample list. For samples with the ⇒*Status (Sample Status)* M (multiple), the time of the last injection is entered. The Dionex Chromatography Management System stores the time stamps as universal time (Greenwich time). However, the date notation is displayed according to the country and system settings chosen in the operating system.
Function:	The kind of entry (empty or time value) indicates whether and when the sample was processed.
***Note**:*	The time difference between successive samples is generally the analysis time plus the time required for injecting the following sample because the report is generated parallel to the online batch. As the injection time is generally minimal, the time value provides a reliable indication as to whether the sample batch was processed without incident (e.g. power failure, third-party interference).

Inj. Vol. *(Injection Volume)*

Type:	**Nonnegative integer**
Dimension:	**µl**
Value Range:	**system-dependent**
Default:	**20.0**
Related Param.:	⇒*Dil. Factor* (dilution factor) ⇒*Weight* (sample weight)
Description:	The ⇒*Sample Variable* **Injection Volume** defines the injection volume in micro liters (µl). In automatic operation, the installed ➢*Driver* converts this value into a volume readable by the autosampler, then the value is sent to the ➢*Autosampler*. By entering different injection volumes, a ➢*Dilution Series* can be created in case of a multiple-point calibration (➢*Single-Point and Multiple-Point Calibration*).
Function:	In a multiple-point calibration, using differing injection volumes, the concentration of the second calibration sample is calculated from the injection volumes of the first and the second sample. The same principle (doubling injection volume equals doubling the amounts of each component) is applied to all subsequent calibration samples. In a multi-point calibration with a "concentration series" (varying injection volume) which was created with an automatic autosampler it is therefore only necessary to enter the component amounts for the first standard sample into the peak table. All additional calibration values, i.e., the corresponding amounts of the subsequent standard samples (Type: **Standard**) are calculated by the data system.
***Note**:*	In order to minimize carry-over effects in such a multiple-point calibration, standard order should always be from lowest to highest concentration.

ISTD Amount *(Amount of the internal standard)*

Type:	**Floating point value**
Dimension:	**---**
Value Range:	**0.001 ... 999999.9999**
Default:	**1.0000**
Related Param.:	⇒*Dil. Factor* (dilution factor) ⇒*Inj. Vol.* (injection volume)
Description:	The ⇒*Sample Variable* **ISTD Amount** is only required for a calibration based on a variable ➢*Internal Standard* (internal or internal/external). In this case, the column serves in the sample list for entering the amount values of the internal standards used for the different samples. Input is directly in the sample list (via the keyboard or the F8 edit dialog box). Editing the column in the QNT editor is not possible. Entering the amount values in the peak table is omitted.
Function:	The **ISTD Amount** parameter is implemented as a multiplication factor in the ➢*Amount Calculation Formula* and is dimensionless.

Method *(QNT Method)*

Type:	**File name**
Dimension:	**---**
Value Range:	---
Default:	**Name of QNT file**
Related Param.:	⇒*Program* (PGM file)
Description:	The **Method** column (in the Browser) contains the name of the **Quantification Method**. The quantification method includes all parameters that are used for evaluating a peak or the entire chromatogram.
Function:	The QNT method serves as the basis for calculation for sample evaluation. It includes: ⇒*QNT Parameters* All parameters required for (qualitative) peak identification and for converting the determined peak areas into amount or concentration values (quantitatively) ⇒*Detection Parameters* All parameters regarding e.g. peak recognition and peak area evaluation ➢*Calibration Variables* All parameters regarding the type and performance of a calibration ➢*Blank Run Subtraction* Information on baseline subtraction Peak Tracking Parameters for comparing spectra to library or sequence spectra Spectra Library Screening Parameters for spectra library screening

Function (Cont'd):

➢*System Suitability Test (SST)*
Parameters for performing the System Suitability Test

MS
Parameters for evaluating ➢*Mass Spectra*

☞ ***Tip***:

Normally it is not necessary to include the QNT method in the sample list before the analysis starts. However, if you want to perform a System Suitability Test, ensure to enter the QNT file into the sample list before starting the analysis. Otherwise, the batch cannot be aborted in case of **Fail Action** - **Abort Batch** because the SST will not yet be performed during the batch run!

Name *(Sample Name)*

Type: **Character String**

Dimension: **---**

Value Range: **All printable characters**

Default: **[Sample] [No.]**

Related Param.: **---**

Description: The ⇒*Sample Variable* **Name** serves to identify a sample and to label graphics and reports.

Function: The **Fill Column** function (F9) allows automatic sample name generation. For this purpose, the currently selected name can be copied or a character string with wild cards as template can be entered. These are names that might include e.g. the sample number (#n, see ⇒*No.*), the position (#p, see ⇒*Pos.*), the replicate number (#r), and the injection volume (#i, s. ⇒*Inj. Vol.*). Thus, telling names can be easily generated using these wild cards! The replicate number is calculated from the repetition of a sample number. Example: If two injections are made from the first two vials the template „Analysis-#p_Repl.#r" yields the following names:

Analysis-1_Repl.1

Analysis-1_Repl.2

Analysis-2_Repl.1

Analysis-2_Repl.2

When creating a sample list using the **Sequence Wizard**, automatic sample name generation is possible as well.

Note: Each line represents an individual analysis. As multiple injections of the same sample also represent multiple analyses, a sample line must be reserved for each injection.

No. *(Sample Number)*

Type:	**Nonnegative integer**
Dimension:	**---**
Value Range:	**1 ... infinite**
Default:	**Ascending number**
Related Param.:	**---**
Description:	The user cannot edit the sample number. Each new line in the sample list (i.e. each analysis) is assigned its own number.
☞ ***Tip***:	Each injection (or replicate) occupies its own line in the sample list and is, therefore, an individual analysis for which an individual raw data file is created.

Pos. *(Sample Position - Sample List)*

Type:	**Nonnegative integer and/or letters**
Dimension:	**---**
Value Range:	**Depending on the autosampler**
Default:	**Sample number**
Related Param.:	**Number**
Description:	The ⇒*Sample Variable* **Pos**. determines the position of the sample in the ➢*Autosampler*. For externally controlled autosamplers, this value is automatically transmitted to the autosampler for sample processing. The sampler approaches the corresponding sample for injection. For non-controllable autosamplers, this value is for documentation purposes only. If the sample position parameter is not entered, the previous (current) value is used.
Function:	Depending on the segment type used, the ASI-100/ASI-100T sampler offers 63 position for semiprep vials, 66 positions for Eppendorf vials, 117 positions for analytical vials, or 192 positions for mini vials. Letters according to their color describes the individual segments: R, G, or B (indicating the red, green, and blue segment, respectively). The different rows are described from the outer to the inner row: A, B, C, or D. The individual positions within the respective rows are number counterclockwise. The position RA1, for example, is in the outer row of the red segment (also, see the ASI-100/ASI-100T Operating Instructions).

Program *(PGM File)*

Type:	**File name**
Dimension:	**---**
Value Range:	---
Default:	**Name of PGM file**
Related Param.:	⇒*Method* (QNT Method)
Description:	The column serves for entering a **Control Program** name. The file contains all information for chromatographic sample processing. These are commands for HPLC instrumentation (flow, %B, etc.), analysis time, acquisition time, etc. For further details, see ➢*PGM File*. Input for a sequence is by directly editing the column in the Browser. The list box offers all program files that are part of the sequence.
Function:	The sample is processed according to the conditions contained in the PGM file.

Replicate ID

Type:	**Text**
Dimension:	**---**
Value Range:	**All printable characters**
Default:	**---**
Related Param.:	⇒*Name* (sample name) ⇒*Sample ID*
Description:	The **Replicate ID** column serves to mark samples as ➢*Replicates*.
Function:	This column is a mere text column and not used for evaluation purposes. The replicate ID is used to identify samples as replicates. If a sequence is generated using the Sequence Wizard (only then), the sample position is entered here. Samples with identical replicate IDs can be grouped in the report by means of suitable settings (Sort Summary by smp.sampleID). Accessing these data for a query (see **How to ...: Actions in the Browser**  **Performing a Query**) is possible as well.

Sample ID

Type:	**Text**
Dimension:	**---**
Value Range:	**All printable characters**
Default:	**---**
Related Param.:	⇒*Name* (sample name) ⇒*Replicate ID*
Description:	The user or a help program enters a sample ID in the Sample ID column.
Function:	This column is a mere text column and not used for evaluation purposes. The sample ID is intended for LIMS connections that usually know sample IDs. Samples with identical sample IDs can be grouped in the report by means of suitable settings (Sort Summary by smp.sampleID). Accessing these data for a query (see **How to ...: Actions in the Browser**  **Performing a Query**) is possible as well.

Status *(Sample Status)*

Type: **Text**

Dimension: **---**

Value Range: **Single/Finished/Multiple/Running**

Default: **Single**

Related Param.: ⇒*Inj. Date/Time (Time of Injection)*

Description: The ⇒*Sample Variable* **Status** determines the current sample processing status. A sample is either unprocessed (Single), or Finished, or due for multiple processing (Multiple).

The Dionex Chromatography Management System also maintains a log of the sample status, i.e., a **Single** sample is automatically assigned the status **Finished** as soon as processing is completed. A sample may also be excluded from processing by assigning the status Finished manually.

The sample status has a special significance for the built-in ➢*Power-Failure Protection*. Upon recovery from a power failure or starting the sample batch after a manual interruption, the Dionex Chromatography Management System continues processing the sample batch according to the selected power-failure handling option.

Functions:

Single The sample is processed only once, after which it receives the status Finished. When loading a sample list for processing (online), only samples with the status Single and Multiple are processed.

If a Single sample contains an entry in the time column, this indicates that the sample was injected but was interrupted before completion.

Finished All original Single samples are automatically assigned the status Finished after successful processing. A sample with the status Finished will be omitted in the renewed processing (also following a ➢*Power Failure*). In ➢*GLP* ➢*Datasources*, it is not possible to reset the sample type Finished to Single.

Multiple The sample can be repeatedly acquired. The system just enters the ⇒*Inj. Date/Time (Time of Injection)* in the **Time** column. Existing ➢*Raw Data* are overwritten with each new data acquisition.

New samples can have the status Multiple assigned only if the **Enable Sample Status Multiple** option of the corresponding datasource is activated. The option is available in the (datasource) **Properties** (via the Properties command of the context menu) on the **General** tab. Samples that have the status Multiple already assigned keep their status even with disabled **Enable Sample Status Multiple** option.

Running A running sample is marked green. Having been processed it gets the status Finished or Multiple assigned (without background color).

☞ ***Tip***: Samples can be opened as well while being analyzed, i.e. while being in **Running** status (see **Opening a Sample**).

☞ ***Tip***: Multiple status samples will be acquired each time. The raw data, therefore, are not protected from accidental overwriting. The **Time** column indicates, however, whether and when the sample was last injected. If this column is empty, the sample has not yet been acquired at all.

Type *(Sample Type)*

Type: **Text**

Dimension: **---**

Value Range: **Blank, Unknown, Standard, Validate, Matrix**

Related Param.: **Amount, Baseline Subtraction**

Default: **Unknown**

Description: The ⇒*Sample Variable* **Type** indicates the sample type:

- Select **Unknown** for an unknown analysis sample:  .
- Select **Standard** for a standard sample with known concentration:  .
- Select **Validate** for a ➢*Validation Sample*: ().
- Select **Blank** for a ➢*Blank Run Sample* (). If a sample is corrected by the ➢*Raw Data* of a blank run sample, this is referred to as ➢*Blank Run Subtraction*.
- Select **Matrix** for a ➢*Matrix Blank Sample*: 

Functions:

Blank The sample should not be analyzed; it serves as a **Blank Run**. In this case, the baseline is stored for subsequent subtraction from a later sample. Thus, if baseline subtraction is switched on for a following sample, the **baseline chromatogram** may be subtracted before the integration.

Unknown The sample should be analyzed (as unknown sample).

Standard The sample is a **calibration standard**. The corresponding ⇒*Amount* values of the single peaks are listed in the corresponding **Amount Table** column.

Validate

Validation samples are treated as ordinary analyses (I), the type, however, is written to the result file. The validation sample points to the amount column in the subordinated peak table. The amount column pointed to by such a validation sample contains the required amount or concentration for each peak of the sample. It can be compared in the report with the calculated actual amount or concentration. For this purpose, the **Amnt. Diff.** (amount difference) and **Rel. Amnt. Diff.** (relative amount difference) peak variables are available.

Matrix

Contrary to blank run samples, **Matrix Blank Samples** are analyzed indeed. The Dionex Chromatography Management System automatically subtracts the peak areas (or peak heights, respectively) of the matrix blind sample from the corresponding peak areas (peak heights) of all samples in the sequence. The resulting areas (heights) are then used for all other calculations (e.g. calibration).

Note:

Thus, matrix blank samples are treated differently from "normal" ➢*Blank Run Samples* for which the chromatogram is subtracted point by point from that of the current sample.

Tip:

Matrix blank samples are subtracted only if they are evaluated in the same QNT method. Otherwise, they will not be taken into account.

Weight *(Sample Weight)*

Type: **Floating point value**

Dimension: **---**

Value Range: **0.0001 ... 999 999.9999**

Default: **1.0000**

Related Param.: ⇒*Dil. Factor* (dilution factor)

⇒*Inj. Vol.* (injection volume)

Description: The ⇒*Sample Variable* **Weight** has two functions. It serves to enter the sample weight but it can also be used as a weight correction factor.

1. **Sample Weight**: Enter the sample weight to calculate the content - normalized to the basic unit - of a substance in a sample

   Should, for example, the calculated concentrations always be valid for 1 mg of a sample, the actual weight is entered, e.g. 124.08 mg. The Dionex Chromatography Management System will then divide all calculated concentrations by 124.08.

2. **Weight Correction Factor:** If you wish to relate the concentrations to be calculated to a specific concentration, enter the corresponding correction factor as **Sample Weight**.

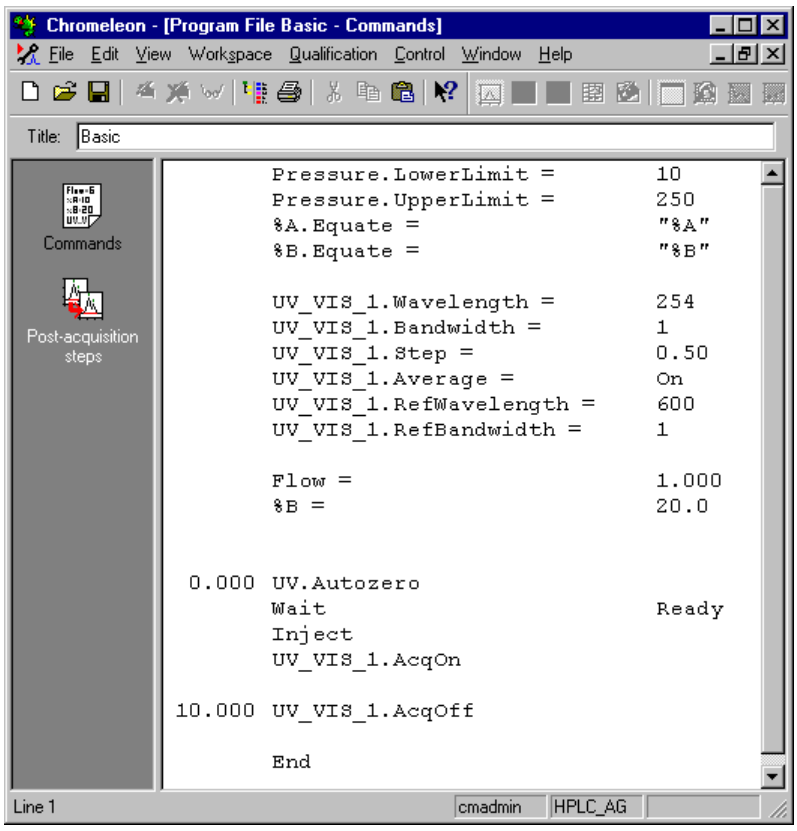
   If, for example, 4.16 mg were weighed instead of 4.0 mg, you must enter 1.04 (not 4.16!) here. This procedure is called **approximate exact weighting**.

Function: Sample Weight is implemented as a multiplication factor in the ➢*Formula for Amount Calculation* of not explicitly entered amount values (dilution series). It is dimensionless.

Program

The **control program** or in short program is part of the PGM file and is displayed in the **Commands** view of the PGM Editor. It contains instrument commands and definitions for chromatographic sample processing. A control file for ➢*Mass Spectrometers* additionally includes the device settings for the MS. The control file has the extension **PGM** and contains a chronological list of instructions (commands) for the chromatography modules or the data system itself (e.g. **End**). The commands are executed in the chronological order.

Creating the basic structure of a PGM file is facilitated by the **Program Wizard**. You may further edit this basic structure via double clicking the PGM file in the Browser. The **Commands** view of the **PGM Editor** (Basic Operations section) opens:



A **control command** contains, first, a time value at which the command should be executed. This value is in *industry minutes*, i.e., "2.500" indicates the time "2 minutes, 30 seconds". Following the time value is the actual program instruction (e.g. ⇒*AcqOn/Off*).

You cannot only integrate control commands into a program but also perform them separately either via the **online toolbar** or via command buttons in the **control panels**.

Should the program instruction require the input of **parameters**, these are entered next in the text line. A comma separates them from instructions. Should several parameters be required, these are specified in the following lines. Each parameter is identified by its parameter name, followed by "=" and then the parameter value. Example:

```
2.500  Pressure.LowerLimit =10
       Pressure.UpperLimit =250
```

Between instruction lines, you may also include any number of **comment lines**. Simply enter a semicolon to commence the line. When a program file is sorted, comment lines are always assigned to the next following instruction line that allows you to explain individual instructions in detail. You may as well include comments at the end of a program instruction. Simply place a semicolon after the last parameter and add the comment.

***Note**:* The injection time, i.e. the time of the Inject command, has, by definition, the time 0 (zero). All preceding commands are assigned negative times, all following instructions positive times.

The advantage is that the PGM time corresponds to the **retention time** of data reduction, e.g. integration, and thus avoids errors such as falsely interpreted gradient profiles. The times of the **AcqOn** and **AcqOff** commands similarly coincide with the time axis of the reduction method.

When processing a program file with the program editor of the Dionex Chromatography Management System, checking the validity of instructions is automatic. You must only enter the commands and their respective parameters: The Dionex Chromatography Management System takes care of the rest, i.e.:

Chronological sorting of lines (use the **Control** command **Sort by Retention Time**)

Examination of input validity (use the **Control** command **Check**), e.g.:

- Does the file contain at least one ⇒*Inject* command?
- Is the first **Inject** command at time 0.000?
- Does the file contain at least one **Acquisition On** command after the first inject (warning)?
- Is a corresponding **Acquisition Off** present for each **Acquisition On** (compulsory)?
- Are total and partial flow rates set at the beginning of the file (required for clearly defined gradients)?
- Are the execution times of preceding instructions considered in the start times of program instructions (otherwise the start times in the program file does not coincide with the actual start time)?
- Is the final instruction an **end** command?

When creating program files with a word processor, you must carry out these checks yourself. It is particularly important to remember that the first line of the file is always interpreted as the header. If no header is required, you must leave a blank line at the beginning of the file.

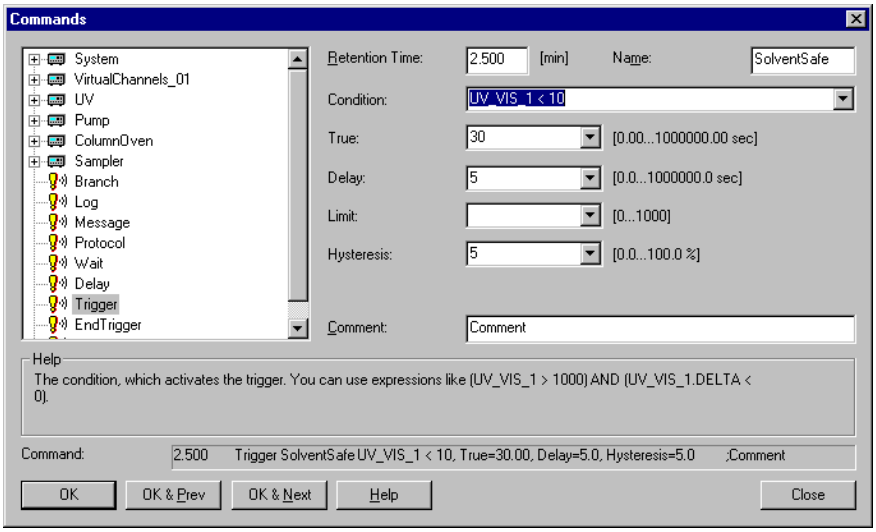
Operation of the PGM Editor

The PGM editor includes three different views that are opened via the respective icons in the left PGM editor section:

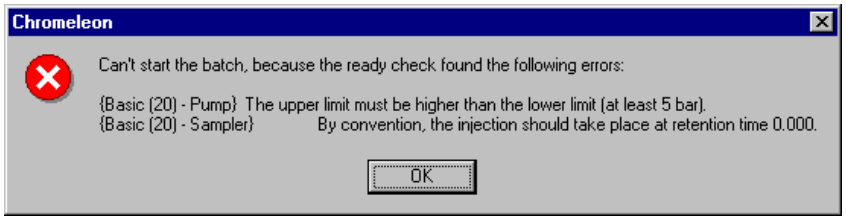
- Commands
- Finnigan AQA (with PGM files for a timebase with MS only)
- Post-acquisition steps

Below please find a description of the **Commands** view where you can enter individual control commands. For details on the **Finnigan AQQ** view, see **How to …: Actions Related to the aQa-MS**  **Creating a Method for the aQa-MS**.

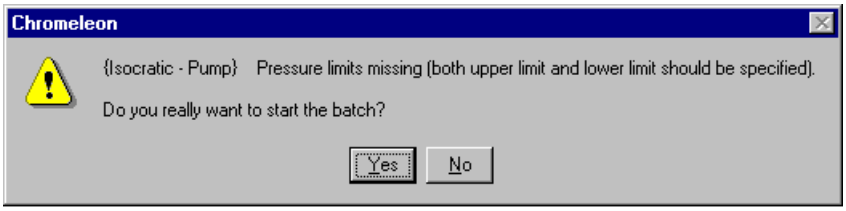
To assist editing control commands, a dialog box is available, which is opened via F8 or **Command** in the **Control** menu. This box allows the individual entry of all instruction components (time, instruction, instrument, parameter, comment). All available instructions and instruments (depending on system configuration) are listed for simple selection.



Before starting a program, a Ready Check is performed. The program is checked (as far as possible) for validity. In case of logical errors (e.g., for the **pressure limits** command, the **lower limit** has to be greater than the **upper limit**) the program cannot start and a message will pop up, such as:



In case of errors, which may affect the course of the program without being critical, a warning is shown. Nevertheless, you may start the batch:



During program file generation, the **Control** command **Sort by Retention Time** can be used to chronologically sort all entries. Therefore, it is possible to simultaneously enter all commands pertinent to a specific instrument (e.g. all flow commands, all signal parameters, etc.) and have them sorted according to time later.

For detailed information, see **How to: Actions in the PGM Editor:**

Control Program

Program Syntax

***Note**:* The command syntax is different from the syntax used by the GynkoSoft Data System. When importing a GynkoSoft PGM file, its syntax will be adapted automatically to the syntax used by the Dionex Chromatography Management System.

Control Commands (Overview)

On the following pages, the most important control commands are described, together with their corresponding parameters. Which commands and parameters are actually available, depends on the individual installation. For example, if a simple UV detector is installed, it is not possible to record a 3D-field.

☞ ***Tip**:* An extensive explanation of all existing commands for all devices, which may be controlled, is far beyond the scope of this reference manual. About 100 commands available just for the hP6890 GC!

In the following topics, commands concerning various devices are explained exemplarily:

⇒*General Commands*

⇒*System Commands*

⇒*Pump Commands*

⇒*Autosampler Commands*

⇒*Detector Commands*

General Commands

The following general commands are available regardless of the installed devices

⇒*Branch*
⇒*Delay*
⇒*End*
⇒*EndTrigger*
⇒*Log*
⇒*Message*
⇒*Protocol*
⇒*Trigger*
⇒*Wait*

System Commands

System control comprises all commands that concern the entire chromatographic process or the entire system. They are partly available via both the online toolbar and the context menu. The most important system commands are:

⇒*Abort Batch*
⇒*AbortSample*
⇒*Acquisition On/Off*
⇒*Continue*
⇒*Hold*
⇒*Sound*
⇒*StopFlow*

Also, see **System Commands.**

Pump Commands

For the most important pump commands, see the topics:

⇒*%A, %B, %C, %D*
⇒*Connect/Disconnect*
⇒*Flow*
⇒*Pressure Limits*

Autosampler Commands

For the most important autosampler commands, see the topics:

⇒*Connect/Disconnect*
⇒*Dispense*
⇒*Draw*
⇒*Inject*
⇒*NeedleUp*
⇒*Position*
⇒*Reset*
⇒*Relay On/Off*
⇒*Temperature*
⇒*Volume*
⇒*Wash*

Detector Commands

For the most important detector commands, see the topics:

⇒*AcqOn/Off*
⇒*Autozero*
⇒*Average*
⇒*Bandwidth*
⇒*Bunch Width*
⇒*Connect/Disconnect*
⇒*Lamp on/off*
⇒*Reference Bandwidth*
⇒*Reference Wavelength*
⇒*Step*
⇒*Wavelength*

%B, %C, %D (Partial Flows)

Instrument Type: **Pump(s)**

Related Comm.: ⇒*Flow*

Description: The amount information for the partial flow is stated in percent of the flow rate. The total sum of all partial flows is 100% (%A+%B+%C+%D=100%), wherein %A is calculated from the remaining partial flows (%A=100%-(%B+%C+%D)). It is therefore sufficient to determine the values for %B, %C, and %D.

Changing the % ratio during the analysis is referred to as ➢*%-Gradient*.

%B, %C, and %D define the **partial flow rates** of the individual pumps in a high pressure mixing system (as %-values of flow), or the partial flow rates on the suction side of a low pressure mixing system. The latter generally refers to a single pump or a separate mixing vessel with controlled proportioning valves. The formation of %-gradients is by the same principle as for Flow.

For each ➢*Timebase*, one or more fluidic systems can be installed. They can be controlled independently, either manually or via a ➢*Program*.

In case a second fluidic system is installed, the corresponding device name has to be specified in the program. Use the F8 key or the Program Wizard to insert the device name automatically.

☞ ***Tip***: The ⇒*Hold*, ⇒*Continue*, and ⇒*StopFlow* commands are always effective for all fluidic systems!

Function: The partial flow rates of B, C, and D change linearly with time between two respective %B, %C, or %D commands. By entering two percent commands at the same time, even step gradients can be programmed.

Function (Cont'd):

When sorting, the editor does not change the order of commands having the same program time! If the partial flow rates are to remain constant during analysis (i.e. isocratic), the appropriate %B, %C, and/or %D commands need only be entered at the beginning of the file.

```
-2.000 Flow =          1.000
         %B =          20.0
...  ...
 0.000 Inject
 0.500 %B =            20.0
       %B =            40.0
...  ...
 8.500 %B.Value =      80.0
 8.500 End
```

In this example, the total flow rate remains constant at 1.0 ml/min. %B also remains constant, at 20% from -2.0 to 0.5 min, then increasing abruptly to 40%, then linearly to 80% with a gradient of 5%/min/min.

Parameter:

Value Percent value [%]

☞ ***Tips:***

The Dionex Chromatography Management System is able to run flow and %-gradients *simultaneously*. However, in high pressure mixing systems, this results in non-linear partial flow rate changes for each individual pump.

Note that due to compressibility and dead volume considerations, high pressure and low-pressure applications are not always interchangeable!

The %-values remain constant from the last %-command to the end of the program. Thus, for isocratic operation, a single %-entry at the beginning of the file is sufficient.

The first %-command (%B, %C, or %D) must be at the beginning of the PGM file immediately following the **Flow** command!

AbortBatch

Instrument Type: **System command**

Related Comm.: ⇒*AbortSample*

Description: The **Abort Batch** command aborts a running sample batch. In combination with the ⇒*Trigger* command, this command offers a possibility to react, for instance, to external errors. Example:

```
0.000 Trigger    Cond=RemErr
        Abort Batch
        EndTrigger
```

Function: Abort batch terminates data acquisition, deletes all triggers, and aborts the current sample batch.

AbortSample

Instrument Type:	**System command**
Related Comm.:	⇒*AbortBatch*
Description:	The **Abort Sample** command interrupts data acquisition and aborts a running sample.
Function:	The batch continues with the next sample. Use this command e.g., if, by mistake, no injection was made for a sample.

AcqOn/Off *(Data Acquisition On/Off)*

Instrument Type: **System command, all detectors**

Related Comm.: ⇒*Inject*

Description: The **AcqOn/Off** command activates/deactivates data recording (➢*Raw Data*) for the selected ➢*Signal* (= channel) of a timebase. Each signal (or channel) is stored in a separate file. The type of data from each signal is determined via signal parameters.

Function: To reduce raw data storage requirements, **AcqOn** can be given some time after the **Inject** command. However, it should be given at least 30 seconds before the elution of the first peak, as the Dionex Chromatography Management System requires a baseline segment of several seconds in order to perform a noise analysis for the auto-optimized ⇒*Step* and ➢*Sampling Rate* functions.

The command can be given manually via the menu command, or automatically via the ➢*Program*.

⇒*Trigger* commands whose conditions depend on signal values or their slope are effective during data acquisition, only.

☞***Tip***: The parameters defined in the program (e.g. ⇒*Step*, ⇒*Average*) can be changed at any time.

☞***Tip*** (cont'd):

For clarity, however, we recommend to use to the following command sequence:

```
-2.000 Flow = 1.000
 ...  ...
 0.000 Inject
 0.500 UV_VIS_1.AcqOn
 ...  ...
 3.270 UV_VIS_1.Wavelength = 275
 ...  ...
12.000 UV_VIS_1.AcqOff
13.500 End
```

The parameters of the 3DFIELD signal may not be altered between AcqOn and AcqOff.

Raw data acquisition is interrupted via the ⇒*Hold* and ⇒*StopFlow* commands. The ⇒*Continue* command is used to resume acquisition. To terminate raw data acquisition, choose the **AcqOff** command.

Autozero

Instrument Type: **All detectors**

Related Comm.: **---**

Description: The **Autozero** command resets physical or ➢*Virtual Signals* to zero.

Function: The subsequently measured data is interpreted and displayed in relation to the new zero point. In the chromatogram, this can be recognized by a sharp increase of the absorption value.

This command applies to all signals delivered from a single detector. Thus, autozeroing a **diode array detector** (e.g. Dionex **UVD 340**) causes the entire **3DFIELD** to be zeroed. Autozero applies to one detector only! When several detectors are present in a system (e.g. in series), they must be autozeroed individually.

☞***Tip***: After an autozero, usually a jump is observed in the baseline. Therefore, we recommend that autozero is carried out before data acquisition, unless this is specifically required during the analysis, e.g. after wavelength switching.

If a wavelength switch has been triggered, an autozero should also be ⇒*trigger*ed to follow! Example:

```
0.000 Inject
0.100 Trigger SwitchWave  UV_VIS_1 > 20
      UV_VIS_1.Wavelength = 280
      Autozero
      EndTrigger
0.500 UV_VIS_1.AcqOn
```

Average

Instrument Type: **Detector**

Default: **ON**

Related Comm.: ⇒*Step*

Description: The **Average** parameter allows averaging signals. This is possible for digital signals the detector sends to the server PC (as with the Dionex Detectors UVD 170S and UVD 340S) as well as for analog signals recorded via the A/D Converter.

The Dionex A/D converter records each analog signal with a frequency of 100 Hz. This corresponds to a ⇒*Step* of 0.01 second or a ➢*Sampling Rate* of 100 data points per second. When increasing the step or decreasing the sampling rate, less data points are stored than theoretically possible.

Function: When activating the **Average** signal parameter, the data points between the stored values are considered as well. The Dionex Chromatography Management System averages all measuring values that are within a step interval. The calculated average is stored in the ➢*Raw Data* file. This generally improves the ➢*Signal to Noise Ratio* (using the **Average** parameter, chromatograms look smoother when there are noisy signals). This parameter has no influence on the precision of the integration.

☞ ***Tip***: Averaging is always performed in a 3D-field.

For almost all detectors, concentration is proportional to peak-area (i.e. integral of the signal over time). A local (time) signal averaging, therefore, does not influence quantitative determination.

Bandwidth

Instrument Type:	**Detector**
Type:	**integer**
Value Range:	**detector-dependent**
Default:	**0 [nm]**
Related Comm.:	⇒*Wavelength* ⇒*Reference Bandwidth* ⇒*BunchWidth*
Description:	Specifies the optical bandwidth in nm with which the chromatogram is recorded. In general, this corresponds to the ➢*Optical Resolution* of a detector.
Function:	The bandwidth can be simulated, i.e. increased, by averaging several single photodiode signals. This process is known as **Photodiode Bunching**. Averaging is performed symmetrically to the selected wavelength. Thus, at a bandwidth of 30 nm and a wavelength of 255 nm, the signals of all photodiodes in the range of 240 to 270 nm are averaged.
☞***Tip***:	In versions of the Dionex Chromatography Management System without control option, the bandwidth cannot be modified during data acquisition. Changing the bandwidth can often lead to an increase in sensitivity. Quadrupling the bandwidth halves the noise. However, normally the linearity decreases.

Branch

Instrument Type: **Processed in PC**

Related Comm.: ---

Description: In the current ➢*Program,* use the **Branch** command to branch into a different program or to start a program via a command button from the ➢*Control Panel*. Combing this command, e.g., with the ⇒*Trigger Commands* allows defining dynamic program runs.

Function: If a **Branch** command is given while a program is running, it stops executing the current control file and continues with the newly selected control file. The times used in this file are automatically corrected by the program time that already passed.

Example1 (within a program):

```
0.000 Trigger        Pressure > 300
      Branch        "Overpressure"
      EndTrigger
```

If the pressure is higher than 300 (bar), the program **Overpressure** will be started in this example. With the Overpressure program you may slow down the flow, switch off the lamp, and deliver the ⇒*Message* that the pressure within the system was too high and thus, the flow has been slowed down.

☞ ***Tip***: In example 1 the program to be started via the **Branch** command has to be stored within the sequence to be started. Otherwise, the location has to be included within the program, using slashes to separate the different levels, as with the command button.

Function (cont'd):

Example 2 (as Command Button within a Control Panel):

Add a **Command Button** in the Control Panel (see **How to ...: Actions in the Control Panel**  **Creating a Command Button**) and branch from there using the corresponding command in the chosen program.

```
Branch
"CM_Seminar/Programs/Equilibration"
```

Via this button, you could start the column equilibration program that is stored in the **CM_Seminar** ➢*Datasource* in the **Programs** directory.

Parameter:

Program Name of the program file used for further processing

☞***Tip***: When making a backup of a sequence, all PGM files that are included in the sequence are also saved. If PGM files, which are pointed to in a Branch command, shall be saved as well, these PGM files need to be included in the sequence.

Bunch Width

Instrument Type:	**Detector**
Type:	**Fixed point value**
Value Range:	**1.9 ... 197.6 [nm]**
Default:	**1.9 [nm]**
Related Comm.:	⇒*Bandwidth*
Description:	To enhance the ➢*Signal to Noise Ratio* of a ➢*Photodiode Array Detector* the signals of several photodiodes can be averaged (or bunched). Bunch Width describes the ⇒*Bandwidth* of a bunch of photodiodes.
Function:	The Bunch Width is closely connected to the **bunch factor**, which refers to the number of photodiode signals of a UV/VIS detector that are averaged. If a detector, for example, has 80 photodiodes distributed on a wavelength range of 160nm, the (theoretical) optical resolution is 2 nm. With a bunch factor of 4, 80 : 4 = 20 photodiodes are averaged to one signal. The theoretical bandwidth is now reduced to 160 : 20 = 8 [nm].
☞***Tip**:*	Averaging the signals improves the signal-to-noise ratio. At the same time, however, ➢*Optical Resolution* decreases.

Connect/Disconnect

Instrument Type: **All**

Related Comm.: **---**

Description: Perform the **Connect Device** command to connect a device with the server to enable remote control.

Execute the **Disconnect** command to separate a user PC (client) from a timebase or to operate an instrument locally.

Functions:

Connect The command checks whether the specified device is actually connected, and then activates the instrument. For all installed instruments, the **Connect** command is executed automatically when server of the Dionex Chromatography Management System is started. Thus, if working in remote operation mode only, you do not need to explicitly issue this command.

When the connect command is activated, the corresponding instrument may now be remotely operated from the PC. On most instruments (e.g. all Dionex instruments) the instrument keyboard is now locked for safety (and ➢*GLP*) reasons, i.e., the instrument can be operated remotely, only. This is to ensure that the selected settings are kept. Input on the instrument itself is possible again after the **Disconnect** command.

Disconnect The corresponding instrument is reverted to local operation mode and the keyboard is unlocked again. The instrument is no longer monitored by the data system, nor can it be operated via the data system.

☞***Tip***: Connect and Disconnect should only be used in interactive (online) mode and not within a ➢*Program*. Otherwise, the ➢*Ready Check* may not be valid.

Continue

Instrument Type: **System command**

Related Comm.: ⇒*StopFlow*

⇒*Hold*

Description: The **Continue** command cancels the **Hold** and **StopFlow** commands.

Function: An interrupted sample ➢*Batch* is continued in the same way as is an interrupted pump flow.

Delay

Instrument Type: **All**

Related Comm.: ⇒*Trigger*

Description: Delays the execution of the following commands for the given time.

☞***Tip***: Usually, Delay is used for Trigger commands, only. Example**:**

```
Trigger PEAK  UV_VIS_1 > 20
Delay  5.0
Sound  Frequency = 440, Duration = 1
EndTrigger
```

Dispense

Instrument Type: ➢*Autosampler*

Related Comm.: ⇒*Inject*

⇒*Draw*

Description: The **Dispense** command causes the autosampler to dispense a specific quantity (volume) from the sample loop into a certain sample vial (⇒*Position*). The amount of time the sampler may take for this operation is determined via the ➢*Duration* parameter.

When the operation is completed, the autosampler sends the signal **Sampler.Ready** (for the ASI-100/ASI-100T sampler, ➢*Sucked* for the GINA 50/GINA 160 samplers) back to the data system. The time interval between the **Dispense** command and the **Sampler.Ready** response signal can vary depending on the instrument (ASI-100/GINA 50).

Parameters:

Position	Sample position
Volume	Sample volume
Duration	This parameter indicates the minimum time required by the sampler for the respective operation.

☞***Tips***: For highly viscous liquids, more time must be allowed for the autosampler to dispense the exact volume.

In manual operation, the commands are selected via the control pull-down of the unit window. When entering the commands to a ➢*Program*, the three parameters need not to be specified. During execution of a PGM file, the missing parameters are replaced by the current sample position, the current inject volume, and by the value 0 (if there is no duration), respectively.

Draw

Instrument Type: ➢*Autosampler*

Related Comm.: ⇒*Inject*

⇒*Dispense*

Description: The **Draw** command (**Draw** for the ASI-100/ASI-100T, **Suck** for the GINA 50/GINA 160) induces the autosampler to draw a specific ⇒*Inj. Vol.* (injection volume) from a certain sample vial (⇒*Pos.* (Sample position)). The amount of time this operation is allowed to take is determined via the ➢*Duration* parameter.

Function: When the operation is completed, the autosampler sends the **Sampler.Ready** signal (for the ASI-100/ASI-100T sampler, ➢*Sucked* for the GINA 50/GINA 160 samplers) back to the data system. The time interval between the **Draw** (or **Suck**) command and the **Sampler.Ready** (or **Sucked**) response can vary depending on the instrument type.

Example:

Via the command sequence

```
-1.000   Draw     Volume=10
   Wait     Sampler.Ready
   Dispense Pos=1, Volume=10
```

10 µl from the current sample are transported to the vial 1. **Dispense** is carried out only after the **draw** process has been completed.

Parameters:

Position Sample position

Volume Sample volume

Duration This parameter indicates the minimum time required by the sampler for the respective operation.

☞ ***Tip***:

For highly viscous or low-boiling liquids, more time must be allowed for the autosampler to draw the exact volume without bubbles.

In manual operation, the commands are selected via the control pull-down of the unit window. When entering the commands to a ➢*Program*, the three parameters need not to be specified. During execution of a program, the missing parameters are replaced by the current sample position, the current inject volume, and by the value 0 (if there is no ➢*Duration*), respectively.

End

Instrument Type: **System Command**

Related Comm.: ⇒*EndTrigger*

Description: Marks the end of a program.

EndTrigger

Instrument Type: **System Command**

Related Comm.: ⇒*Trigger*

Description: Marks the end of a block of triggered commands.

Function: All commands between **Trigger** and **EndTrigger** are executed when the trigger condition becomes true.

☞***Tip***: Define the Trigger identified by its name with the new condition „0" and mark the end of this trigger block with the EndTrigger command to finish an active Trigger.

```
Time Trigger Name  0

  EndTrigger
```

This is necessary for each trigger separately. It is not possible to finish all triggers together.

Equate

Instrument Type: **Processed in PC**

Related Comm.: ⇒*%A, %B, %C, %D*

Description: **Equate** is used to assign different designations to the three partial flows of the fluidics, %A, %B, %C, and %D. Example:

```
0.000 %A.Equate =    "Water"
0.000 %B.Equate =    "MeOH"
0.000 %C.Equate =    "ACN"
```

Function: In the unit windows, you can assign the partial flows the actual eluent names. The equate commands are logged in the audit trail. This to keep track of the chromatographic conditions at any time. Consider that a PGM file which contains equate commands may itself serve as a protocol!

☞***Tip***: It is up to the user to check the consistency of %A, %B, %C, and %D with the eluents actually used!

Flow (Flow Rate)

Instrument Type: **Pump**

Related Comm.: **%B, %C, %D**

Description: Defines the total flow rate (in [ml/min]) through the column, i.e., the sum of ⇒*Partial Flows* (%A+%B+%C+%D=100%). The value entered represents the **current value**. For isocratic systems, this value remains constant during the program. In **flow-gradient** systems, this value represents an interpolation point of a polygonal line to which the previous and following flow values are adjoined by straight lines.

Function: The total flow rate alters linearly with time, between two flow commands. By entering two flow commands at the same time, even step gradients can be programmed. When sorting, the editor does not change the order of commands having the same program time! If the flow is to remain constant for the entire analysis, a single entry at the beginning of the ➢*Program* is sufficient.

```
-2.000 Flow=    0.500
 ... ...
 0.000 Inject
 0.500 Flow=    0.500
 0.500 Flow=    1.000
 ... ...
 8.500 Flow=    5.000
  8.500 End
```

In this example, the flow rate remains constant at 0.5 ml/min between -2.0 and 0.5 min. Then it increases abruptly to 1.0 ml/min and then linearly to 5 ml/min with a gradient of 0.5 ml/min.

Function (Cont'd):

In case a second fluidic system is installed within the same ➢*Timebase*, the corresponding device name has to be specified in the program. By using the F8 key for generating command lines, the device name is inserted automatically.

☞***Tip***: The ⇒*Hold*, ⇒*Continue*, and ⇒*StopFlow* commands are always effective for both fluidic systems!

☞***Tip***:

The Dionex Chromatography Management System is able to run flow and %-gradients *simultaneously*. However, in high pressure mixing systems this results in non-linear partial flow rate changes for each individual pump.

As there are pressures up to 400 bars in the chromatography column and as solvent mixtures are subject to volume compression (e.g. methanol/water), the delivered volume in ➢*High-Pressure Gradient Systems* does not correspond to the volume transported via the column. However, the number of delivered and transported solvent particles is not changed by this fact.

The flow rate remains constant from the last flow command to the end of the program. Thus, for isocratic operation, a single flow entry at the beginning of the file is sufficient.

The first flow command must be *at the beginning* of the PGM file!

Normal flow rates are in the range 0.5 to 10 ml/min. Flow rates deviating from this range are achieved by using special micro pumps (0.1 - 0.5 ml/min) or preparative pumps (as from 10 ml/min).

Hold

Instrument Type: **System command**

Related Comm.: ⇒*StopFlow*

⇒*Continue*

Description: The Hold command

- Stops ➢*Data Acquisition*
- Interrupts a running ➢*Gradient* program
- Stops automatic ➢*Batch Processing*

Function: In the **Hold** mode, no data is acquired, the pump continues delivery with the current solvent composition, and evaluation of the batch samples is stopped.

☞***Tip***: All processes can be completely aborted via the **StopFlow** command or continued with the **Continue** command.

Inject

Instrument Type: ➢*Autosampler*

Related Comm.: ⇒*AcqOn*

⇒*Draw*

⇒*Dispense*

Description: Defines the beginning of a chromatogram, i.e., determines the time at which the sample enters the high-pressure system. Thus, the time of the first inject command is 0 by definition. The advantage is that the ⇒*Retention Time*, as appearing in chromatograms and reports, coincides with program execution times. All commands before inject, are assigned **negative execution times**.

Between the Inject command and the actual injection process (Inject response by the sampler or the hand-operated valve), a system-dependent interval is required for reaching the rack and to draw the sample. During this time, the pump is kept in the ⇒*Hold* state (i.e., a possibly running gradient is stopped). This **Inject Wait** state is canceled only by an **Inject Response** signal. The response signal is delivered either automatically (via an interface) or via a remote input signal. Only from this point, time keeping is started.

Function: The function is dependent on the individual installation. For manual injection, the Dionex Chromatography Management System simply holds the analysis time and waits for inject response. For a controlled autosampler, the inject command (at least) is relayed to this. For autosamplers with **variable injection volumes** and **random sample access** (e.g. **ASI-100**), the inject volume and vial position are relayed as well. Such autosamplers are ideal for automated **multipoint calibration.**

Function (Cont'd):

For **interactive operation** (online) of the inject command, the **Sample Position** and **Inject Volume** parameters must be entered as well. During **automated batch operation**, these values are read from the sequence. Thus, parameters do not have to be set individually in the ➢*Program*.

Parameters:

(When a hand-operated valve is used for injection, this information can be used for documentation purposes.)

Position

Vial ⇒*Position* in the autosampler

Inject Volume

Injection ⇒*Volume* in µl

Blank

Specifies whether ➢*Blank Run Samples* are actually injected:

Skip: no injection

Inject: Injection is performed.

☞***Tip***:

Data acquisition (⇒*AcqOn/Off*) should be started after the Inject signal, at least 30 seconds before the first peak. Also, there should be ➢*Isocratic* conditions during the injection process.

A program should only contain *one* inject command.

Lamp On/Off

Instrument Type: **All optical detectors**

Related Comm.: **---**

Description: This command switches the lamp of an optical detector on and off. UV/VIS detectors often have a separate lamp (deuterium/halogen) for each range. Then, the commands are as follows: UV_Lamp = On/off and Visible_Lamp = On/Off.

Function: The lamp is switched on or off.

☞***Tip***: Practically all optical detectors require a considerable warm-up period for high sensitivity, drift-free operation. The inject command should, therefore, be placed several minutes (minimum) after this command. Note also that lamp(s) should never be switched off during a sample batch. It is common practice is many laboratories to operate detectors 24 hours a day with the lamp being switched on.

Detector lamps are subject to aging. Do not use the **LampIntensity** variable, e.g., to receive the value of the current lamp intensity at 254 nm via the ⇒*Log* command. If a value was measured when the lamp was new, the value indicates how much the intensity decreased since then.

Log

Instrument Type: **Processed in PC**

Related Comm.: ⇒*Message*

⇒*Protocol*

Description: The **Log** command allows you to document the values of variables in the ➢*Audit Trail* at any time.

Function: This option is especially useful to log information that is not periodically retrieved.

If, for example, the pressure at the time t = 5.000 min during sample processing should be logged, include the following line in the **Control Program**:

```
5.000 Log    Pressure.Value
```

In the example mentioned above, the current pressure will be logged. In exceptions, the **Log** command is sent directly by the device driver (e.g. fraction collector).

Message

Instrument Type: **Processed in PC**

Related Comm.: ⇒*Wait*

⇒*Protocol*

⇒*Log*

Description: During execution of the program, a message pops up on the screen that is to be acknowledged by the user with **Ok**. Only then the program is continued.

The Message command allows the user to enter reminders for things to do or to consider while executing a ➢*Program*.

Function: When executing the program, a window containing the respective message text is displayed. The program is interrupted until the user acknowledges the message. Besides, the command and the message are written to the Audit Trail.

If, for example, a user should be reminded to check and, if necessary, refill eluents prior to the analysis, the following command can be included in the program:

```
-1.000 Message "Check eluent containers!"
```

When executing the program, the text in quotation marks is displayed on the user's screen at the specified time (in the above example one minute prior to injection). Simultaneously, the command and the message are included in the Audit Trail. The server is then in **Hold** mode. During this time, the monitor icon indicates this status by its yellow/red coloring.

Function (cont'd):

If the Dionex Chromatography Management System is operated in a network, the message appears on the client that currently has control privileges.

The program continues operating as soon as the message is confirmed!

Parameter:

Text The message to be displayed.

☞***Tip***: For as long as the message dialog box is displayed on the screen, the time is interrupted, the flow conditions are in Hold mode.

NeedleUp

Instrument Type: ➢*Autosampler*

Related Comm.: ⇒*Wash*

Value Range: **Depends on device and installed syringe**

Description: The **NeedleUp** command enables lifting the sample needle.

Function: Then the internal sample valve is switched (see the example for a load/inject process in the Autosampler).

When lifting the needle, a running ⇒*Wash* process is automatically interrupted, i.e., the solvent flow is not through the sample loop but directly from the pump onto the column. Use the **Load** command to perform the same operation without moving the needle up.

☞ ***Tip***: Use the **Wash** and **NeedleUp** commands to prevent crystallization of substances (e.g. buffers) by washing the sample loop.

Position

Instrument Type: ➢*Autosampler*

Related Comm.: ⇒*Inject*

⇒*Volume*

Value Range: **Depends on device and installed carrier segment**

Description: Specifies the position of the vial from which a sample shall be injected.

Function: If you use a controllable autosampler, the entered position is transmitted automatically to the sampler. The sampler approaches the corresponding sample for injection. If using a non-controlled autosampler or a hand-operated valve, this column only serves for documentation purposes. If the sample position parameter is not entered, the previous (current) value is used.

Pressure Limits

Instrument Type: **Pump**

Related Comm.: ⇒*Flow*

Description: Define the pressure limits within which the pump(s) is permitted to operate.

Function: Should the pressure go beyond a set limit, **the Dionex Chromatography Management System turns off the flow**, displays an error message, and terminates the current sample batch.

Parameters: (The values that can be entered depend on the pump type.)

Lower Limit Lower pressure limit in **Bar**.

Upper Limit Upper pressure limit in **Bar**.

☞***Tip***: Pressure limits apply to *all* connected pumps on the high-pressure side.

Exceeding the upper pressure limit can be due to a blocked column or capillary or to a defective injection valve.

If the pressure is below the lower limit, this is usually due to a leak in the fluidic system.

Protocol

Instrument Type: **Processed in PC**

Related Comm.: ⇒*Message*

⇒*Log*

Description: Writes a comment to the audit trail (without screen message). Thus, program steps can be additionally commented or chromatographic conditions can be written to the audit trail (PGM comments are not written to the audit trail).

```
-2.000 Protocol "Separation
according to DFG-method, residue
analysis"

-2.000 Protocol "0.05 M
Natriumdihydrogenephosphate buffer"

-2.000 Protocol "Column: LiChrospher
RP-18"
```

Function: Unlike simple green comments starting with a semicolon, which are only part of the program, the **Protocol** text is included in the Audit Trail and is thus directly linked with the corresponding sample. The **Protocol** text can thus be used for commenting individual samples. The program run is not affected by a **Protocol** command.

Parameter:

Text The text that is written to the audit trail.

Tip: Event-controlled execution of the command is also possible. Example:

```
0.000  Trigger Protocol UV_VIS_1 > 1000

       Protocol     "Valid absorption
                    range exceeded"

       EndTrigger
```

RefBandwidth (Reference Bandwidth)

Type:	**Integer**
Value Range:	**Detector-dependent**
Default:	**0 [nm]**
Related Comm.:	⇒*Reference Wavelength* ⇒*Bandwidth*
Description:	The reference bandwidth can be selected separately for each channel. The 3D-field of a photodiode array detector also has its own reference bandwidth. Analogous to the conventional bandwidth of a channel, the reference bandwidth serves to average several photodiode signals of the Reference Wavelength.
Function:	For example, if the reference wavelength is 350 nm and the reference bandwidth is 5 nm, wavelengths in the range of 348 - 352 nm are averaged and used as the reference.
☞***Tip***:	For **UVD 160S/320S** and **UVD 170S/340S** detectors, alter the reference bandwidth only if the reference wavelength cannot be set to 600 nm (i.e., for substances clearly absorbing at 600 nm, especially blue substances). This is the only case where using a higher bandwidth can improve the signal to noise ratio. For **PDA-100** detectors and other two-lamp PDA detectors, select a reference bandwidth that includes a majority of light from the same lamp as the sample wavelength. For the PDA-100, the deuterium lamp provides wavelengths of 190 nm to 380 nm and the tungsten lamp provides wavelengths of 380 nm to 800 nm. Select a reference bandwidth that is narrow enough not to interfere with nearby compounds and select an area of the spectrum where the sample does not absorb.

RefWavelength (Reference Wavelength)

Instrument Type	**Detector**
Type:	**Integer**
Value Range:	**Detector-dependent**
Default:	**Off**
Related Comm.:	⇒*Reference Bandwidth* ⇒*Wavelength*
Description:	With Dionex Photodiode Array Detectors, the reference wavelength is used to correct the absorption values of the wavelength that has been selected for the analysis.
Function:	If the absorption of the reference wavelength changes during the analysis, absorption values of the analysis wavelengths are adjusted up or down accordingly. The selected reference wavelength should be in a quiet area of the spectrum where little absorption occurs. Each change in the absorption then indicates substantially changed conditions, for example, a reduction of the lamp energy (lamp drift). Each change can be used to correct the absorption in the remaining wavelength range even during the analysis (the recorded signal is reduced or amplified accordingly, as necessary). Reference wavelengths are especially useful for gradient analyses because as the light intensity changes over time (due to the gradient), absorption values are adjusted, thus minimizing baseline drift. Peaks are not detected in the reference wavelength range where the system is "blind" per definition. Should peaks be detected, nevertheless, select a different reference wavelength. You can deliberately use this as well to inhibit peaks.

Function (Cont'd): If the reference wavelength is chosen in a light-deficient range, it is recommended to average the signals of several photodiodes by increasing the Reference Bandwidth and thus improve the signal to noise ratio.

☞ ***Tip***: Do not confuse the reference wavelength with the ➢*Reference Channel* used for ➢*Baseline Correction*.

Settings: Details about reference wavelengths vary depending on the type of detector:

Dionex UVD 160/320S PDA and UVD 170S/340S PDA Detectors

For Dionex UV/PDA Detectors UVD 160S/320S PDA and UVD 170S/340S PDA, a reference wavelength of 600nm should be selected because relatively small absorption values are observed there. In addition, these Dionex Detectors have a special noise optimum at this value. However, when the reference wavelength is changed, the special noise optimum of the Dionex detectors no longer applies.

☞ ***Tip***: Referencing the measured wavelength range, i.e., verifying whether the actual nanometer value corresponds to the nominal value is via a ➢*Holmium Oxide Filter* (**Spectra Calibration**).

Dionex PDA-100 Detector

By default, the reference wavelength is turned off for the PDA-100. With UV channels (≠ 3D-Field), the absorption at the first scan after the autozero is used as a reference. This results in lower noise but less drift compensation. The **Reference_Wavelength=Off** command in a program or on the control panel turns off the reference wavelength.

Settings (Cont'd):

During collection of ➢*3D-Field* data, the absorption after autozero is always used as a reference (as described above). After data collection, a reference wavelength can be applied to the data. The reference wavelength in this case defaults to the highest wavelength in the analysis range. For example, if the analysis wavelength range is 190 - 350 nm, the default reference wavelength is 350 nm. If you select a different reference wavelength, the selected reference must be within in the stored wavelength range.

Relay On/Off

Instrument Type: **All relays**

Related Comm.: ---

Description: **Relay-Name.On (Off)** closes (opens) a relay output (closure contact) for a specific instructed time. Switching valves are treated as relays also.

Function: The specified relay is opened or closed for a specified time in seconds. **Relay-Name.On** opens the relay upon completing a certain period (➢*Duration*), **Relay-Name.Off** closes the relay after completing the duration. If no duration is specified for **Relay-Name.On (Off)**, the relay remains closed (open) until the next relay command is given.

Parameter:

Duration Closure or opening time in seconds [s] (optional).

☞***Tip***: Relay On/Off duration for the same relay may not overlap!

Reset

Instrument Type: **All**

Related Comm.: ⇒*Autozero*

Description: Resets an instrument to its initial conditions, as attained after power-up, i.e. **standby mode**.

Function: Activates (in general) a "warm start", i.e. the instrument regains its initial state as immediately after power-up. The reset command is particularly useful when an instrument has been operated locally, or has an undefined status (to the data system), e.g. after an instrument fault.

☞***Tip***: Activating the reset of an autosampler may require a considerable time to completion, as generally this involves a mechanical recalibration and a complete wash cycle.

Sound

Instrument Type: **Processed in PC**

Related Comm.: **---**

Description: Sound generates a tone (of selectable frequency) on the internal loudspeaker of the PC. This may be used to acoustically monitor the progress of a program, by setting sound commands at key-points in the file. Combining this function with the ⇒*Trigger* command allows, for example, "hearing" eluting peaks. By selecting different frequencies for ascending and descending peak flanks, these can be acoustically distinguished!

Example:

```
-2.000 Flow =        1.000
-2.000 %B =          50
 0.000 Inject
 0.000 Trigger Up    UV-VIS-1 > 20
       Sound    Frequency=440, Duration=1
       EndTrigger
       Trigger Down  UV-VIS-1 < 40
       Sound    Frequency=880, Duration=1
       EndTrigger
 0.500 Acquisition On
 ...  ...
 8.000 Acquisition Off
 9.000 Program End
```

Function: Sound generates a tone of selectable frequency and duration on the PC loudspeaker. If the command cannot be performed due to a missing sound card, a default sound is generated at the PC speaker.

Also, see **How to ...: Device Control**  **Trigger Commands**.

Parameters:

File	Sound File (normally WAV file)
Frequency	In Hertz [Hz] (concert pitch a = 440 Hz
Duration	In seconds [sec].

Step

Instrument Type: **Detector**

Type: **Fixed point value**

Value Range: **Depending on the channel (e.g. for a UV channel: 0.01 ... 4.8 [sec] or Auto)**

Default: **0.25 s (GC: 0.05 s)**

Note: For uncontrolled GCs: 0.25 s.

Related Comm.: ➢*Data Collection Rate*

Description: Determines the time interval between two consecutive data points within the signal's **Raw Data** file. This value can be fixed or auto (i.e. variable). A fixed sampling rate is especially required in the event that the recorded raw data are to be exported where the recipient program can only process **equidistant** data points.

Function: **Fixed Step [0.01 .... 4.8 sec]**

Every *step* seconds, a data point is stored in the export **Raw Data** file. For example, selecting step = 0.5 means that 2 data points per second are acquired and stored. The smaller the step, the more data points will be recorded per time unit (regardless whether there is a baseline segment or a peak).

For the 3D field, **step** (here 0.1 - 4.0 sec) defines the data rate with which the connected ➢*Photodiode Array Detector* collects spectra.

The distance between individual data is as follows: for the Dionex UV Detector = 0.01 s, the ➢*A/D Converter* = 0.01 s; ➢*3D-Field* = 0.1 s.

Function (Cont'd):

Automatic Step [auto]

At a variable sampling rate, the last 10 seconds of a chromatogram are temporarily stored in system memory with the highest sampling rate. For each new data point (every 0.01 s), the oldest data point can be removed.

A complex algorithm allows determining and storing only those data points in the raw data file that are actually required. All "unnecessary" datapoints are filtered out and the chromatogram is stored almost without a loss in representation (!).

Depending on whether there are narrow or wide peaks or a baseline segment, between 0.2 and 100 data points per second are stored as the result. Thus, the step is automatically varied between 0.01 and 5 seconds.

Saving raw data with automatic step reduces the storage requirement up to 75% and thus increases data processing.

In the Report, you can view the chosen raw data points via the **Raw Data Point** option on the **Peak Decoration** tab of **Decoration** in the context menu.

☞ ***Tip***:

Select the step in such a way that 20 data points are placed on the narrowest, relevant peak of your chromatogram. If you acquire more data points, this will use unnecessary disc capacity and the integration might become incorrect, especially with heavier baseline noise.

Use the step **Auto** for fast peak chromatograms for which you do not know the width of the expected peak. For a precise and reproducible analysis, always use a fixed step (see above). Especially with heavier baseline noise, using **Auto** may result in an incorrect integration.

StopFlow

Instrument Type: **System Command**

Related Comm.: ⇒*Hold*

⇒*Flow*

⇒*Continue*

Function: The **Stop Flow** command switches off the pump flow; data acquisition is interrupted. A running batch is stopped, as in the hold mode.

Use the **Continue** command to undo this command.

Temperature

Instrument Type:	**Column Oven / Autosampler / GC**
Related Comm.:	**---**
Description:	**Temperature** adjusts the required temperature for a column thermostat, autosampler, or GC.
Function:	If the program file contains more than one Temperature command, you will get a step profile instead of linear interpolation between two commands, which is happening with all temperature commands. In other words: Every new temperature command drives the thermostat to the new temperature as fast as possible (device-dependent). With GCs, the temperature is changed according to the desired temperature program.
Parameters:	
Value	Actual column thermostat temperature
Nominal	Required temperature for the column oven.
Upper/LowerLimit	Upper/lower limit for the temperature of the column oven.
***Tip**:*	As with all device parameters, the Dionex Chromatography Management System tries to display the status on the screen! Whether this is possible depends on the column oven connected.

Trigger

Instrument Type: **System Command**

Related Comm.: ⇒*EndTrigger*

Description: Executes the command immediately following once defined conditions are satisfied, e.g. a defined signal voltage threshold and/or your time gradients exceeds a specified threshold. The condition is defined via the **Condition** parameter.

In the program, the entire Trigger block is indicated in blue color.

Examples

- A typical use for this function is the control of a ➢*Fraction Collector*. If the absorption signal of a given channel exceeds a threshold value, a relay is activated, switching to the next collection vial. Further important applications are
- Signal-dependent ➢*Wavelength Switches*, e.g. immediately after completion of a peak. Thus, retention time variations can be neglected!
- Programs can be ⇒*Branched* off according to external conditions, e.g. a digital input or the value of an analog signal. Thus, the chromatographic reaction to external conditions (pressure, conductivity, etc.) can be flexibly determined.
- Acoustic signals can be generated when certain conditions become true (⇒*Sound*). Thus, your peaks can be made audible!

Function:

The trigger condition is active from the time of the trigger command and has to be specifically deactivated. However, signal values are received only after the ⇒*AcqOn* command of the program. The following command is executed every time the specified conditions are satisfied (**flank triggering**), i.e. from each transition from false to true. Thus, in the previous example, the trigger condition must be entered only once in the program; the fraction collector will then be switched for each new peak.

Trigger commands can only be activated from programs or programmable buttons but not in the online control. The following syntax is valid:

```
Time Trigger NAME Condition, True,
                  Delay,       Limit,
Hysteresis
     Triggered command 1
     Triggered command 2
     Triggered command 3
     ...
     EndTrigger
```

As a response to a ➢*Trigger* condition becoming true, virtually any instruction can be performed. Examples:

- AbortBatch
- Acquisition.on/off
- BranchTo
- ⇒*Message*
- ⇒*Protocol*
- Relayname.on/off
- Signalname.Parameter
- Sound

Function (Cont'd):

Triggering the flow rate and the solvent composition is also possible. However, a gradient will be interrupted, and the analysis will be continued under isocratic conditions. Yet, you can use the **Branch** command to start a new gradient program.

The inject command cannot be triggered, as it is linked to t = 0.000 and can be given dependently from the time.

Even trigger commands can be triggered!

Parameters:

Name

The name of the trigger command is obligatory. It serves for its identification. Therefore, the name must be unique, i.e., the trigger cannot have the same name as a device or another command. Then, several triggers with different names can be activated simultaneously.

***Tip**:* To be able to find the trigger in an Audit Trail or a Report, it is recommended to include the trigger name in capital letters in the program.

Condition

Defines the **trigger condition** and can have two forms:

<Parameter><Comparison Operator><Value> or <Signal.Delta><Comparison Operator><Value>

or

<Remote-Input-Name>

<Parameter>
All installed channels, but also parameters such as **Temperature** (column temperature), **Pressure** (system pressure), **Flow** (flow rate), and **%A, %B, %C**, and **%D** can be used.

Condition (Cont'd):

<Signal.Delta>
For signals, the first derivative of the parameter can be evaluated. This is achieved by adding the signal property ➢*DELTA*.

<Comparison Operator>
<, >, =, <=, >= and <>

<Value>
Fixed-point number. The dimension of the <Value> corresponds to the signal dimension. Parameters that are combined with DELTA have the dimension [signal dimension / sec].

<Remote-Input-Name>
is reported from the instrument to the data system, e.g. **Sample.Ready** or **Leak**

If several parameters are to be linked, this can be realized via mathematical (+, -, *, / , **) or logical (AND, OR, NOT, XOR) operators. Parenthesis show combinations and hierarchy, e.g.:

- (UV_VIS_1>100) AND (UV_VIS_2>100)
- (UV_VIS_1+UV_VIS_2)>200

Logical links of entire conditions are also possible.

- (UV_VIS_1>100) AND NOT (UV_VIS_2>200)

True

Validity in seconds. The trigger condition must be true for this time, to activate the trigger. Example:

```
Trigger DIGIN1 Remote1, True=2.0
```

The input signal must be active for at least 2 seconds to trigger DIGIN1.

The **True** parameter is also used as a criterion for the truth of signals, e.g., to differentiate between **true** signals and spikes.

Delay

In seconds. Indicates the delay time between fulfillment of the conditions and execution of the command, e.g.:

```
1.220 Trigger SIGNAL UV_VIS_1>20, Delay=5.0

1.220 Relay On FracCol
```

The FraCol relay is switched 5 seconds after trigger activation only.

The **Delay** parameter is usually used for switching a fraction collector with a time delay. Thus, the dead volume between the detector and the fraction collector is taken into account.

If the **Delay** parameter is used in combination with the **True** parameter, the command is executed only <TRUE> + <DELAY> seconds after the condition is true.

Limit

The upper limit for executing the trigger command. Without the limit parameter, a trigger command is carried out any number of times until the trigger off command is activated. The limit parameter automatically deletes the trigger after a corresponding number of activations. Example:

```
1.220 Trigger BRANCH RemoteIn, Limit=1

      Branch NEWPGM
```

The trigger command is only carried out once, and then the trigger is deleted.

Hysteresis

To prevent multiple trigger execution with very noisy signals, each trigger receives the **Hysteresis** parameter in addition to the **True** parameter.

In contrast to the **True** parameter, **Hysteresis** is not time but signal-dependent. The parameter can vary between 0 and 100%. The default value is 5%.

Hysteresis (Cont'd):

A 5 % hysteresis causes, e.g., the condition

```
Cond = UV_VIS_1 > 20,0
```

To change from FALSE to TRUE when reaching the value 20.0, but only changing from TRUE to FALSE at 19.0. Thus, a difference is made between signal increases and decreases. This corresponds to the different paths of a hysteresis loop.

If the operator < is used instead of >, the calculation is reversed! For the above example, this means that the condition

```
Cond = UV_VIS_1 < 20,0
```

Becomes TRUE immediately when the value falls below 20, but is reset from TRUE to FALSE only at 20 + 5% = 21.

☞***Tips***:

While acquisition is switched off or interrupted, signal values cannot be evaluated.

If the **True** and **Delay** parameters are used, the command is switched only <TRUE> + <DELAY> seconds after the condition becomes true.

End program automatically deactivates all trigger conditions!

Triggering of the commands **Flow**, **%B**, **%C**, and **%D** is restricted to isocratic separations.

Example:

When the trigger condition becomes true, the following program switches the flow to 0.1 ml/min and sets %B to 0.

```
-1.000 Trigger ELUENT    UV_VIS_1 > 20
       Flow =            0.100
       %B.Value =        0.0
       EndTrigger
 0.000 Inject
 0.000 UV_VIS_1.AcqOn
 .....  ........
15.000 UV_VIS_1.AcqOff
15.000 End
```

Volume

Instrument Type: ➢*Autosampler*

Related Comm.: ⇒*Inject*

⇒*Position*

Value Range: **Depends on device and installed syringe**

Description: Specifies the injection volume in micro liters (µl).

Function: In automatic operation, the installed ➢*Driver* converts this value into a volume readable by the autosampler, then the value is sent to the autosampler.

By entering different injection volumes, a ➢*Dilution Series* can be created in case of a multiple-point calibration (➢*Single-Point and Multiple-Point Calibration*).

☞ ***Tip***: In order to minimize carry-over effects in multiple-point calibrations, you should always start with the sample with the highest dilution or the smallest injection volume.

Wait

Instrument Type: ➢*Remote Input*

Related Comm.: ⇒*Message*

⇒*Inject*

⇒*AcqOn/Off*

Description: The **Wait** command interrupts program execution until the specified remote input signal arrives.

Function: Wait stops the program time and the acquisition; the pump(s) are in hold-mode. For examples for using the **Wait** command see **How to ...: Device Control**:

Control - Autosampler

Mixed Commands

Parameter:

Condition Condition for the realization of which the system waits (see ⇒*Trigger*)

Wash

Instrument Type: ➢*Autosampler*

Related Comm.: ⇒*Inject*

⇒*NeedleUp*

Value Range: **Depends on device and installed syringe**

Description: The **Wash** command serves for rinsing the autosampler.

Function: It causes the autosampler to lower the needle into the needle seat and to rinse the sample loop and needle with solvent in the **Inject** state. This corresponds to the normal solvent flow following an **Inject** command.

☞ ***Tip***: Use the **Wash** and **NeedleUp** commands to wash the sample loop and thus prevent crystallization of substances in the sample loop.

Wavelength

Instrument Type:	**Detector**
Type:	**Integer**
Value Range:	**Detector-dependent**
Default:	**0 [nm]**
Related Comm.:	⇒*Bandwidth* ⇒*Reference Wavelength*
Description:	Specifies the wavelength at which the chromatogram is recorded.
Function:	For controlled detectors (e.g. Dionex detectors) this value is automatically transferred to the detector (requires **control option**). The wavelength can also be entered manually during the analysis or in the program. In configurations of the Dionex Chromatography Management System without control option, the selected wavelength remains fixed during the analysis. In controlled versions, the wavelength can be altered during analysis.

QNT Editor

The QNT editor allows defining the method of quantification (in short: **QNT Method** or just method). The quantification method defines parameters that identify the peaks within a chromatogram (assign substances - peak identification) and others that enable the calculation of amount/concentration from the recorded peak areas (calibration).

Peak Identification

The Dionex Chromatography Management System has two possibilities for identifying detected peaks, i.e. assignment of substance names.

Generally, peaks are identified by their ⇒*Retention Times*. If a peak elutes within a defined time window, it is assigned the corresponding name, calibration function, etc.

In the event that many peaks are obtained in rapid succession, or their order is altered by a change in chromatographic conditions (e.g. pH-value), identification by the **UV spectrum** or the ➢*Mass Spectrum* is considerably more reliable.

☞***Tip:*** Peak identification by UV spectra requires use of a ➢*Photodiode Array Detector* (e.g. Dionex UVD 340 or PDA-100) and the appropriate software configuration.

Mass spectra acquisition requires an aQa ➢*Mass Spectrometer* and the ➢*Xcalibur* software in addition to the Dionex Chromatography Management System software.

Calibration

The peak table contains all information for the calibration. Using the amount column and the recorded peak areas, the offset, slope, and curve parameters are calculated.

☞***Tip:*** With each new calibration the results are recalculated automatically for the report, as the calibration constants and the recorded integration values are entered to the peak table by the integration programs.

To save the user from having to determine the retention time of each peak manually, peak tables can be generated automatically (see **How to ...: Actions in the QNT Editor Autogenerating the Peak Table**).

The QNT editor offers the following tabs for parameter input:

- **General** (general settings)
- **Detection** (⇒*Detection Parameters*)
- **Peak Table** (general peak table)
- **Amount Table** (parameters to determine the amount)
- **Peak Tracking** (parameters for peak assignment via UV reference spectra)
- **MS Tracking** (parameters for peak assignment via ➢*Mass Spectra*)
- **Calibration**
- **Spectra Library Screening** (spectra search parameters)
- **SST** (➢*System Suitability Test (SST)* parameters)
- **MS** (parameters for mass spectra evaluation)

The **General** tab lists those parameters that apply to all peaks, e.g.

- ⇒*Use Recent Retention Time*: automatic correction of expected retention times during calibration runs.
- ⇒*(Calibration) Mode*: Specification which sample is calibrated using which standard(s).
- ⇒*Dimension of Amounts*

The peak table (on the **Peak Table**, **Amount Table**, **Peak Tracking**, and **MS Tracking** tabs) lists peak-specific parameters, e.g.

- **Expected retention time**
- **Peak name**
- **Integration type (area/height)**
- **Calibration type (linear, exponential, etc.)**

The general and the peak table parameters are described below.

QNT Parameters (Overview)

The QNT editor allows you to define general, peak table, and detection parameters. For a description of the latter ones, see ⇒*Detection Parameters (Overview)*. For information on the general parameters and the peak table parameters, see the following topics:

⇒*Amount*
⇒*Calibration Mode*
⇒*Calibration Type*
⇒*Check Derivative*
⇒*Check Extrema*
⇒*Comment (Peak)*
⇒*Dead Time*
⇒*Delay Time*
⇒*Dimension of Amounts*
⇒*Group* (*Peak Group)*
⇒*Integration Type*
⇒*Kovats Index*
⇒*Left/Right Limit*
⇒*Match Criterion*
⇒*Maximum/Minimum Wavelength*
⇒*Name* (*Peak Name*)
⇒*Reference Spectrum*
⇒*Relative Maximum Deviation*
⇒*Response Factor*
⇒*Retention Index*
⇒*Retention Time*
⇒*Standard*
⇒*Threshold*
⇒*Type* (*Peak Type)*
⇒*Use Recently Detected Retention Time*
⇒*Window*

Amount

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **Floating point number**

Dimension: Determined by the **Dimension of Amounts** parameter on the **General** tab

Value Range: **0.000001 ... 9999999.999999**

Default: **1.000000**

Related Param.: ⇒*Dimension of Amounts*

Description: Determines the content (amount, concentration) of a standard sample or a ➢*Validation Sample* of a particular mixture component. For multi-point calibration with various standards (i.e. not via the variation of the injection volume), several values must be entered for each peak. Thus, a matrix of standard contents is created, whose lines correlate to the peaks and the columns to the various standards.

Function: The amount can be entered either as concentration value (e.g. µg/µl) or as absolute amount (e.g. µg). In the report, the result is displayed accordingly, either as concentration value or as an absolute amount. Use the respective inverse function for calculation (see: **Calculating the Peak Variable Amount**).

In absolute amounts, the result always relates to the injected volume, e.g. 17.6µg per 20µl injection volume. Use the ➢*Concentration* peak result variable to receive normalization to 1 µl (e.g. 17.6 / 20 = 0.88 µg/µl) by dividing the absolute value by the injection volume.

Tip: If a concentration unit has been chosen as **Dimension of Amount**, the **Concentration** peak variable has lost its sense.

Function (Cont'd):

In a single-point calibration, only one standard is used. This means that there is only one value per component (peak).

In a "real" multiple-point calibration (➢*Single-Point and Multiple-Point Calibration* - no variation of the injection volume), the number of amount values for each component must correspond exactly to the number of standards.

☞ ***Tip***:

In a multiple-point calibration, the values of the **Amount** columns are corrected by the ratio of the injection volumes (for which the reference volume defined on the **General** tab of the QNT editor is used) and the dilution factors in comparison to the first standard. You can thus combine the amount values with the ➢*Dilution Series*!

Even for multi-point calibration normally only one peak table is required!

Calibration Mode

Location: Tab **General** / Report Variable **(Peak Calibration)**

Type: **Character**

Dimension: **No dimension**

Value Range: **Fixed / Total / Group / Additional / Bracketed**

Default: **Total**

Related Param.: ⇒*Calibration Type*

Description: The calibration mode determines which standards are used for calibrating a specific sample of a sequence. The Dionex Chromatography Management System has five different calibration modes.

The mode is selected on the  **General** sheet in the QNT editor.

Function:

Fixed This setting enables the calibration using various standards (also from other sequences).

The desired standards are entered via the **Insert Standard** or **Append Standard** commands to the **Calibration** sheet of the QNT editor. The sequence the standards are taken from is included in the **Sequence** column.

Entering individual calibration coefficients is possible as well via the c0, c1, and c2 columns in the amount table.

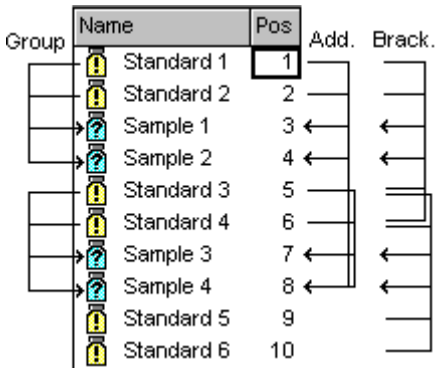
☞ ***Tip***: Always perform the calibration manually (**Calibrate**). The **Auto-Recalibrate** option is not available.

Total Calibration is performed using all valid standard samples of a sequence. The standard samples deactivated in the **Enabled** column of the **Calibration** sheet (QNT editor) are not included.

Group The calibration of a sample series from the sample list (e.g. samples 3 to 50) is performed based on the standard samples listed directly before this series (e.g. no. 1 and 2). If this sample list includes further standards (e.g. no. 51 and 52), the following samples (e.g. 53 to 100) will be evaluated based on these. The standard samples in lines 1 and 2 will no longer be considered (For an example, see below.)

Additional For calibrating a sample, all standard samples that are listed *before* this sample in the sample list are used. The further down the sample is listed in the table, the more standard samples will be considered. (For an example, see below.)

Bracketed Samples are evaluated based on all standard samples immediately surrounding. In case of an alternating list of two standards, two samples, two standards, two samples, etc. the samples 1 and 2 (located at positions 3 and 4) are evaluated with the standards 1, 2, 3, and 4 (located at positions 1, 2, 5, and 6) while the samples 3 and 4 are evaluated using the standards 3, 4, 5, and 6 (located at positions 5, 6, 9, and 10), etc. (For an example, see below.)



Calibration Type

Location: Tab **Peak Table** / Report Variable **(Peak Calibration)**

Type: **Code**

Dimension: **---**

Value Range: **Linear (Lin) / Linear with Offset (LOff) /**
Quadratic (Quad) / Quadratic with Offset (QOff) /
Exponential (Exp) / Point-to-Point (P-P)

Combine with: **No Weights, 1/Amount (X), 1/Amount² (XX), 1/Response (Y), 1/Response² (YY)** (with **Average all response values...** additionally **1/Rel.Std.Dev., 1/Rel.Std.Dev.²**)

Default: **Linear**

Related Param.: ⇒*Standard*

⇒*Calibration Mode*

Description: The Calibration Type determines the ➢*Calibration Function* and the ➢*Weights*. In calibration, for each peak up to three calibration constants are entered into the calibration file, defining the peak area/amount ratio. The minimum number of required samples depends on the type of calibration curve chosen. A maximum of 20 samples from different sample files may be marked and used as calibration samples. The calibration points can also be weighted with 1/Amount, 1/Amount², 1/Response, and 1/Response². The type of the weight function is entered together with the curve type. We recommend using the F8 box for selecting the desired specifications, e.g. the field value *XXQOff* stands for quadratic with offset and weight function $1/amount^2$.

Function: A series of methods, differing with respect to their model function and the number of coefficients is available. The number of calibration samples needs to be at least equal to the number of coefficients to be determined.

Calibration functions:

Linear (Lin)

Minimum number of standards: 1

The model function presents a straight line passing the origin. For more than one standard, the regression line is calculated. The calibration curve is based on the following equation:

Model function: $f(A) = c1 \, x \, A$

Where x is the peak area and a(x) the calculated amount.

c1 (linear coefficient, slope) is calculated and stored.

Linear with offset (LOff)

Minimum number of standards: 2

The calibration curve presents a straight line, crossing the ordinate at a finite value.

Model function: $f(A) = c0 + c1 \, x \, A$

c0 and c1 are calculated and stored.

Quadratic (Quad)

Minimum number of standards: 2

The calibration curve presents a parabola passing the origin. For more than two calibration samples, the regression parabola is calculated.

Model function: $f(A) = c1 \, x \, A + c2 \, x \, A^2$

c1 and c2 are calculated and stored.

Quadratic with offset (QOff)

Minimum number of standards: 3

The calibration curve presents a parabola crossing the ordinate at a finite value. For more than three calibration samples, the regression parabola is calculated.

Model function: $f(A) = c0 + c1 x A + c2 x A^2$

c0, c1, and c2 are calculated and stored.

Exponential (Exp)

Minimum number of standards: 2

The calibration curve presents an exponential function.

Model function: $f(A) = c0 x A^{c1}$

c0 and c1 are calculated and stored.

Point-to-Point

Minimum number of standards: 1

The calibration curve is polygon, i.e. a linear interpolation between two calibration points. If there are several replicates of a calibration level, they are averaged before interpolation.

Weighting:

No Weights

Default: higher weighting of higher amounts / signal values.

1/Amount (X)

Nearly cancels out the weighting of higher amounts.

1/Amount² (XX)

Causes over-proportional weighting of smaller amounts.

1/Response (Y)

Nearly cancels out the weighting of higher signal values. In this case, the Y-values (dependent signal values) of the calibration points are used as weight factors instead of the X-values (nominal amounts).

1/Response² (YY)	Causes over-proportional weighting of smaller signal values. In this case, the Y-values (dependent signal values) of the calibration points are used as weight factors instead of the X-values (nominal amounts).
1/Rel.Std.Dev. (S)	Weights signal values with small relative standard deviations more than those with large relative standard deviations.
1/Rel.Std.Dev. ² (SS)	Weights signal values with small relative standard deviations clearly more than those with large relative standard deviation.
Options:	**Average all response values of each calibration level before curve fitting** averages the calibration level points before calculating the calibration curve from the average values. **Include point (0,0) for curve fitting** includes the origin into the calibration curve calculation for calibration functions with offset without forcing the calibration curve through the origin.
☞ ***Tip***:	All procedures are possible both, with the area method and the height method. Note that integration and calibration should fit together, i.e. either area method in both cases, or height method. Only the area method can be substantiated by physics.

For further information on the available calibration types, see the following topics in the **Theory of Calibration** section:

Calibration Types (Linear)

Calibration Types (Non-Linear)

Check Derivative

Location: Tabs **Peak Tracking** and **Spectra Library Screening /** Report Variable **(Peak Table)**

Type: **Selection**

Dimension: **-**

Value Range: **Off; 1st derivative; 2nd derivative**

Default: **Off**

Related Param.: Additional parameters for comparing spectra:

⇒*Check Extrema*
⇒*Match Criterion*
⇒*Maximum/Minimum Wavelength*
⇒*Relative Maximum Deviation*
⇒*Threshold*

Description: Comparison of two or more spectra with each other can be performed in three different ways (comparison functions):

- Based on the curve shape of the spectrum itself
- Based on the curve shape of the first derivative of the spectrum
- Based on the curve shape of the second derivative of the spectrum

Function: Comparing the curve shape of the first or second derivative of the spectrum is more characteristic (shoulders become extremes). However, the ➢*Signal to Noise Ratio* decreases considerably. Depending on the comparison function different ⇒*Threshold* values are useful.

***Note**:* Differentiating once or twice can lead to well matching hits, although the absorption heights of the original spectra differ significantly.

Check Extrema

Location:	Tabs **Peak Tracking** and **Spectra Library Screening /** Report Variable **(Peak Table)**
Type:	**Selection**
Dimension:	**-**
Value Range:	**Off; On**
Default:	**Off**
Related Param.:	Additional parameters for comparing spectra: ⇒*Check Derivative* ⇒*Match Criterion* ⇒*Maximum/Minimum Wavelength* ⇒*Relative Maximum Deviation* ⇒*Threshold*
Description:	The parameter indicates whether the spectra search compares the number of extrema in the reference spectra with the ones in the peak spectrum.
***Note**:*	If there is strong noise (see ➢*Signal to Noise Ratio*), it is possible that noise peaks are considered extrema. In this case, it is recommended to deactivate the **Check Extrema** option.

Comment (Peak)

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **Text**

Dimension: **---**

Value Range: **All printable characters**

Default: **---**

Related Param.: ⇒*Name* (*Peak Name*)

Description: In addition to the peak name, further comments can be entered. Double-clicking or pressing the F8 key opens an enlarged entry field.

***Note**:* If the peak table is generated in the QNT editor via the *Autogenerate Peak Table* function (for details, see the respective Online Help topic), this will be automatically indicated in the **Comment** column of the peak table:

- If **Enumerate peaks of current chromatogram** is selected, the comment will be **Autogenerated**.
- If **Use spectra library screening results** is selected, the corresponding comment will be **Autogenerated, Spectrum: *Name of Reference Spectrum*, Match:** ➢*Match Factor* ***number***.

Dead Time

Location:	Tab **General** / Report Variable **(Quantification Method)**
Type:	**Floating point value**
Dimension:	**Minutes**
Value Range:	**0.000 ... 9999.999**
Default:	**Not chosen**
Related Param.:	⇒*Retention Time* ⇒*Delay Time* ⇒*Window*
Description:	The Dead Time To is defined as the time required for the peak maximum of an unretained substance to reach the detector from the point of injection. The dead time thus corresponds to the residual time (of all substances) in the mobile phase. Enter the dead time in the **QNT Editor** on the **General** tab.
Function:	The adjusted retention time, T'(S), of a substance is defined as the time this substance remains in the stationary phase. The sum of the residual times in the mobile and stationary phases is the ➢*Retention Time*: T(S) = T'(S) + To. The dead time is required to calculate the ➢*Capacity Factors* and the ⇒*Kovats Indexes*.

Delay Time

Location:	Tab **General** / Report Variable **(Quantification Method)**
Type:	**Floating point value**
Dimension:	**Minutes**
Value Range:	**-9999.999 ... 9999.999**
Default:	**Not selected**
Related Param.:	⇒*Dead Time* ⇒*Retention Time*
Description:	The time needed by a substance to travel from the detector cell of one detector to the detector cell of a second detector is referred to as Delay Time.
Function:	Usually, a constant ⇒*Flow* is used. With constant flow, the delay time between two detectors is constant as well. In this case, it can be measured and entered on the **General** tab of the ⇒*QNT Editor*. The entered delay times can be positive or negative depending on whether the detector directly following the column or any other detector is defined as **2nd detector**.
***Tip**:*	Entering a delay time for ➢*Flow Gradients* does not make sense because the delay is not constant in this case. Proceed as described under **Defining the QNT Method for Several Detectors**. You cannot use the **Delay Time** parameter in MT2 and GynkoSoft datasources or in any raw data that are imported from them.

Dimension of Amounts

Location:	Tab **General /** Report Variable **(Peak Table)**
Type:	**String**
Dimension:	**---**
Value Range:	**All printable characters**
Default:	**---**
Related Param.:	⇒*Amount*
Description:	This parameter defines the physical dimension of the amount values. Usually, it should be an amount dimension but you may as well choose a concentration dimension.
Function:	The chosen dimension is entered in the column header of the amount column of the report table. It is only relevant to the documentation of results and has no influence on the calculation algorithms.
☞ ***Tip**:*	Consistency of dimensions is entirely up to the user. If weight was read as g, do not enter mg here. There will be no automatic conversion! For the calculation of the concentration in the report or the printer layout, the Dionex Chromatography Management System presumes that a dimension of amount was chosen. If a dimension of concentration was entered as **Dimension of Amounts**, this calculation does not make sense.

Group (Peak Group)

Location:	Tab **Peak Table /** Report Variable **(Peak Table)**
Type:	**String**
Dimension:	**---**
Value Range:	**All printable characters**
Default:	**---**
Related Param.:	⇒*Peak Group Start/End* ⇒*Integration Type* ⇒*Calibration Type*
Description:	Peaks may be grouped and then be calibrated and integrated together. You may assign the group any name, whilst it is recommended to use the name of the group's most "important" member. The members must not necessarily succeed one another. (If you wish to group peaks that lie close together, use the **Peak Group Start** and **Peak Group End** detection parameters (on the **Detection** tab of the QNT editor.)
Function:	During calibration (not during peak detection), the peak group is treated as one non-resolved peak: The calibration constants of the amount value and the area sum of all peaks being part of the group are calculated. The calibration curve, therefore, is identical for all peaks. During integration, the amount/concentration values for each peak are calculated individually for each peak from its area and calibration constants.
☞ ***Tip:***	The **Integration** and **Calibration** types must be identical for all peaks within a peak group.

Also see: **How to ...: Actions in the QNT Editor**  **Grouping Peaks**

Integration Type

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **Selection**

Dimension: **No dimension**

Value Range: **Area / Height / Relative Area / Relative Height / CE Area**

Can be combined with: **All peaks, identified Peaks only / Exclude ISTD peaks** (only with **Relative Area / Relative Height**)

Default: **Area**

Related Param.: ⇒*Calibration Type*

⇒*Group*

Description: Indicates the peak property to be used for the calculation of quantitative results. Different Area and height methods are the alternatives.

Functions:

Area Peak area integration.

All amount calculations refer to the peak area which itself is calculated numerically according to the trapezoidal method. Area delimiters in this case, consist of chromatogram, baseline and, if necessary, perpendiculars in order to exclude adjacent non-resolved peaks. In case of ➢*Riders*, an appropriate skimming tangent substitutes the baseline.

Height Peak height integration.

All amounts refer to the peak height, i.e., the height of the peak maximum as related to the baseline.

Relative Area Relative peak area integration. The area can be chosen relative to the area of

- **All peaks** or
- **Identified peaks only**

In both cases the internal standard(s) may be excluded (**Exclude ISTD peaks**).

Relative Height Relative peak height integration. Reference corresponding to the relative peak area integration is possible.

CE Area Integration type for capillary electrophoresis

CE-Area = Area / Ret. Time in [mAU])

☞ ***Tip:*** Integration and calibration always require the same method!

All peaks of a **Group** require the same method.

Only the area methods can be substantiated by physics.

Kovats Index

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **Integer**

Dimension: **No dimension**

Value Range: **0 ... 999.999**

Default: **-**

Related Param.: ⇒*Retention Time*

⇒*Dead Time*

Description: Data exchange between laboratories for substance identification based on relative retention times is not exact. Therefore, especially in gas chromatography, retention indexes are used. They use a series of chemically similar standard substances to achieve uniform scaling of the **Retention Time**.

Advantage is taken of the fact that within a homologous series of compounds the logarithms of the adjusted retention times are proportional to the number of carbon atoms (adiabatic and isothermal conditions presumed). The most frequently used **Kovats Index** is defined as follows:

$$KI = 100 * n + 100 \frac{[\log T'(x) - \log T'(n)]}{[\log T'(n+1) - \log T'(n)]}$$

Wherein:

KI: Kovats index

T'(x): Adjusted retention time (with: T'(x) = T(x) -)To)

T(x): Retention time

To: Dead time

n: Number of carbon atoms (normally of n-alcane)

x: substance of interest

While the following must be true:

T(n) < T(x) < T(n+1).

Function:

As the Kovats indexes for the markers are freely selectable the following formula is used for the calculation:

$$KI = KI(z) + (KI(z+1) - KI(z)) \frac{[\log T'(x) - \log T'(z)]}{[\log T'(z+1) - \log T'(z)]}$$

With KI = Kovats index (usually KI = 100 * n is entered) and

z = number of the marker peak.

If no marker peaks or no dead time is determined, the Kovats index is not defined (n.a.). In addition, the Kovats index is not defined for any peaks that occur before the first and behind the last marker peaks. For further information on how to enter marker peaks and dead time see **How to …: Actions in the QNT Editor**  **Defining the Retention Index and the Kovats Index**.

☞ ***Tip:***

In the Dionex Chromatography Management System, the substances of interest must be between two marker peaks.

Left/Right Limit

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **Fixed point number**

Dimension: **Minutes**

Value Range: **0 ... 999.999 [min]**

Default: **0 (no function)**

Related Param.: ⇒*Retention Time*

Description: Normally, peak integration is performed automatically. It is possible to limit or extend integration on the left, right, or on both sides with the appropriate peak table parameters. This may be done in the peak table via a left and/or a right limit.

Function: The peak is integrated between left and right limit, i.e. between:

RT - LL ... RT + RL

Wherein:

RT = Retention Time

LL = Left Limit

RL = Right Limit.

The value 0 deactivates the limitation.

Example 1:
For the right and the left integration limit, the value 0.5 min is entered. The peak maximum is at the retention time of 8 min. The peak is integrated from 7 min 30 sec to 8 min 30 sec.

☞ ***Tip:*** The limits LL and RL can also be activated/deactivated independently.

Example 2:
For the left integration limit the value 0.5 min and for the right integration limit the value 0 is entered. As before, the peak maximum is at the retention time of 8 min. The peak is integrated from 7 min 30 sec. The end of the integration is automatically determined then.

Match Criterion

Location: Tabs **Peak Table** and **Spectra Library Screening** / Report Variable **(Peak Table)**

Type: **Selection**

Dimension: **no dimension**

Value Range: **Least Square, Weighted Least Square, or Correlation**

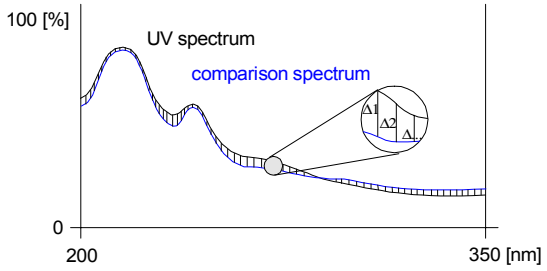
Default: **Least Square**

Related Param.: Additional parameters for comparing spectra:

⇒*Check Derivative*
⇒*Check Extrema*
⇒*Maximum/Minimum Wavelength*
⇒*Relative Maximum Deviation*
⇒*Threshold*

Description: The match criterion defines the mathematical method with which two standardized spectra are compared with each other.

Function: The signal deviation, i.e., the difference between the UV spectrum and a reference spectrum at defined wavelength, is checked (Δ1, Δ2, ...). Since the square of the deviations is calculated as well, the direction of the subtraction does not matter.



The method provides a value of similarity (match) between completely different (= 0) and identical (= 1000).

Function (Cont'd): The following mathematical methods are available in the Dionex Chromatography Management System:

Least Square: Forms the sum of the squared signal deviations at each wavelength and determines the average square deviation between two spectra (standard method)

Weighted Least Square: Analogue to Least Square; the squared deviations are weighted by the signal height (for spectra extracted close to the detection limit).

Correlation: Usual match criterion in statistics if a linear correlation between two curves is presumed (similar to Least Square; usually provides the same result).

Maximum/Minimum Wavelength

Location:	Tab **Peak Tracking** and **Spectra Library Screening /** Report Variable **(Peak Table)**
Type:	**Floating point number**
Dimension:	**nm**
Value Range:	**Auto; 190.0 - 900.0 nm**
Default:	**Auto**
Related Param.:	Additional parameters for comparing spectra: ⇒*Check Derivative* ⇒*Check Extrema* ⇒*Match Criterion* ⇒*Relative Maximum Deviation* ⇒*Threshold*
Description:	The **Maximum**/**Minimum Wavelength** (= **Max**./**Min. WL**) column allows you to enter the upper/lower wavelength limits for spectra screening. In case of **Auto,** the respective limits will not be considered.
☞ ***Tip**:*	The value entered here has no significance for any currently displayed peak spectrum.

Name (Peak Name)

Location:	Tab **Peak Table /** Report Variable **(Peak Table)**
Type:	**String**
Dimension:	**no dimension**
Value Range:	**All printable characters**
Default:	With automatic table generation: **<Name of the QNT Method>x**, wherein **x** is the current peak number. When appending a new cell: **Peak-x**
Description:	In this column, you may enter the chemical name of the substance that created the peak at the time t (default is used with auto-generated peaks, only).
Function:	The substance name is taken for the report and the ➢*Printer Layout*.
☞ ***Tip**:*	Only letters, numbers, and punctuation marks should be used, since the complete MS-DOS character set is not available on all printers.

Reference Spectrum

Location:	Tab **Peak Tracking** / Report Variable **(Peak Table)**
Type:	**Selection**
Dimension:	**No dimension**
Value Range:	**---**
Default:	**Empty**
Related Param.:	⇒*Window*
Description:	Reference spectra are used for substance identification. For each peak such a reference spectrum can be chosen. Such spectra are acquired with the DAD license of the Dionex Chromatography Management System. Identifying peaks by means of peak tracking can be activated via an input in the **Window** column. In the corresponding F8 dialog box (press the F8 key or double-click in the **Window** column), select one of the options **Spectrum** or **Spectrum and time** of the group **Peak Match**.
Function:	Peak tracking is performed (limited to the specified time window in the case of **Spectrum and time**) using the reference spectra in the corresponding column (see **How to ...: Actions in the QNT Editor** **Peak Tracking**).
☞ ***Tip:***	Spectra acquisition is possible with the DAD license, only.

Relative Maximum Deviation

Location:	Tab **Peak Tracking** and **Spectra Library Screening /** Report Variable **(Peak Table)**
Type:	**Floating point number**
Dimension:	**nm**
Value Range:	**Off; 0.0-100.0 nm**
Default:	**Off**
Related Param.:	Additional parameters for comparing spectra: ⇒*Check Derivative* ⇒*Check Extrema* ⇒*Match Criterion* ⇒*Maximum/Minimum Wavelength* ⇒*Threshold*
Description:	The column **Relative Maximum Deviation** allows you to enter the maximum permissible deviation of the wavelength maxima of the reference spectra from the maximum of the current peak spectrum.
Function:	If the setting is **Off**, the deviation is not checked.

Response Factor

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **Floating point number**

Dimension: **---**

Value Range: **0.000000 ... 9999999.999999**

Default: **1.000000**

Related Param.: ⇒*Weight* (sample weight)
⇒*Dil. Factor* (dilution factor)

Description: The response factor is a peak-specific dimensionless, multiplicative factor, used to compensate for absorption differences in the case of differing wavelengths.

Function:

Absolute Select **Absolute** to correct the amount value received from the peak area via the ➢*Formula for Amount Calculation* by the entered factor. In this way, e.g. absorption differences at different wavelengths can be compensated. Besides, losses of readily volatile samples can thus be considered in the calculation (especially common in gas chromatography).

Relative To Peak Select **Relative To Peak** for a correction in relation to a reference peak. As a reference peak, all peaks that are assigned a peak name in the peak table can be used. As the **normal** (absolute) response factor, the value of the relative response factor is used as a multiplicative factor in the amount evaluation. The basis of the evaluation is not the calibration curve of the peak in the peak table, but that of the selected reference peak.

Relative To Peak (Cont'd):

Example: Relative to Peak

Under certain conditions, an active agent in a tablet decomposes into various products. As standards for these products are difficult to produce or very expensive, the active agent and the decomposition products are calibrated e.g. once a year.

If the active agent and the decomposition products are calibrated via the **linear without offset** function, there is a direct correlation between the slope of the active agent calibration curve and the calibration curves of the individual decomposition products. This proportionality between the calibration coefficient c1 of the active agent and that of the decomposition product is expressed as the Response Factor and must be determined by the user.

Should the active agent and/or the decomposition product be determined in an analysis, the existing calibration and the Response Factor determined for each decomposition product is used. The factors are entered as *relative* values (**Response Factor** column) in the peak table, i.e., the active agent in the tablet is used as the reference peak.

Calculating the amount values of all decomposition products is according to the calibration coefficients of the active agent, corrected by the Response Factor.

☞ ***Tip**:*

The response factor is peak-specific!

In contrast to this, the Sample Weight and the Dilution Factor of the sequence table are sample specific, i.e., they apply to all peaks.

Retention Index

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **Integer**

Dimension: **No dimension**

Value Range: **0 - 999.999**

Default: **-**

Related Param.: ⇒*Retention Time*
⇒*Dead Time*
⇒*Kovats Index*

Description: Retention indexes are used to facilitate positive assignment of substances in inter-laboratory data exchange. For programmed GC as well as for HPLC linear retention indexes are defined.

Function: The Dionex Chromatography Management System calculates the following linear retention index:

$$RI(x) = RI(z) + \frac{[RI(z+1) - RI(z+1)] * [T(x) - T(z)]}{T(z+1) - T(z)}$$

With

RI: Retention index (usually RI = 100, 200, 300 is entered)

z: number of the marker

The following is true:

T(z) < T(x) < T(z+1).

If the peak occurs before the first maker peak, the following formula is used:

RI (x) = RI(1) * [T(x) / T(1)]

If the peak occurs behind the last marker peak, the following formula is used:

RI (x) = RI(last) * [T(x) / T(last)]

For information how to determine marker peaks see, **How to ...: Actions in the QNT Editor Defining the Retention Index and the Kovats Index**.

Retention Time

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **Floating point value**

Dimension: **Minutes**

Value Range: **0.000 ... 9999.999**

Default: **0.000**
With **Autogenerate Peak Table**, the retention time of the current chromatogram is used.

Can be combined with: **Absolute time; Time distance / ratio to reference peak; Reference peak**

Related Param.: ⇒*Window*
⇒*Use Recently Detected Retention Times*
⇒*Dead Time*

Description: The retention time is used for peak identification. The peak **Retention Time** variable refers to the time (in minutes) that passed since the injection (also see ⇒*Dead Time*).

By definition, the injection time always equals zero. Therefore, control commands issued before this time will have negative times. The advantage is that the times stated in the ➢*PGM File* (file type .PGM) are compatible with the retention times, rather than being delayed by the injection time.

Peak retention times are generally interpreted as time between injection and peak maximum. However, indication of the distance to a reference peak is possible as well. As the reference peak does not need to be at the beginning of the chromatogram, such difference retention times can also have negative values. Relative retention times are time quotients in percent as to a reference peak.

Function:

On the page **Peak Table** in the QNT editor, the retention time can be entered either manually by the user or automatically by the system. The latter is possible via the **Autogenerate Peak Table** command from the **Edit** or context menus.

The user enters the expected retention time, while the system enters the actually detected retention time of the actually analyzed sample.

Interpretation

Input in the **Retention Time for Peak X** dialog box (to be opened via **F8** or double-clicking the **Ret. Time** column)

Absolute time

Select **Absolute time [min]** to display the retention times as usual (time period between injection and peak maximum).

Time distance to reference peak [min]

Select **Time distance to reference peak [min]** to express the time difference to the reference peak in minutes. All peak lines except the line for the reference peak show time differences in the time column.

Time ratio to reference peak [%]

Select **Time ratio to reference peak [%]** to express the retention time relatively to the reference peak in % values. The retention times are indicated as time ratio (percent) to the reference peak. All peak lines except the line for the reference peak show the time ratios to the reference peak in percent.

Reference peak

Select a peak from the peaks listed in the selection box. The reference peak line in the peak table is highlighted in light blue. It **always** shows the **absolute retention time**!

☞***Tips***:

If the **Use Recently Detected Retention Time** option (retention time correction) is activated in the peak table, the retention times entered manually on the page **Peak Table** are no longer used as nominal retention times for all identified peaks. Instead, the values detected for the previously analyzed sample (its nominal times) are used.

☞***Tips** (Cont'd):*

It is to be distinguished between:

- The originally expected retention time which was entered on the **Peak Table** sheet,
- The nominal retention time which, in this case, corresponds to the actual retention time of the previously analyzed sample, and
- The actual retention time of the actually analyzed sample.

⇒*Retention Windows* are also interpreted as percentage value of the absolute retention time for both, difference, and relative retention times! Only the retention times of identified peaks are corrected!

In the Peak Table, you can toggle the three options. The retention time column is automatically re-calculated.

Standard

Location: Tab **Peak Table /** Report Variable **(Peak Table)**

Type: **String**

Dimension: **---**

Value Range: **External; Internal; Internal/External; Use this peak as internal Standard**

Default: **External**

Can be combined with: **Use sample amount as reference (**only with **Use this peak as internal Standard)**

Related Param.: ⇒*Amount*

Description: Indicates the standard method to be used for calibration. For a detailed description including numerical examples, see **How to ...: Actions in the QNT Editor Calibration**

Function:

External The calibration curve determines the area/amount ratio. During calibration, the calibration coefficients (see ➢*Calibration Function* and **Standard Methods**) are calculated from mixtures of known components.

Internal Calibration corresponds to the External Standard method. In addition, an ➢*Internal Standard* is added. The internal standard itself is calibrated as all other peaks. When performing the integration, the calculated amounts of the remaining peaks are corrected by the nominal/actual ratio of the internal standard.

The Dionex Chromatography Management System recognizes any number of internal standards. Theoretically, each peak may have its own internal standard! Furthermore, the standard method may be selected for each peak individually.

Internal (Cont'd):

During calibration, the amount ratio (instead of amount against area) is given in the diagram with regard to the respective peak. From these data points, the calibration function is calculated.

During integration also, the area ratio is inserted into the stored calibration function and the amount ratio is calculated.

☞ ***Tip:*** Before you can use this option, at least one internal standard must be defined (see **Use this peak as internal Standard**). Select the desired ISTD peak in the **Associated ISTD Peak** checkbox.

Entering Several Internal Standards

It is also possible to define several internal standards. Via the F8 box, define the respective peaks of the peak table in the Standard column of the peak table as ISTD peaks. A yellow background will highlight the corresponding line of the peak table. For the remaining peaks, enter the standard method to be used (external, internal/external, internal). If this should be performed in relation to an ISTD peak, it is possible to choose between the previously defined ISTD peaks.

Internal/External

When calibrating with an internal standard, calculation is with area and amount ratios instead of absolute areas and amounts. During integration, the area ratio is inserted into the saved calibration function to calculate the amount ratio. The result is the amount in relation to its reference peak. Each peak can have its own internal standard.

Calibration does not vary from the external standard method, except for a defined peak (i.e. internal standard) being added to the analyses. The internal standard is calibrated as all other peaks.

Internal (Cont'd):

During integration, the calculated amounts of the other peaks are corrected according to the relation of the internal standard to the actual peak.

☞ ***Tip***: Before you can use this option, at least one internal standard must be defined (see **Use this peak as internal Standard**). Select the desired ISTD peak in the **Associated ISTD Peak** checkbox.

Use this peak as Internal Standard

This option allows you to define the current peak as ISTD peak. Use the **Use sample amount as reference** checkbox to use the amount of the internal standard from the ISTD amount column of the sample list (instead of the **Amount** columns of the QNT peak table). In this way, you can enter a different amount of internal standard for each sample.

☞ ***Tip***:

For internal standard as well as internal/external standard methods, a substance whose concentration is known, must be added to the standards and to the analyses. This can be conveniently carried out by means of an appropriate ➢*Autosampler*. Quantitative accuracy reached with this method, exceeds that of the external standard method by one dimension.

For these two options, the name of the internal standard must be indicated.

Internal standard methods compensate even small injections deviations, since possible loss or excess apply to the internal standard as well.

Threshold

Location: Tab **Peak Tracking** and **Spectra Library Screening /** Report Variable **(Peak Table)**

Type: **Integer**

Dimension: **No dimension**

Value Range: **0 - 1000**

Default: **950**

Related Param.: Additional parameters for comparing spectra:

⇒*Check Derivative*
⇒*Check Extrema*
⇒*Match Criterion*
⇒*Maximum/Minimum Wavelength*
⇒*Relative Maximum Deviation*
⇒*Threshold*

Description: This parameter defines the threshold of the ➢*Match Factor* above which two spectra may be accepted as matching.

Function: Depending on the comparison function the following settings can usually be recommended:

Spectrum (Off): 950

1st derivative: 900

2nd derivative: 800

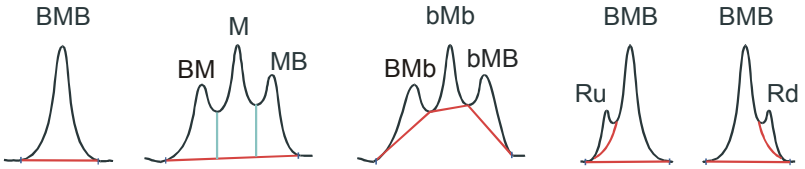
Type (Peak Type)

Location:	Tab **Peak Table /** Report Variable **(Peak Table)**
Type:	**Alternatives**
Dimension:	**No dimension**
Value Range:	**Autodetect (Auto) / Rider (R) / Main (M) / Baseline-Main (B-M) / Main-Baseline (M-B) / Baseline-Main-Baseline (B-M-B)**
Default:	**Autodetect**
Related Param.:	⇒*Rider Threshold* ⇒*Maximum Rider Ratio* ⇒*Valley to Valley* ⇒*Lock Baseline*
Description:	Determines the type of baseline contact and the separation of other, non-resolved peaks. An integration program algorithm usually defines the peak type. The peak type can also be altered as desired via the detection parameters (see **How to ...: Actions in the QNT Editor Modifying Detection Parameters**). In order to determine the peak type regardless of other factors, this should be done in the peak table. Type specifications of the peak table have **priority**.
Functions:	
Autodetect (Auto)	The peak type is determined via an algorithm, or via detection parameters.
Determine at Calibration	Not yet implemented
Rider (R) / Main (M)	The peak is integrated as rider or main peak without baseline contact. This, of course, applies to non-resolved peaks, only. In the case of rider peaks, an additional distinction is made between peaks on the ascending edge (**u** = up) and peaks on the descending edge (**d** = down). Of course, this does not affect the type of baseline contact of the reference peak.

Baseline-Main(B-M) / Main-Baseline(M-B) / Baseline-Main-Baseline (M-B-M)

The peak is integrated as main peak with left, right, or bilateral baseline contact.

A further distinction between **b** and **B** is made in the report: If a main peak has direct baseline contact on the left and/or right side, this is indicated by a capital **B**. If the baseline below non-resolved peaks is drawn from minimum to minimum (⇒*Valley to Valley*), i.e. from peak end to peak end, this type of baseline contact is characterized by a small **b**.



☞ ***Tip**:*

The peak type determined here can only be realized with non-resolved peaks. For resolved peaks, peak type is always *Baseline-Main-Baseline*!

The distinction between **b** and **B** is made only in the report output. The baseline is checked automatically. Then, the baseline contact is determined. In the peak table, the classification is always **B**.

The peak type that is defined in the peak table has priority over the type assignments of the **Rider Threshold** and **Maximum Rider Ratio** detection parameters.

Use Recently Detected Retention Time

Location: Tab **General** / Report Variable **Use Prev. Retention Time (Peak Table)**

Type: **Check-box**

Dimension: **---**

Value Ranges: **Marked / not marked**

Use recently detected ret. times of last sample / standard

Set reference time to Last value / Average of last n values / Global average

Defaults: **Not marked**

Last sample

Last value

Related Param.: ⇒*Retention Time*

⇒*Window*

Description: This QNT file parameter (**General** sheet) defines whether the retention time stored in the peak table (nominal time) is used by default to identify a peak or whether the actual retention time of a peak in the last sample is used. Thus, many types of drift phenomena can be compensated (e.g. evaporation of volatile components in pre-mixed solvents or column age).

If the peak is not found in this sample, the chronologically previous sample in the sequence is searched, etc. (The chronological order is important and not the order in the sample list).

If you have chosen this option, you may select whether you want to use the retention times of the last unknown sample (**Sample**) or of the last **Standard**.

Via the **Options** button, you can also define whether you want to use the last retention time (**Last value**), the average of the last x retention times (**Average of last x values**), or the average of all retention times (**Global average**).

Function:

If the check box **Use Recently Detected Ret.Time** is selected, the Dionex Chromatography Management System always stores the last actual retention time of the peak and positions the **Window** specified in the peak table around this actual value, not around the nominal value stated in the peak table.

This allows positive identification of peaks even when the retention time changes due to column trends, and thus the peak leaves the defined retention time window.

Example:

The first sample of a sequence containing 10 samples is processed in an automatic batch. Based on the retention times stated in the peak table and the selected window values (e.g. 0.2G), four peaks are identified in the first sample (A, B, C, and D). Each one of these peaks may have an actual retention time that deviates from the nominal retention time. The Dionex Chromatography Management System stores these actual values and uses them as the basis for positioning the time window in the second sample. If single peaks are then identified in the second sample, the "stored" actual values are replaced by the current actual values. The time window is repositioned accordingly. If, for example, the retention time of peak A from the first sample (1 min) is delayed by 10 sec in each sample, the peak will be appear at 1 min + 9 x 10 sec = 150 sec or 2.5 min in the tenth sample. As the time window is also moved by 10 sec with each sample, peak A can be clearly identified in the tenth sample, although the peak is no longer within the originally specified time window (48 sec to 1 min 12 sec).

☞***Tip***:

Only retention times of identified peaks are corrected!

Window *(Retention Window)*

Location:	Tab **Peak Table /** Report Variable **(Peak Table)**
Type:	**Positive floating point number or string**
Dimension:	**Minutes or %**
Value Range:	**0.000 ... 999.999 or 0 - 100%** **Absolute / Relative** and **First / Greatest / Nearest / Spectrum / Spectrum and time**
Default:	**Autogenerate Peak Table**: A third of the distance to the preceding or the succeeding peak depending on which distance is smaller **Else: 0.100 min or %** **Absolute Greatest**
Can be combined with:	**Check the best hits only** (with the peak match options **Spectrum** and **Spectrum and Time** only)
Related Param.:	⇒*Retention Time*
Description:	Defines a tolerance interval within which the peak is expected. The start and end times of the retention window result from adding the window value to and subtracting it from the retention time (retention time +/- window value), i.e., the window width is always twice as wide as your input. A peak outside this window is not identified. The window value defined here is either interpreted as absolute (minutes) or relative (percentage) value by the integration programs. For each peak, the interpretation can be individually specified, by adding a suffix to the window time.

Function: The dimension W of the time windows is calculated according to the following formula:

Absolute time window: W = TW

Relative time window: W = T x TW / 100

Where T is the retention time of the table and TW the entered **window** value. All peaks whose maximum falls into the time interval T+W belong to the time window.

Function of the suffixes:

- Select **Absolute** or add a capital **A** to the window value to indicate the window width in minutes.
- Select **Relative** or add a capital **R** to the window value to indicate the window width relative to the retention time.

If a peak is registered within this window, it is assigned the peak name entered in the peak table. If several peaks are located in the same window, the window parameter can be extended to determine which peak is identified:

- Select **First** to identify the first peak within the window (F).
- Select **Greatest** to identify the largest peak within the window (G).
- Select **Nearest** to identify the peak nearest to the specified retention time (N).
- Select **Spectrum** to identify a peak by a spectrum. The reference spectrum is specified in the **Spectrum** column of the peak table (S).
- Select **Spectrum and time** to identify a peak within a specific window width by a spectrum. The reference spectrum is specified in the **Reference Spectrum** column of the peak table (ST).

Via the **Check the best hits only** option, **Spectrum** and **Spectrum and time** allow you to check the hits with the largest ➢*Match Factors* for the respective peaks only (= checkbox selected, default). The abbreviation for this is **B** (**SB** or **STB**).

If you have MS options installed, you can also enable the **Check mass ratios** option to check whether the masses indicated on the **Mass Tracking** tab are found in the defined ratio range.

Examples:

Window Values: 0.2 AF / 0.2 AG / = 0.2 AN

If the expected retention time of the peak is Ret.Time = 5.0min and the window value is 0.2 A, the time window is 5.0min +/- 0.2min = 4min 48sec to 5min 12sec. By adding the suffix F, the first peak in the time window, by adding the suffix G, the greatest peak in the window, and by adding the suffix N, the peak nearest to the expected retention time is assigned.

Window Values: 10 RF / 10 RG

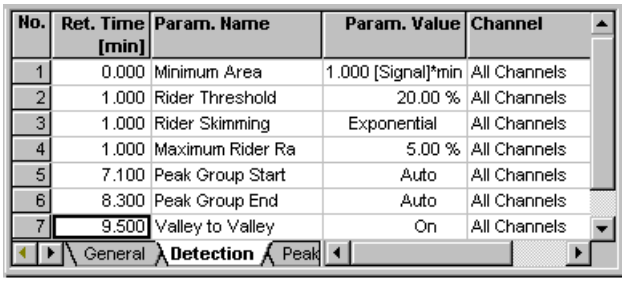
If the expected retention time of the peak is Ret.Time = 5.0min and the window value is 10 R, the time window has the range 5.0 min ± 10% = 5 min ± 0.5 min = 4 min 30 sec to 5min 30 sec. By adding the suffix F, the first peak in the time window, by adding the suffix G, the largest peak in the window is assigned.

☞ ***Tip***:

The absolute time interval of the window is twice as wide as the window value entered, since the interval reaches from T-W to T+W!

QNT: Detection

Integration and detection parameters are determined on the **Detection** page of the QNT method. They control peak detection, baseline treatment, peak classification, and inhibition (**integration parameters**). The values of these parameters are assigned time-dependently and channel-dependently; thus, they may be altered several times during a chromatogram.



No.	Ret. Time [min]	Param. Name	Param. Value	Channel
1	0.000	Minimum Area	1.000 [Signal]*min	All Channels
2	1.000	Rider Threshold	20.00 %	All Channels
3	1.000	Rider Skimming	Exponential	All Channels
4	1.000	Maximum Rider Ra	5.00 %	All Channels
5	7.100	Peak Group Start	Auto	All Channels
6	8.300	Peak Group End	Auto	All Channels
7	9.500	Valley to Valley	On	All Channels

General | Detection | Peak

Example of a detection table

Generally, about 90% of all chromatograms are integrated correctly by the system. In critical cases (e.g. **wavelength switching**), the user may influence the baseline or the peak type (e.g. rider or main peak), or he can inhibit detection entirely for certain periods. The figure illustrates a detection table.

Besides, detection parameters can be defined graphically. This is extremely useful for the two parameters ⇒*Sensitivity* and ⇒*Peak Slice*. For details, see **How to ...: Actions in the Chromatogram Defining Detection Parameter Graphically**.

Each of the 26 differing parameters described in detail below, can be assigned a new value at any time. The last value is valid for the duration of a sample, then the parameters are assigned their original default values. The assignment of a new value to a parameter is called an **event**. Events can be printed in the Report, with identification and a numerical value at the respective execution time.

Events need not be entered in chronological order. They are sorted automatically in chronological (ascending) order before being stored.

Parameter tables include the following columns:

No.	Line number, cannot be edited.
Ret. Time [min]	Retention time, specified in minutes within a range of 0.000 - 9999.999.
Param. Name	**Parameter name**; dialog box (F8 or double click) displays a list of all available parameters.
Param. Value	**Parameter value**; contains detailed information concerning all permitted values of the selected parameter type.
Channel	Via the arrow or the dialog box (open via F8), all options available can be chosen. In addition to **All Channels**, the single channels that have been recorded can be chosen.

Many parameters can only have the values ON or OFF. They are called **switches**. All other parameters are called **variables**.

The parameters are described in detail on the following pages (the order of description corresponds to the order in which they can be selected in the QNT editor).

For details on how to define individual detection parameters, see:

How to ...: Actions in the QNT Editor Defining Detection Parameters.

Detection Parameters (Overview)

The Dionex Chromatography Management System provides the following detection parameters:

⇒*Baseline Point*
⇒*Detect Negative Peaks*
⇒*Front Riders to Main Peaks*
⇒*Inhibit Integration*
⇒*Lock Baseline*
⇒*Maximum Area Reject*
⇒*Maximum Height Reject*
⇒*Maximum Peak Height*
⇒*Maximum Rider Ratio*
⇒*Maximum Width*
⇒*Minimum Area*
⇒*Minimum Height*
⇒*Minimum Width*
⇒*Peak Group Start/End*
⇒*Peak Purity Start/End Wavelength* (*PWIStart/PPWIEnd*)
⇒*Peak Purity Threshold (PPTrshold)*
⇒*Peak Shoulder Threshold*
⇒*Peak Slice*
⇒*Rider Skimming*
⇒*Rider Threshold*
⇒*Sensitivity*
⇒*Tailing/Fronting Sensitivity Factor*
⇒*Valley to Valley*

For details on how to define detection parameters, see **How to ...: Actions in the QNT Editor** **Defining Detection Parameters**.

Baseline Point

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Command**
Dimension:	**---**
Value Range:	**---**
Default:	**---**
Related Param.:	⇒*Lock Baseline* ⇒*Valley to Valley* ⇒*Inhibit Integration* ⇒*Type (Peak Type)*
Description:	The **Baseline Point** detection parameter defines a baseline point at the indicated time.
☞***Tips**:*	When setting a baseline point, keep in mind that this point will be valid for all chromatograms that are evaluated with the respective QNT method. If in one of these chromatograms a peak maximum occurs by coincidence at the time of your hard entered baseline point, the peak maximum will be defined as base point and the peak will not be detected. This command has priority over ⇒*Lock Baseline* and ⇒*Valley to Valley*, but not over ⇒*Type (Peak Type)* from the peak table.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor**  **Defining Detection Parameters**.

Detect Negative Peaks

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Switch**
Dimension:	**---**
Value Range:	**On / Off**
Default:	**Off** (i.e., negative peaks are not detected)
Description:	Enables/disables detection of negative peaks ON or OFF. When turned on, negative as well as positive peaks are detected.
Function:	Enabling detection of negative peaks automatically activates the ⇒*Lock Baseline* parameter. Disabling negative peak detection locks the baseline to the default again. In the result report, the area of negative peaks is indicated as a positive value. To correct the baseline without labeling the peaks or including peaks in the peak list, select the **Don't label** option.
***Tip**:*	In order to be effective, this switch must be activated before the peak start.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Front Riders to Main Peaks

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Selection**
Dimension:	**-**
Value Range:	**Off, On**
Default:	**Off**
Rel. Param.:	⇒*Rider Threshold* ⇒*Maximum Rider Ratio* ⇒*Type (Peak Type)*
Description:	The **Front Riders to Main Peaks** detection parameter allows you to change rider peaks on the ascending edge of a peak into main peaks.
Function:	Set the parameter value to **On** to change upward riders to main peaks even if riders are enforced (e.g., ⇒*Rider Threshold* = 0.00%, ⇒*Maximum Rider Ratio* = 100.0%).
***Tip**:*	This parameter has priority over the **Rider** peak type in the peak table (see ➢*Rider*).

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Inhibit Integration

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Switch**
Dimension:	**---**
Value Range:	**On / Off**
Default:	**Off**
Description:	The **Inhibit Integration** detection parameter serves to fade out certain chromatogram areas. When turned on, peak detection is de-activated,.
Function:	If the value is set to **On** before the first peak to inhibit, no peak detection will take place until the parameter is deactivated (**Off**), i.e., no peaks are recognized in this area. The chromatogram is displayed on the screen, but it is not integrated. Inhibit Integration can be used to inhibit the injection peak by activating the criterion at the start time of the chromatogram and by deactivating it after the dead time.
***Tip**:*	To have any effect, this switch must be activated before the start of the first peak to be inhibited.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Lock Baseline

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Alternatives**

Dimension: **---**

Value Range: **Off / On / At current level /**

At global minimum

Default: **No**

Related Param.: ⇒*Valley to Valley*
⇒*Inhibit Integration*
⇒*Baseline Point*
⇒*Type (Peak Type)*

Description: In case this parameter is set to Off, the detection program calculates the baseline below non-resolved peaks according to a complex pattern recognition process. The other values are used to lock the baseline on different levels.

Function:

Off Below non-resolved peaks, the baseline is determined automatically. The **Valley-to-Valley** parameter is effective in this mode, only. With all other lock-values, lock baseline has priority, while valley-to-valley is ignored.

On In the case of non-resolved peaks, the baseline is **not** pulled up to the relative minima (valleys). The baseline connects the start of the first with the end of the last non-resolved peak.

If one of the valleys in between is located below the baseline, the baseline is connected with this minimum to avoid cutting off a peak foot. The **Valley-to-Valley** parameter is not effective.

At current level	The baseline is fixed at the current signal level and is extrapolated horizontally to the right. The **Valley-to-Valley** parameter will not take effect.
At global minimum	The Dionex Chromatography Management System searches to the right for the next absolute minimum. The search is performed either to the end of the chromatogram or to the next **Lock Baseline**. Within this interval, the baseline is locked on the found minimum and is horizontal. The **Valley-to-Valley** parameter is not effective.
***Tips**:*	The end of the last non-resolved peak in a series of peaks is always a baseline point, since the chromatogram itself forms the baseline outside the peak! Lock baseline needs to be turned off, before switching from **At global minimum** to another lock baseline value. The classification criterion ⇒*Type (Peak Type)* in the peak table has priority. The criterion specified here is effective only for Peak Type = AUTO!

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor**  **Defining Detection Parameters**.

Maximum Area Reject

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Fixed point number**
Dimension:	**Signal dimension ∗ Minute**
Value Range:	**0.000 ... 1,000,000.000**
Default:	The default setting is **Off**, i.e. all peaks are integrated.
Related Param.:	⇒*Minimum Area* ⇒*Maximum Height Reject*
Description:	The **Maximum Area Reject** parameter allows limiting the number of integrated peaks. This parameter is very similar to ⇒*Minimum Area*.
Function:	The parameter defines the maximum peak area up to which a peak is rejected. No peaks with a peak area below the defined value are integrated.
☞ ***Tip:***	Contrary to the **Minimum Area** the **Maximum Area Reject** parameter does not affect the baseline course.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Maximum Height Reject

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Fixed point number**
Dimension:	**Signal dimension (e.g. mAU)**
Value Range:	**0.000 ... 1,000,000.000**
Default:	The default setting is **Off**, i.e., all peaks are integrated.
Related Param.:	⇒*Minimum Height* ⇒*Maximum Peak Height* ⇒*Maximum Area Reject*
Description:	The **Maximum Height Reject** parameter allows limiting the number of integrated peaks. This parameter is very similar to ⇒*Minimum Height*.
Function:	The parameter defines the maximum peak height up to which a peak is rejected. Not all peaks with a peak height below the defined value are integrated. (Determination of the height is always relatively to the baseline).
☞ ***Tip***:	Contrary to **Minimum Height** the **Maximum Height Reject** parameter does not affect the baseline course.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor** **Defining Detection Parameters**.

Maximum Peak Height *(MaxHght)*

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Fixed point number**
Dimension:	**Signal dimension (e.g. mAU)**
Value Range:	**Off; 0.000 ... 1,000,000.000**
Default:	The default setting is **Off**, i.e., all peaks are integrated.
Related Param.:	⇒*Minimum Height* ⇒*Maximum Area Reject*
Description:	Positive peak identification is via the ⇒*Minimum Height* parameter. *All* peaks above this height value are identified. The **Max. Peak Height** detection parameter is used as a maximum criterion determining the height threshold above which peaks are not identified.
Function:	All peaks above the specified peak height are classified as **Unknown**; i.e., despite the positive identification, they are not assigned a name from the peak table (the height is always determined relative to the baseline). This option is very useful when working with two detectors switched in series. Peaks that are clearly identified in the channel of the first detector (e.g. a UV detector) can cause problems in the second detector (e.g. a fluorescence detector) due to an excessive concentration. These peaks are outside the linear range. Due to the positive identification, they would be considered in the calibration and they would falsify the result. If they are classified as **Unknown**, they are not considered.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor**  **Defining Detection Parameters**.

Maximum Rider Ratio

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Fixed point number**

Dimension: **Percent [%]**

Value Range: **0 ... 99.99**

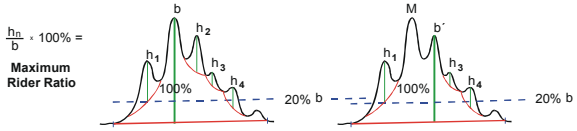
Default: **20**

Related Param.: ⇒*Rider Threshold*

⇒*Type*

Description: If one or several peaks (h1 to h4) are above the **Rider Threshold** in a series of non-resolved peaks, the Dionex Chromatography Management System determines via the **Maximum Rider Ratio** detection parameter, whether a peak is classified as main peak or ➢*Rider*.

Function: For this, the height of the peak to classify is put in relation to the height of the greatest peak in the series (reference peak).



As can be seen in the figure, not the "real" peak height of the peak to be classified is evaluated but the distance between the peak maximum and the skimming tangent.

If the ratio h/b multiplied by 100 percent produces a value *larger* than the one defined as maximum rider ratio, the peak is a main peak.

If the ratio h/b multiplied by 100 percent produces a value *smaller* than the one defined as maximum rider ratio, the peak is a rider peak.

Function (Cont'd):

Starting with the largest peak in the series (reference peak), all adjacent peaks are then classified. As soon as another main peak is recognized, this peak automatically becomes the new reference peak (b´). The maximum rider ratio is recalculated considering b´. The remaining peaks are classified again. The process is continued until all peaks of the series are classified.

Riders can be recognized as such by the skimming tangent drawn in the chromatogram plot and by a Ru (Rider up) or Rd (Rider down) entry in the **Type** column of the report (tab **Integration)**.

☞***Tip***:

In order to be effective, the criterion must be activated before the peak start!

The criterion ⇒*Type (Peak Type)* in the peak table has priority! The criterion specified here, is effective only in combination with PEAK TYPE = AUTO!

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Maximum Width

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Fixed point number**
Dimension:	**min**
Value Range:	**0.01 ... 999.99**
Default:	**The presetting is 999.99 min so that all peaks are considered.**
Related Param.:	⇒*Minimum Width* ⇒*Maximum Peak Height*
Description:	The **Maximum Width** detection parameter defines the maximum width above which peaks are ignored during peak detection. The peak width is measured on the baseline. For peaks that do not reach the baseline, the width is extrapolated.
☞ ***Tip**:*	The criterion must be activated before the peak end. The maximum width influences peak recognition and thus the baseline! In order to avoid this and to inhibit small peaks in the report only, choose the **Properties** command from the **Table** menu and activate the **Reject peak with smaller area than ...%** option.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor** **Defining Detection Parameters**.

Minimum Area

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Fixed point number**
Dimension:	**Signal dimension ∗ Minute**
Value Range:	**0.000 ... 1,000,000.000**
Default:	The default setting is **0.001**, i.e. all peaks with an area > 0.001 [*Sig.dimension x minutes*] are integrated.
Related Param.:	⇒*Maximum Area Reject* ⇒*Minimum Width* ⇒*Minimum Height*
Description:	The **Minimum Area** detection parameter is used as a minimum criterion determining the area threshold below which peaks are identified during peak detection or integration.
Function:	Should only this inhibition criterion be applied, peak numbers in the integration report table may not be consecutive, because two detection phases are carried out for a chromatogram (i.e. peak detection and area calculation). The minimum area parameter might be effective in the second run only, i.e., a peak may be sorted out only then, the result being a gap. The **No**. column of the result file thus indicates which criterion was responsible for inhibiting a peak.
☞ ***Tip***:	This parameter must be activated at a retention time before the start of a peak. It influences peak recognition and, therefore, also the baseline! In order to avoid this and to inhibit small peaks in the report only, choose the **Properties** command from the **Table** menu and activate the **Reject peak with smaller area than ...%** option.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor**  **Defining Detection Parameters**.

Minimum Height

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Fixed point number**

Dimension: **Signal dimension**

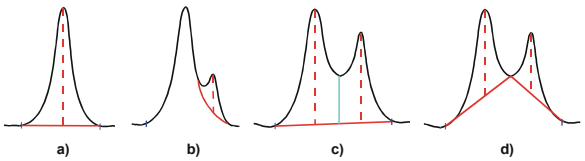
Value Range: **0.000 ... 1,000,000.000**

Default: The default setting is zero, i.e. all peaks with the height > 0 [*Sig.dimension*] are integrated.

Related Param.: ⇒*Maximum Height Reject*
⇒*Minimum Area*
⇒*Minimum Width*
⇒*Maximum Peak Height*

Description: The **Minimum Height** detection parameter is used as a minimum criterion determining the height threshold below which peaks are identified.

Function: The peak height is measured relative to the baseline (a). For ➢*Rider Peaks*, the height measurement is relative to the profile of the carrier peak (b). The baseline can strongly influence these criteria (c,d).



☞ ***Tip:*** This parameter must be activated for a retention time before the start of a peak. It influences peak recognition and, therefore, also the baseline! In order to avoid this and to inhibit small peaks in the report only, choose the command **Properties** from the **Table** menu and activate the **Reject peak with smaller area than ...%** option.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Minimum Width

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Fixed point number**
Dimension:	**Minute**
Value Range:	**0.000 ... 1,000,000.000**
Default:	The default setting is zero, i.e. all peaks with the width > 0 [*minutes*] are integrated.
Related Param.:	⇒*Minimum Area* ⇒*Minimum Height*
Description:	The **Minimum Width** detection parameter is used as a minimum criterion defining the minimum width below which peaks are ignored during peak detection. Peak width is measured on the baseline. In the case of peaks not reaching the baseline, the width is extrapolated
☞ ***Tip**:*	This parameter must be activated for a retention time before the start of a peak. It influences peak recognition and, therefore, also the baseline! In order to avoid this and to inhibit small peaks in the report only, choose the **Properties** command from the **Table** menu and activate the **Reject peak with smaller area than ...%** option.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Peak Group Start / Peak Group End

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Selection**

Dimension: **---**

Value range: **Auto, Fixed**

Default: **Auto**

Related Param.: ⇒*Baseline Point*
⇒*Lock Baseline*
⇒*Inhibit Integration*

Description: The two detection parameters **Peak Group Start** and **Peak Group End** allow identification of several successive peaks as one peak group. A peak group that has been defined in such a way is treated as one single peak. The peak maximum of the largest peak becomes the peak maximum of the entire group. For the group, only one name and number is entered in the chromatogram. Parameters such as area value, peak height, etc. are determined and displayed only once.

Function: The **Peak Group Start** parameter (**Peak Group End** parameter, respectively) defines the start (end) of such a group. The QNT editor sheet **Detection** allows you to set the start of the peak group automatically (**Auto**). If you choose the **Fixed** mode, the baseline will start and end exactly at the mentioned retention times. The setting made for the **Peak Group Start** parameter is also adopted for **Peak Group End**. The system toggles between **Peak Group Start** and **Peak Group End** when appending a line.

Function (Cont'd): Within one group, the entire peak detection algorithm is switched off; i.e., the **Rider Threshold** and **Maximum Rider Ratio** detection parameters are not considered. The area defined by **Peak Group Start** and **Peak Group End** only indicates the limits in which the algorithm is not active. Peak start and end as well as the baseline are determined as usual.

☞***Tip***: The time interval defined by peak group start and peak group end defines only the limits within which the algorithm is disabled. Peak start, peak end, and baseline course are determined as usual!

Instead of setting the peak group start and peak group end, you can group individual peaks that are not necessarily consecutive. To do so, use the ⇒*Group* column of the peak table in the QNT editor. Contrary to a peak group that has been defined via peak group start and peak group end the individual peaks of this group are still indicated.

Also see: **How to ...: Actions in the QNT Editor** **Grouping Peaks**.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor** **Defining Detection Parameters**.

Peak Purity Start/End Wavelength (PPWlStart/*PPWlEnd*)

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Floating point number**
Dimension:	**nm**
Value range:	**190.0 - 900.0**
Default:	**Start: 190.0 nm; End: 900.0 nm**
Related Param.:	⇒*Peak Purity Threshold*
Description:	The two detection parameters **Peak Purity Start Wavelength** and **Peak Purity End Wavelength** limit the wavelength range for peak purity calculations.
Function:	For calculating the ➢*Peak Purity Index (PPI)* and the ➢*Peak Purity Match Factor*, only the wavelength range within the values limited by start and end is used.
☞***Tip**:*	As the default limits, the values 190nm (Start) and 900nm (End) are used. The actually recorded wavelength range is used for the calculation if the recorded range of the 3D-field is smaller.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Peak Purity Threshold (PPTrshold)

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Command**

Dimension: **---**

Value range: **0.00 ... 100.00**

Default: **10.00**

Related Param.: ⇒*Peak Purity Start/End Wavelength*

Description: The **Peak Purity Threshold** detection parameter determines the threshold for the signal height above which spectra comparison is performed for the UV and ➢*Mass Spectra*. The parameter is important for the Peak Purity Analysis (PPA) and the Peak Ratio.

Peak Purity Analysis (PPA)

When determining the ➢*Peak Purity Index (PPI)* or the ➢*Peak Purity Match Factor*, the parameter defines the signal height above the baseline, from which the spectra are extracted for calculation.

Peak Ratio

For the Peak Ratio, the **PPTrshold** parameter defines the signal height above which the ratio is formed.

Function: **Peak Purity Analysis (PPA)**

The value is stated in percent of the peak height, i.e. at the value 20%, only the spectra are used to determine the match factor for which the signal height of the peak is at least 20%.

Function (Cont'd): The smaller the selected value, the wider the match factor curves. The calculation may include spectra that no longer have an optimum ➢*Signal to Noise Ratio*. The match factor curve then has "fringes" at the margins (peak start and peak end). This can be avoided by a smaller threshold value.

Limiting the wavelength range that is used for calculating the center wavelength of the PPI is possible via the ⇒*Peak Purity Start/End Wavelength* detection parameters. A corresponding limitation to a specified mass range is not possible for the MS Peak Purity Match.

Peak Ratio

A value of 10% means that the signal ratio between two channels is only formed where the signal intensity exceeds 10% in two channels (!).

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor** **Defining Detection Parameters**.

Peak Shoulder Threshold

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Fixed point number**
Dimension:	**-**
Value Range:	**Off; 0.01 ... 1000.00**
Default:	**Off** (i.e., shoulders without relative maximum are not recognized as peaks. Only if value ≠ Off, shoulders are detected.)
Rel. Param.:	⇒*Rider Threshold* ⇒*Type (Peak Type)*
Description:	The **Peak Shoulder Threshold** parameter defines a threshold value for peak shoulder recognition.
Function:	First, the average baseline curvature is determined for the entire chromatogram. The curvature threshold value is the product of the average baseline curvature and the threshold value. Detected peak shoulders with a maximum curvature above this threshold value are not considered. The ⇒*Sensitivity* detection parameter allows you to influence the determination of the average baseline curvature. Higher sensitivity results in a smaller average baseline curvature and thus effects peak shoulder recognition.
☞***Tip***:	Peak shoulders are treated like "normal" peaks. All other detection parameters (such as rider criteria, minimum criteria as well as peak recognition via peak table) except the peak group parameters (⇒*Peak Group Start / Peak Group End*) and the ⇒*Valley to Valley* parameter are used for peak shoulders as well.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Peak Slice

Location:	Tab **Detection** / Report Variable **(Detection Parameters)**
Type:	**Floating point number**
Dimension:	**Seconds [sec]**
Value Range:	**0.01 ... 100,000.00**
Default:	**0.05**
Related Param.:	This parameter should always be considered in combination with the ⇒*Sensitivity*!
Description:	The **Peak Slice** detection parameter determines the width (= time span) from which several successive data points are interpreted as peak or as noise. The presetting is 5/100 seconds.
Function:	**General Rule** If a specific peak should "just" be interpreted as a peak and if this was not reached via the Auto setting, a manual peak slice value can be specified by selecting the peak width.
☞***Tip**:*	This parameter only refers to peak detection, not to integration. For area calculation, the original signal is used. To change the variables, *Sensitivity* and *Peak Slice*, is only necessary in case of chromatograms comprising very wide (many minutes) or very narrow (< 0.1 sec) peaks. Under normal conditions, the default values should not be changed**.** Graphical definition is recommended above all for **Sensitivity** and **Peak Slice**. For details see. **How to ...: Actions in the QNT Editor / Modifying the Peak Recognition Algorithm**.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Rider Skimming

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Selection**

Dimension: **-**

Value Range: **Tangential at lower peak end, Tangential at both peak ends** or **Exponential**

Default: **Tangential at lower peak end**

Rel. Param.: ⇒*Rider Threshold*
⇒*Maximum Rider Ratio*
⇒*Type (Peak Type)*

Description: This parameter indicates how ➢*Rider Peaks* are skimmed.

Function: There are three options:

- **Tangential at lower peak end** (default and the common skimming method): For ascending rider peaks, the peak start, and for descending rider peaks, the peak end is defined in such a way that rider skimming is tangential to the chromatogram.
- **Tangential at both peak ends**: Peak start and peak end are determined so that rider skimming is tangential at both chromatogram ends.
- **Exponential**: The chromatogram is approximated by an exponential function, so that the slope of the chromatogram and the exponential function correspond at the peak start and the peak end of the rider peak. This option clearly distinguishes from the two others. In most cases, **Exponential** maps the actual course of the curve very accurate. With this option, the rider peak will usually receive a more realistic larger area. A sufficient number of data points must be available to ensure that this option can be used.

☞***Tip:*** When reprocessing a chromatogram, the skimming function can be set manually for each rider peak. The required commands are included in the context menu of the selected peak.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Rider Threshold

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Fixed point number**

Dimension: **Percent [%]**

Value Range: **0.00 ... 100.00**

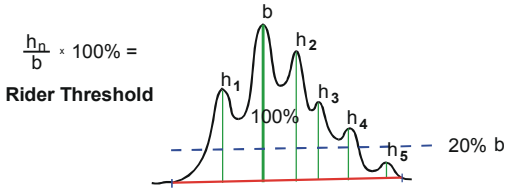
Default: **10.00**

Related Param.: ⇒*Maximum Rider Ratio*

⇒*Type (Peak Type)*

Description: Both rider variables **Rider Threshold** and **Maximum Rider Ratio** decide whether individual peaks in a series of non-resolved peaks are classified as ➢*Rider* (skimming peak) or as main peaks.

Function: The classification as rider or main peak is decided via the ➢*Peak Height* ratio of each individual peak (here h1 to h5) to the largest peak (b) in the series (reference peak).



If the height ratio h/b multiplied by 100 percent produces a value below the defined rider threshold, the corresponding peak is by definition a main peak. Here, this is only the case for the h5 peak.

If the height ratio h/b multiplied by 100 percent produces a value above the defined rider threshold, the **Rider Threshold** criterion is not sufficient for a clear classification.

Function (Cont'd):

In this case, the ⇒*Maximum Rider Ratio* is established. The resulting value allows the classification of the remaining peaks as rider or main peaks.

Riders can be recognized as such by the skimming tangent drawn in the chromatogram plot and by a Ru (Rider up) or Rd (Rider down) entry in the **Type** column of the report (**Integration** tab).

☞***Tips***:

In order to be effective, the criterion must be activated before the peak start!

The ⇒*Type (Peak Type)* classification criterion in the peak table has priority! The criterion specified here, is effective only in combination with PEAK TYPE = AUTO!

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Sensitivity

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Floating point number**

Dimension: **Signal dimension**

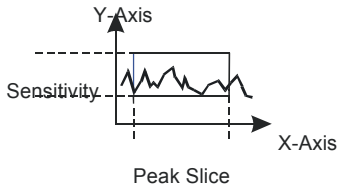
Value Range: **0.0001 ... 10,000,000.0**

Default: **0.0010**

Related Param.: Always consider this parameter in combination with the ⇒*Peak Slice*

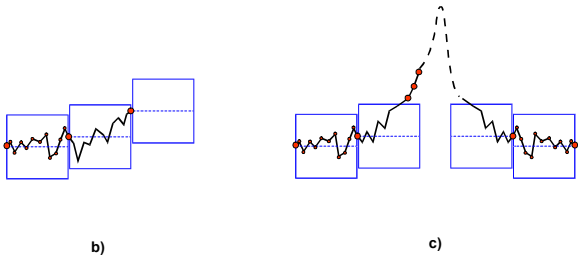
Description: Sensitivity determines in combination with **Peak Slice** the **granularity** of the peak detection algorithm, i.e., when using small values, even the smallest signals (e.g. pump pulsation) are interpreted as peaks, whereas such signals are ignored when using higher values.

Function: Peak recognition is performed using a rectangle formed by the granularity of the y-axis (**Sensitivity**) and the granularity of the x-axis (**Peak Slice**) (see figure a):



As shown in figure a), this rectangle is placed with its lower left corner on the first data point, and is duplicated by mirroring in the direction of negative y-values. As long as none of the subsequent data points is above or below the mirrored rectangle, the last data point will be used for positioning further rectangles (b). The measured signal is interpreted as noise.

Function (Cont'd):



If three successive data points are located above or below the rectangle (simplified!), the peak recognition algorithm will recognize a peak. When the signal difference of one data point to the next one becomes so small that they are within the bandwidth again, the peak end is indicated (c).

Manually Setting the Parameters Sensitivity and Peak Slice

You can manually modify the granularity of the peak recognition, i.e., determine the size of the rectangle or the bandwidth. The larger the area, the lower the sensitivity of the system. Smaller peaks are likely to be interpreted as noise.

General Rule

If a specific peak shall "just" be interpreted as a peak and if this was not achieved via the Auto setting, specify a manual Sensitivity value of a third of the signal height of the peak.

☞***Tip***:

This parameter refers to peak detection only, not to integration. For area calculation, the original signal is used.

Using the **Sensitivity** and **Peak Slice** variables is only necessary in case of chromatograms comprising very wide (many minutes) or very narrow (< 0.1 sec) peaks. Under normal conditions, the default values should not be changed.

☞***Tip** (Cont'd):* Sensitivity is always interpreted in the dimension installed (e.g. mAU)!

Graphical definition is recommended above all for **Sensitivity** and **Peak Slice**. For details, see **How to ...: Actions in the QNT Editor / Modifying the Peak Recognition Algorithm**.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Tailing/Fronting Sensitivity Factor

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Floating point number**

Dimension: **---**

Value range: **Off; 1.0 ... 100.0**

Default: **Off**

Related Param.: **Baseline Point, Lock baseline, Inhibit Integration**

Description: This detection parameter is an implicit threshold for setting the peak end. In the case of the **Fronting sensitivity factor**, the options refer to the peak start.

Function: The following paragraphs describe the **Tailing sensitivity factor** options. The **Fronting sensitivity factor** behaves in the same way.

Off (=0): The peak end is moved on the time axis until the slopes of the chromatogram and of the baseline correspond in the peak end.

Factor 1 - 100: Determining the time for the peak end is as described in the above case (Off). Then, the right baseline width is determined. (This is the ➢*Right Width* peak variable, **Baseline Level** parameter or **peak.right_width(0)**). This value is then multiplied by the **Tailing sensitivity factor** and forms the upper limit for the distance between peak retention time and peak end. If this limit is exceeded, the peak end is corrected and is **reset** accordingly.

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor**  **Defining Detection Parameters**.

Valley to Valley

Location: Tab **Detection** / Report Variable **(Detection Parameters)**

Type: **Switch**

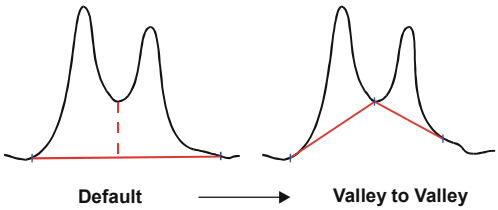
Dimension: **---**

Value Range: **On / Off**

Default: **Off**

Description: Usually, the baseline is determined with an algorithm. This switch enables baseline treatment from valley-to-valley, i.e., from minimum to minimum, in a series of non-resolved peaks.

Function: When turned on, the baseline below non-resolved peaks leads from peak end to peak end.



☞***Tips:*** The end of the last non-resolved peak in a series of peaks is always a baseline point since the chromatogram itself forms the baseline outside the peak!

This parameter is invalidated by ⇒*Lock Baseline*!

The ⇒*Type (Peak Type)* criterion of the peak table has absolute priority!

For a description on how to use individual detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Report Definition File (RDF)

Report Definition Files (**RDFs**) have two functions: They serve to display and reprocess your results on the screen (**Report**) on the one hand and to prepare the printout (➢*Printer Layout*) on the other.

All settings regarding user-specific representation of chromatographic data in different windows are stored in the Report Template (= **Report Definition**). In connection with the ➢*Workspace,* this enables the user to arrange the screen according to individual requirements.

If no workspace is loaded, each new window is opened based on the most recently used RDF. If no Report Definitions were stored, the default RDF included in the Dionex Chromatography Management System (**DEFAULT-RDF**) is used. It is located in the **Report** directory.

Each RDF contains specific information on window sections and views, window presentations, and captions, color, size of individual elements, and the presentation of reports. This regards the following questions:

- Is the window contents (e.g. a chromatogram) shown in the zoomed view or in the full-scale view?
- Which type of axis scaling is used?
- Which additional objects (e.g. grid, comparison chromatogram, units, etc.) are displayed?
- Which colors are used for comparison chromatograms, captions, etc.?
- Are other window sections displayed (Spectra Plot, Calibration Curve, Report, etc.)?
- Which worksheet make up the report and how is the report formatted?
- Which columns does the worksheet include?

etc.

On the following pages, you will find a table listing the various ⇒*Report Categories* as well as tables for the individual categories with brief explanations on the individual report variables.

Report Categories

Proceed as described under **How to ...: Actions in the Report** **Linking Report Variables** to link report variables listed on the following pages via the four basic arithmetic operations, and thus create user-defined report variables.

The report variables belong to the following categories:

Category	Formula	Variables
⇒*General*	gen.*	General variables (in the ➢*Printer Layout* only)
⇒*Sequence*	seq.*	⇒*Sequence* variables
⇒*Sample*	smp.*	Sample variables
⇒*Audit Trail*	AUDIT.*	**Audit Trail** variables (protocol variables)
⇒*Chromatogram*	chm.*	Chromatogram variables
⇒*Detection Parameters*	det.*	⇒*Detection Parameters* variables
⇒*Peak Results*	peak.*	Peak result variables
⇒*Peak Calibration*	peak.*	Calibration variables
⇒*Peak Table*	peakTab.*	Peak table variables
⇒*Mass Spectrometry*	ms.*	➢*Mass Spectra* variables
⇒*Peak Purity*	peak.*	Peak purity variables
⇒*Quantification Method*	qnt.*	Quantification method variables (in the Printer Layout only)
⇒*System Suitability Test*	sst.	➢*System Suitability Test (SST)* variables (in the Printer Layout only)
⇒*History*	history.*	➢*History* variables (in the history report only)
⇒*Integration/Summary Table*	table.group*	Variables for statistics concerning sample groups / replicates (named **Summary Table** from the sheet Summary - else: **Integration Table**)

Category	Formula	Variables
⇒*Mass Spectrum*	msspec.*	Mass spectra variables (accessible via the **Select Spectrum** variable of the **Mass Spectrometry** category)
⇒*Spectrum Data*	peak.spectrum.*	Peak spectra variables (accessible via the **Reference Spectrum** variable of the **Peak Table** category)
⇒*Hit Spectrum*	hitSpec.*	Variables concerning spectra of spectra libraries (accessible via the **SLS Hit** variable of the **Peak Purity** category)
⇒*Spectra Library*	specLib.*	Spectra library variables (accessible via the **Library Record** variable of the **Hit Spectrum** category)
⇒*User Information*	~.*	Variables concerning the corresponding user (accessible via all **Operator** variables of the different categories. ~: Formula depends on the way you opened the category.)

These Help pages briefly describe the respective variables of the corresponding categories.

Category "General"

The **General** category is available only in the ➢*Printer Layout*. It contains the following variables:

Variable	Formula	Description
Version Number	gen.version	
Operator Name	gen.operator	User name - branches to the ⇒*User Information* category
Serial Number	gen.serialNo	
Key Code	gen.keyCode	
Computer Name	gen.computerName	

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "⇒*Sequence*"

Variable	Formula	Description
Name	seq.name	Sequence name
Directory	seq.path	Directory in which the sequence is stored
Datasource	seq.dsn	Name of the corresponding ➢*Datasource*
Timebase	seq.timebase	➢*Timebase* of last run
Title	seq.title	Sequence header
Number of Samples	seq.nSamples	
Creation Date & Time	seq.creation_time	(See➢ *Time*)
Creation Operator	seq.creation_operator	Branches to the ⇒*User Information* category
Last Update Date & Time	seq.update_time	
Last Update Operator	seq.update_operator	Branches to the **User Information** category
Preferred RDF File	seq.prefRdf	Preferred ⇒*Report Definition File*
Preferred Channel	seq.prefChl	Preferred ➢*Channel*
Sign Status	seq.signStatus	Status of the➢ *Electronic Signature*
Submit Date & Time	seq.submitTime	Date and time when submitting the electronic signature

Variable	Formula	Description
Submit Operator	seq.submitOperator…	User who submitted the electronic signature - branches to the **User Information** category
Submit Comment	seq.submitComment	Comment when submitting the electronic signature
Review Date & Time	seq.reviewTime	Date and time when checking the electronic signature
Review Operator	seq.reviewOperator…	User who checked the electronic signature - branches to the **User Information** category
Review Comment	seq.reviewComment	Comment when checking the electronic signature
Approve Date & Time	seq.approveTime	Date and time when the approving the electronic signature
Approve Operator	seq.approveOperator…	User who approved the electronic signature - branches to the **User Information** category
Approve Comment	seq.approveTime	Comment when approving the electronic signature

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "⇒*Sample*"

Variable	Formula	Description
Sample Number	smp.number	⇒*No.*
Sample Name	smp.name	⇒*Name*
Raw Data ID	smp.id	
Sample ID	smp.ident	⇒*Sample ID*
Comment	smp.comment	⇒*Comment*
Sample Type	smp.type	⇒*Type* (sample type)
Vial Number	smp.position	See ⇒*Pos.* (sample position)
Replicate ID	smp.replicate	⇒*Replicate ID*
Status	smp.status	⇒*Status* (sample status): Single/Finished/Multiple/Running
Date & Time Sample Run	smp.time	See: ⇒*Inj. Date/Time* and ➢*Time*
Inject Volume	smp.inject_volume	⇒*Inj. Vol.* (injection volume)
Dilution Factor	smp.dilution_factor	See: ⇒*Dil. Factor*
Sample Weight	smp.weight	⇒*Weight* (sample weight)
ISTD Amount	smp.amount	See: ⇒*ISTD Amount* (amount of the ➢*Internal Standard (ISTD)*)
Program	smp.program	➢*PGM File*
Quantification Method	smp.method	➢*Quantification Method* (QNT method)

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Audit Trail"

Depending on the connected instrumentation hundreds of ➢*Audit Trail* variables are available. The list below shows those variables only that are available during data acquisition with a P580 pump and an UVD 340 detector.

Variable	Formula	Description
Lower Limit (Pressure)	AUDIT.Pressure.Lower Limit	Lower ⇒*Pressure Limit*
Upper Limit (Pressure)	AUDIT.Pressure.Upper Limit	
Equate (%A)	AUDIT.%A.Equate	Name of eluent component A
Max. Wavelength (3DFIELD)	AUDIT.3DFIELD.Max Wavelength	Max. wavelength of the ➢*3D-Field*
Min. Wavelength (3DFIELD)	AUDIT.3DFIELD.Min Wavelength	Min. wavelength of the 3D field
Bunch Width	AUDIT.3DFIELD.Bunch Width	⇒*Bunch Width* of the diode bundle
Wavelength	AUDIT.Wavelength	⇒*Wavelength*
Bandwidth	AUDIT.BandWidth	⇒*Bandwidth*
Step	AUDIT.Step	⇒*Step*
Average	AUDIT.Average	Status of Averaging (see:⇒ *Average*)
Ref Wavelength	AUDIT.RefWavelength	⇒*Reference Wavelength*
Ref Bandwidth	AUDIT.RefBandwidth	⇒*Reference Bandwidth*
Flow	AUDIT.Flow	⇒*Flow* rate
%A (%B, %C or %D)	AUDIT.%A	Percentage of the respective component in the eluent (⇒*%B, %C, %D*)

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Chromatogram"

Depending on the connected detector(s), several different chromatogram variables are available. The list below shows those variables only that are available during data acquisition with an UVD340 detector or an aQa ➢*Mass Spectrometer*.

Variable	Formula	Description
Channel Name	chm.channel	
Raw Data File Path Name	chm.rawpath	See: ➢*Raw Data*
Number of Peaks	chm.nPeak	
Select Peak	chm.peak(***OPT***)	⇒*Select Peak* selects peak in the chromatogram according to input; opens the ⇒*Peak Results* category
Count Peaks if ...	chm.countIF	Counts the peaks which ...
Sum Peak Results if ...	chm.sumIF	Adds up the peak characteristics of peaks which ....
Start Time (relative to Inject Time)	chm.start_time	Chromatogram start time [min]
End Time (relative to Inject Time)	chm.end_time	Chromatogram end time [min]
Signal Value	chm.sig_value	Signal value [e.g. in mAU]
Signal Dimension	chm.sig_dim	
Signal Noise	chm.noise	[in mAU]
Sample Rate	chm.sig_step	
Modified?	chm.manipulated	(Yes/no)
Modification Time	chm.manip_time	Corresponding date/time
Modification Operator	chm.manip_operator	Corresponding operator - branches to the ⇒*User Information* category
XXXXX Start Value	chm.XXXXX	Start value of the signal parameter XXXXX when acquiring data.
Delay Time Value	chm.delayTimeValue	⇒*Delay Time* between two detectors
Delay Time Detector	chm.delayTimeDetector	Name of the second detector
Average	chm.Average	⇒*Average* (for UV channels only)
Step	chm.Step	⇒*Step* (for UV channels only)

Variable	Formula	Description
Wavelength	chm.Wavelength	⇒*Wavelength* (for UV channels only)
Bandwidth	chm.Bandwidth	⇒*Bandwidth* (for UV channels only)
RefWavelength	chm.RefWavelength	See ⇒*Reference Wavelength*) (for UV channels only)
RefBandwidth	chm.RefBandwidth	See ⇒*Reference Bandwidth*) (for UV channels only)
MassRange	chm.MassRange	Mass range of the mass spectrometer channel (for MS channels only)
Polarity	chm.Polarity	Polarity of the ➢*Mass Spectrometer* channel (for MS channels only)
Source Voltage	chm.Voltage	Voltage of the mass spectrometer channel (for MS channels only)
Smoothing	chm.Smoothing	Smoothing algorithm (in parenthesis: number of smoothing points) (for MS channels only or if explicitly performed)

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Detection Parameters"

Variable	Formula	Description
Minimum Area	det.minArea	⇒*Minimum Peak Area*
Maximum Area Reject	det.maxAreaRj	⇒*Maximum Area Reject*
Minimum Height	det.minHeight	⇒*Minimum Height*
Maximum Height Reject	det.maxHeightRj	⇒*Maximum Height Reject*
Maximum Peak Height	det.maxHeight	⇒*Maximum Peak Height*
Minimum Width	det.minWidth	⇒*Minimum Width*
Maximum Width	det.maxWidth	⇒*Maximum Width*
Rider Threshold	det.riderMin	⇒*Rider Threshold*
Maximum Rider Ratio	det.riderRatio	⇒*Maximum Rider Ratio*
Rider Skimming	det.riderSkim	➢*Rider⇒ Skimming*
Peak Shoulder Threshold	det.shoulderThrshld	⇒*Peak Shoulder Threshold*
Front Riders to Main Peaks	det.frontRiderToMain	⇒*Front Riders to Main Peaks*
Detect Negative Peaks	det.negDetect	⇒*Detect Negative Peaks*
Lock Baseline	det.lockBl	⇒*Lock Baseline*
Valley to Valley	det.valval	Baseline from ⇒*Valley to Valley*
Inhibit Integration	det.noInteg	⇒*Inhibit Integration*
Sensitivity	det.noise	⇒*Sensitivity*
Peak Slice	det.filter	⇒*Peak Slice*
Fronting Sensitivity Factor	det.frontFac	⇒*Fronting Sensitivity Factor*
Tailing Sensitivity Factor	det.tailFac	⇒*Tailing Sensitivity Factor*
Part of a Peak Group?	det.isInGroup	See: ⇒*Group*
Peak Purity Threshold	det.ppThrshld	⇒*Peak Purity Threshold*
Peak Purity Start Wavelength	det.ppStartWl	⇒*Peak Purity Start Wavelength*
Peak Purity End Wavelength	det.ppEndWl	⇒*Peak Purity End Wavelength*

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Peak Results"

Variable	Formula	Description
Number	peak.number	
Name	peak.name	⇒*Name* (Peak Name)
Group	peak.group	⇒*Group* (Peak Group)
Link Count	peak.linkCount	Number of substances assigned in one peak
Retention Time	peak.retention_time	⇒*Retention Time* in [min]
Retention Deviation	peak.retention_deviation	Deviation in [min] or [%], depending on parameter (**abs** or **rel**)
Relative Retention Time	peak.rel_retention_time	
Retention Window Width	peak retention windows	Width of the Retention⇒ *Window*
Area	peak.area	Peak area for UV detectors in [min * mAU]
Relative Area	peak.rel_area	Parameters: **total**, **identified**, **group**, **istd**, **rel**
Group Area	peak.groupArea	Total of the peak ⇒*Group* areas
Height	peak.height	Peak height for UV detectors in [mAU]
Relative Height	peak.rel_height	Parameters **total**, **identified**, **group**, **istd**, **rel**
Group Height	peak.groupHeight	Total of the heights of the peak group
Amount	peak.amount	⇒*Amount* or concentration
Amount Deviation	peak.amount_deviation	Deviation analogous to retention_deviation
Concentration	peak.concentration	Concentration: amount/injection volume
Relative Amount	peak.rel_amount	Parameters **total**, **group**, **istd**, **rel**
Group Amount	peak.groupAmount	Peak ⇒*Group* amount
Width	peak.width	Peak width (Parameters 0, 5, 10, 50 in % of signal height above baseline - 0 base width with tangent method)
Left Width	peak.left_width	For the parameters, see Width
Right Width	peak.right_width	For the parameters, see Width

Variable	Formula	Description
Peak Start Time	peak.start_time	In [min]
Peak Stop Time	peak.stop_time	In [min]
Signal Value at Peak Start	peak.start_value	➢*Signal Value at Peak Start* in [mAU]
Signal Value at Peak End	peak.stop_value	➢*Signal Value at Peak Stop* in [mAU]
Baseline Value at Peak Start	peak.start_value_baseline	➢*Baseline Value at Peak Start* in [mAU]
Baseline Value at Peak End	peak.stop_value_baseline	➢*Baseline Value at Peak Stop* in [mAU]
Detection Code at Peak Start	peak.start_detection_code	➢*Det. Code (AIA) -Peak Start*
Detection Code at Peak End	peak.stop_detection_code	➢*Det. Code (AIA) -Peak Stop*
Type	peak.type	Peak⇒ *Type*
Modified	peak.modified	Modified peak?
Manually Assigned	peak.assigned	Manually assigned peak?
Resolution	peak.resolution	➢*Resolution* (parameters **EP** and **USP**)
Asymmetry	peak.asymmetry	Peak ➢*Asymmetry*, parameters **EP** and **AIA**
Theoretical Plates	peak.theoretical_plates	➢*Theoretical Plates* (parameters **EP** and **USP**)
Skewness	peak.skewness	➢*Skewness*
K'	peak.kValue	➢*Capacity Factor*
Retention Index	peak.ri	Linear ⇒*Retention Index*
Kovats Index	peak.ki	⇒*Kovats Index*

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Peak Calibration"

Variable	Formula	Description
Calibration Mode	peak.calMode	⇒*Calibration Mode*
Auto Recalibrate	peak.autoRelCal	Auto calibration On/Off
Reference Inject Volume	peak.reference_inject_volume	Reference Injection Volume
Calibration Type	peak.calibration_type	⇒*Calibration Type*
Weights	peak.calibration_weight	➢*Weights*
Offset (c0)	peak.offset	➢*Offset c0*
Slope (c1)	peak.slope	➢*Slope c1*
Curve (c2)	peak.curve	➢*Curve c2*
RF-Value (Amount/Area)	peak.rf_value	(1/c1) (see: ➢*RF-Value (Amount/Area)*)
Number of Calibration Points	peak.nCalpoints	➢*Number of Calibration Points*
Number of Disabled Calibr. Points	peak.nCalDisabled	➢*Number of Disabled Calibration Points*
Variance	peak.variance	➢*Variance*
Variance Coefficient	peak.variance_coefficient	➢*Variance Coefficient*
Standard Deviation	peak.standard_deviation	➢*Standard Deviation*
Relative Standard Deviation	peak.rel_standard_deviation	➢*Relative Standard Deviation*
Correlation Coefficient	peak.correlation_coefficient	➢*Correlation Coefficient*
Coefficient of Determination	peak.rQuadrat	➢*Coefficient of Determination*
DOF-Adj. Coefficient of Determination	peak.rQuadratAdj	➢*DOF-Adjusted Coefficient of Determination*
Calibration Point x	peak.calPointX	
Calibration Point y	peak.calPointY	
Calibration Point Weight	peak.calPointWeight	➢*Calibration Point* weighting
Evaluation of Calibration Function	peak.calPointFX	
Residual for Cal. Point x	peak.calPointDist	
Calibration Point Status	peak.calPointStatus	
Relative Retention Index	peak.rri("lin")	Linear rel. retention index
	peak.rri("log")	logarithmic rel. ret. index

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Peak Table"

Variable	Formula	Description
Number	peakTab.number	Peak number
Peak Name	peakTab.name	Peak ⇒*Name*
Retention Time	peakTab.retention_time	⇒*Retention Time* in [min]
Retention Time Interpretation	peakTab.retention_type	Specification of retention times
Use Prev. Retention Time	peakTab.use_previous_rettime	Status of corresponding variable in QNT file (see ⇒*Use Recent Retention Time*)
Window	peakTab.window	Time ⇒*Window* width
Standard Method	peakTab.standard_method	see ⇒*Standard*
Integration Type	peakTab.integration_type	⇒*Integration Type*
Calibration Type	peakTab.calibration_type	⇒*Calibration Type*
Peak Type	peakTab.type	See ⇒*Type*
Left Limit	peakTab.left_limit	⇒*Left Limit*)
Right Limit	peakTab.right_limit	See ⇒*Right Limit*)
Peak Group	peakTab.group	See ⇒*Group*
Response Factor	peakTab.response_factor	⇒*Response Factor*
Amount	peakTab.amount	⇒*Amount*
Amount Dimension	peakTab.amount_dimension	
C0 Value	peakTab.C0	Y ➢*Offset* of the calibration curve
C1 Value	peakTab.C1	➢*Slope* of the calibration curve
C2 Value	peakTab.C2	Curvature of the calibration➢ *Curve*
Reference Spectrum	peakTab.reference_spectrum.**x**	⇒*Reference Spectrum*, opens the category ⇒*Spectrum Data*
Match Criterion	peakTab.spec_compare_method	⇒*Match Criterion*
Check Derivative	peakTab.spec_derivative	⇒*Check Derivative*
Minimum Wavelength	peakTab.spec_min_wavelength	Lower limit of the compared wavelength range (see ⇒*Minimum Wavelength*)
Maximum Wavelength	peakTab.spec_max_wavelength	Upper limit of the compared wavelength range (see ⇒*Maximum Wavelength*)

Variable	Formula	Description
Threshold	peakTab.spec_threshold	⇒*Threshold* value for spectra search
Relative Maximum Deviation	peakTab.spec_relmaxdev	⇒*Relative Maximum Deviation* during spectra search
Check Number of rel. Extrema	peakTab.spec_check_extrema	Checking the number of extrema during spectra search (see ⇒*Check Extrema*)
Comment	peakTab.comment	⇒*Comment*
Retention Index	peakTab.ri	Linear ⇒*Retention Index*
Kovats Index	peakTab.ki	⇒*Kovats Index*
Mass Peak x	peakTab.ms_peakx	Mass of Peak x
MS Threshold	peakTab.ms_threshold	Threshold for Mass
MS Filter	peakTab.ms_filter	Mass Filter
Check of mass ratios	peakTab.ms_enable_rejection	
Check of MS retention times	peakTab.ms_check_traces	

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Mass Spectrometry"

Variable	Formula	Description
Spectrum Enhancement	ms.spec_enhanced	Indicates whether ➢*Mass Spectra* averaging is activated
Peak Top Region	ms.nSpec_peak_top	Number of averaged single spectra at peak maximum
Left Background Subtraction Region	ms.nSpec_left_BG	Number of single spectra that are averaged for the left background spectrum
Right Background Subtraction Region	ms.nSpec_right_BG	Number of single spectra that are averaged for the right background spectrum
Delay Time	ms.delay_time	⇒*Delay Time* of the ➢*Mass Spectrometer*
Instrument Information	ms.instrument	Information on the mass spectrometer
Tune Data	ms.tune	Tune data of the ➢*Xcalibur* raw data file
Instrument Method	ms.method	MS method
Status Log	ms.statusLog	Information on the status of the MS system at a specified time
Spectra Count	ms.spec_count	Number of mass spectra
Select Spectrum	ms.spectrum	Opens the ⇒*Mass Spectrum* category

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Peak Purity and Identification"

Variable	Formula	Description
Peak Purity Index	peak.ppi	Average ➢*PPI (Peak Purity Index)* in nm over the entire peak (from a specific height)
RSD Peak Purity Index	peak.rsd_ppi	Correspond. Rel.Std.Dev.
Peak Purity Match	peak.match	Average ➢*Peak Purity Match Factor* (0..1000) over the entire peak (from a specific height detection parameter)
RSD Peak Purity Match	peak.rsd_match	Corresponding Rel.Std.Dev.
Peak Ratio Mean Value	peak.ratio	Average ratio value (BL-corrected) with the "next" channel.
RSD Peak Ratio	peak.rsd_ratio	Corresponding Rel.Std.Dev. value
Peak Spectrum	peak.spectrum.**x**	Opens the ⇒*Spectrum Data* category
Reference Spectrum Match	peak.refMatch	(See: ➢*Match Factor*)
Number of SLS Hits	peak.nSlsHits	No. of reference spectra
SLS Hit	hitSpec.**x**	Opens the ⇒*Hit Spectrum* category
Mass of n-th MS peak	peak.ms_peak_ mass(n)	
Intensity of n-th MS peak	peak.ms_peak_ intens(n,"peak1")	
Position of mass peak maximum	peak.ms_peak_ maximum(n."retTime")	
Mass of MS base peak	peak.ms_base_peak_mass	(See: ➢Base Peak and ➢Mass Spectrum
Intensity of MS base peak	peak.ms_base_peak_ intens	
Mass Spectrum	peak.msspectrum	Opens the □Mass Spectrum category

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Quantification Method"

The **Quantification Method** category is available only in Summary tables and in individual cells in the ➢*Printer Layout*. It contains the following variables:

Variable	Formula	Description
Name	qnt.name	QNT file name
Directory	qnt.path	Directory where the QNT file is saved
Datasource	qnt.dsn	Name of corresponding datasource
Title	qnt.title	QNT file description
Creation Date & Time	qnt.creation_time	
Creation Operator	qnt.creation_operator.x	Branches to the ⇒*User Information* category
Last Update Date & Time	qnt.update_time	
Last Update Operator	qnt.update_operator	Branches to the **User Information** category
Parent Sequence Name	qnt.seq_name	
Sequence Header Record	qnt.sequence.x	Opens the ⇒*Sequence* category
Dead Time	qnt.deadTime	⇒*Dead Time*
Delay Time Value	qnt.delayTimeValue	Also, see ⇒*Delay Time*
Delay Time Detector	qnt.delayTimeDetector	Corresponding detector
Blank Run Subtraction	qnt.blankRun Mode	Status of ➢*Blank Run Subtraction*
Blank Run Sample Record	qnt.blankRunSample.x	Opens the ⇒*Sample* category
Number of Detection Parameters	qnt.nDet	
Number of Peaks in the Peak Table	qnt.nPeaks	
Select Peak in the Peak Table	qnt.peakTabLine("**OPT**")	⇒*Select Peak in the Peak Table* selects peak in chromatogram according to the included option - opens the ⇒*Peak Table* category

Variable	Formula	Description
SST Result	qnt.sst-result	Total result of all single ➢*System Suitability Tests (SST)*
SST Rows	qnt.sst_rows	Number of lines (= number of single System Suitability Tests) on the SST page in the QNT editor
Select SST	qnt.sst(n).x	Opens the category: ⇒*SST*. You can then select a variable for the chosen single System Suitability Test with the number n.

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "System Suitability Test"

Usually, the ➢*System Suitability Test* category is available only in the ➢*Printer Layout* or in the SST Report. However, it can be opened as well via the **Select SST** variable of the ⇒*Quantification Method*. In this case, the formulas start with **qnt.sst(n).x** instead of **sst.x** and the variables refer to the single SST referenced by the number n in brackets. Otherwise, the variables refer to the current single SST.

The System Suitability Test category contains the following variables:

Variable	Formula	Description
Number	sst.number	Number of the SST
Name	sst.name	Name of the SST
Sample Condition	sst.sample_condition	Sample condition for the SST
Test Condition	qnt.test_condition	
Aggregate Condition	qnt.aggregate	Aggregate function
Operator	qnt.operator	
Value	qnt.value	
Channel	qnt.channel	
Peak Condition	qnt.peak	
N.A.	qnt.n_a	User defined test result if the condition cannot be evaluated.
Fail Action	sst.fail_action	
Aggregated Samples	sst.agg_number_real	
Sample Condition Result	sst.sample_cond_result	
Test Results	sst.results	
List of Aggregated Samples	sst.agg_list	
Result List for Aggr. Samples	sst.agg_list_results	
Results of Test Condition or Aggregate	sst.test_cond_result	
Result of Compare Value	sst.value_result	

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "History"

The ➢*History* category is available in the History Report only. It contains the following variables:

Variable	Formula	Description
Object Name	history.name	
Object Path	history.path	Data path, object path and name.
Object Version	history.version	Version of the modified object.
Date/Time	history.time	Date and Time (see➢ *Time*) of the modification.
Operator	history.operator	User - branches to the ⇒*User Information* category.
Operation	history.operation	Short description of the modification.
Comment	history.comment	
Detail Number	history.detail_number	
Detail Object	history.detail_object	
Detail Column	history.detail_column	
Detail Old Value	history.detail_old_value	Old value of the modified field.
Detail New Value	history.detail_new_value	New value of the modified field.
Detail Comment	history.detail_comment	

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Categories "Integration Table" and "Summary Table"

The variables of the **Integration/Summary Table** category allow you to calculate various statistical values of samples/replicates. Using these variables makes sense only if the table has been sorted before applying them.

The category contains the following variables:

Variable	Formula	Description
Group Sum	table.groupSum	Total number of report lines with identical group criterion
Group Count	table.groupCount	Number of report lines with identical group criterion
Group Average	table.groupAverage	Average of report lines with identical group criterion
Group Standard Deviation	table.groupStdev	Standard deviation of report lines with identical group criterion
Group Relative Standard Deviation	table.groupRelStdev	Relative standard deviation of report lines with identical group criterion

 ***Note***: On the sheet Summary the category is named Summary Table. Else, it is called Integration Table.

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Spectrum Data"

Open the **Spectrum Data** category via the **Reference Spectrum** variable of the ⇒*Peak Table* category. It contains the following variables:

Variable	Formula	Description
Lambda Min	peak.spectrum.wlmin	Lower limit of wavelength range
Lambda Max	peak.spectrum.wlmax	Upper limit of wavelength range
Lambda Resolution	peak.spectrum.wlResolution	Wavelength resolution
Sample Rate	peak.spectrum.acqStep	
Absorbance Value	peak.spectrum.sig_value("max")	
Absorbance Extremum at [nm]	peak.spectrum.extremum("relMax")	

For an overview on the different report variable categories including links to the lists for the respective categories, see: ⇒*Report Categories*.

Category "Mass Spectrum"

Open the **Mass Spectrum** category via the **Select Spectrum** variable of the ⇒*Mass Spectrometry* category. It contains the following variables:

Variable	Formula	Description
Number of Data Points	mspec.mass_count	
Mass	mspec.mass	Mass [amu]
Intensity	mspec.intensity	Intensity [counts]
Relative Intensity	mspec.rel_intensity	Relative Intensity (%)
Minimal Mass	mspec.mass_min	Minimal mass [amu]
Maximal Mass	mspec.mass_max	Maximal mass [amu]
Spectrum Type	mspec.type	Spectra type (centroid / profile)
Resolution	mspec.resolution	Resolution of the ➢*Mass Spectrum*
Total Ion Current	mspec.TIC	Number of ➢*TIC* channels
Noise Removed	mspec.threshold.* (z.B. mspec.threshold.mass)	Opens the ⇒*Mass Spectrum* category for spectra with reduced ➢*Signal to Noise Ratio*

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Hit Spectrum"

Open the **Hit Spectrum** category via the **SLS Hit** variable of the ⇒*Peak Purity* category. It contains the following variables for the matching reference spectrum:

Variable	Formula	Description
Substance Name	hitSpec.name	
Match Factor	hitSpec.match	➢*Match Factor*
Library Name	hitSpec.lib_name	Spectra library name
Library Record	hitSpec.specLib.**x**	Opens the ⇒*Spectra Library* category
Number of rel Extrema	hitSpec.nExtrema	
Solvents	hitSpec.solvent	
Comment	hitSpec.comment	➢*Comment*
Sequence Name	hitSpec.seq_name	
Sequence Header Record	hitSpec. sequence.**x**	Opens the ⇒*Sample* category
Sample Name	hitSpec.smp_name	
Sample Record	hitSpec.sample.**x**	Branches to the ⇒*Sample* category
Acquisition Time	hitSpec.acqTime	
Timebase	hitSpec.timebase	➢*Timebase*
Program	hitSpec.program	➢*PGM File* used for recording the library spectrum.
Sample Rate	hitSpec.acqStep	
Retention Time	hitSpec.retention_time	⇒*Retention Time*
Lambda Min	hitSpec.wlMin	Lower limit of wavelength range
Lambda Max	hitSpec.wlMax	Upper limit of wavelength range
Lambda Range	hitSpec.wlRange	Wavelength range
Lambda Resolution	hitSpec.wlResolution	Wavelength resolution
Detector Name	hitSpec.detectorName	
Detector Serial No.	hitSpec.detectorSerNo	
Extract Time	hitSpec.extrTime	
Extract Operator	hitSpec.operator	Branches to the ⇒*User Information* category
Retention Index (lin)	hitSpec.ri	Linear ⇒*Retention Index*
Kovats Index	hitSpec.ri	⇒*Kovats Index*

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "Spectra Library"

Open the **Spectra Library** category via the **Library Record** variable of the ⇒*Hit Spectrum* category. It contains the following variables:

Variable	Formula	Description
Name	specLib.name	Spectra library name
Directory	specLib.path	Directory in which the spectra library is saved
Datasource	specLib.dsn	Name of corresponding datasource
Timebase	specLib.timebase	Timebase where the reference spectrum was recorded
Title	specLib.title	Spectra library description
Number of Spectra	specLib.nSpectra	
Creation Date & Time	specLib.creation_time	(See ➢*Time*)
Creation Operator	specLib.creation_operator	Branches to the ⇒*User Information* category
Creation Software Version	specLib.creation_ version	
Last Update Date & Time	specLib.update_time	
Last Update Operator	specLib.update_operator	Branches to the **User Information** category
Last Update Software Version	specLib.update_version	
Retention Index (lin)	specLib.ri	Linear ⇒*Retention Index*
Kovats Index (log)	specLib.ki	⇒*Kovats Index*

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

Category "User Information"

You can open the **User Information** category via all **Operator** variables of the different categories (e.g. via the Creation Operator variable of the ⇒*Sequence* category except the **Operator** variable of the **System Suitability Test** Category). The category contains the following variables (formulas according to the above mentioned example):

Variable	Formula	Description
User ID	seq.creation_operator.userID	ID of the user
User Name	seq.creation_operator.userName	Name of the user
Job Title	seq.creation_operator.jobTitle	Job title of the user

For an overview on the different report variable categories including links to the lists for the respective categories, see ⇒*Report Categories*.

"Select Peak" Options (OPT)

For the **Select Peak** and **Select Peak in the Peak Table** report variables, you can choose between various options in the **Formula** field. These variables are included in the ⇒*Chromatogram* and ⇒*Quantification Method* report categories. Depending on the category, the options have different meanings:

Report Category "Chromatogram":

"Formula": chm.peak(OPT, [Name, Number])

OPT = "By Number" (default)**:**	Searches the chromatogram for the peak with the indicated number. Example: **chm.peak("By Number," 1).area** determines the area of the first peak in the chromatogram.
OPT = "By Name":	Searches the chromatogram for the peak with the indicated name. Example: **chm.peak("By Name," "Benzene").amount** determines the amount of benzene in the sample.
OPT = "By Tab.Number":	Searches the chromatogram for the peak that was identified by the corresponding line in the peak table. Example: **chm.peak("By Tab.Number," 2).height** searches the chromatogram for the peak that was identified by the second peak in the peak table, and then it determines its height.
OPT = "By Group":	Searches the chromatogram for the first peak in a specific peak group. Example: **chm.peak("By Group," "CKW").amount** searches the chromatogram for the first peak in the ⇒*Group (Peak Group)* called CKW and then determines its ⇒*Amount*.

OPT = "By SLS-Hit":	Searches the chromatogram for a peak for which at least one SLS hit is available. Example: **chm.peak("By SLS-Hit," 2).hitSpec(1).name** selects the second peak in the chromatogram for which at least one SLS hit is available. In addition, the name of the respective library spectrum with the best match is indicated.
OPT = "ISTD":	Searches the chromatogram for the ➢*Internal Standard* peak. If there are several ISTD peaks, the number of the ISTD peak can be indicated by a second parameter. Example: **chm.peak("ISTD").area** searches the chromatogram for the first ISTD peak and then calculates its area. **chm.peak("ISTD," 2).area** calculates the area of the second ISTD peak.
OPT = "Ref":	Searches the chromatogram for the reference peak (Retention Time Interpretation as **Time Distance to ...** or **Time Ratio to...**). For example: **chm.peak("Ref").retention_time** searches for the reference peak and then calculates the corresponding retention time.

Report Category "Quantification Method"

"Formula": qnt.peakTabLine(OPT, [name, number])

OPT = "By Name":	Searches the peak table for the first line with the corresponding name. Example: **qnt.peakTabLine("By Name," "Benzene").amount(1)** returns the value in the first amount column for the peak 'Benzene'.
OPT = "By Number" (default):	Searches the peak table for the line with the corresponding number. Example: **qnt.peakTabLine("By Number," 1).name** returns the name of the first peak in the peak table.
OPT = "By Group":	Searches the peak table for the first line with the specified group entry. Example: **qnt.peakTabLine("By Group," "CKW").amount(1)** returns the value in the first amount column for the first peak in the group called CKW.
OPT = "ISTD":	Searches the peak table for the line with the ISTD peak. If there are several ISTD peaks, the corresponding number can be specified via the second parameter. If no number is specified, the first ISTD peak will be used. Example: **qnt.peakTabLine("ISTD," 2).name** returns the name of the second ISTD peak.
OPT = "Ref":	Searches the peak table for the line with the reference peak (Retention Time Interpretation as **Time Distance to ...** or **Time Ratio to...**). Example: **qnt.peakTabLine ("Ref").name** returns the name of the reference peak.

Glossary

%B, %C, %D (Partial Flows)

The amount information for the partial flow is stated in percent of the ⇒*Flow Rate*. The total sum of all partial flows is 100% (%A + %B + %C + %D = 100%), where %A is calculated from the remaining partial flows (%A = 100% - (%B + %C + %D)). It is therefore sufficient to determine the values for %B, %C, and %D.

Changing the % ratio during the analysis is referred to as ➢*%-Gradient*.

Also, see ⇒*%B, %C, %D (Partial Flows)*.

%-Gradient

If the composition of the delivered solvent mixture changes during the analysis, this is referred to as %-gradient. The composition can be modified immediately (➢*Step Gradient*) or over a certain period.

⚠ ***Caution***: Depending on the dead volume of the pump, the required time for changing the mixing ratio varies. The greater the dead volume, the later the new mixing ratio will be realized and the later the solvent mixture will reach the column. The user should therefore take care to perform gradient courses in sensible intervals.

3D-Field

A ➢*Photodiode Array Detector* (PDA) simultaneously measures the different absorptions in a wavelength range at the time t. The two-dimensional view of a chromatogram (retention time and absorption height) is extended by another dimension (wavelength). Each recorded data point contains information on the detected wavelength (λ) in addition to the retention time (t) and the absorption value (A).

The resulting 3D-field stretches in x, y, and z-direction.

Dionex Photodiode Array Detectors record data points via the **3DFIELD** signal. Similar to other signals, the recorded signals can be influenced via ➢*Signal Parameters*.

Depending on the selected ➢*Sampling Rate*, the ➢*Optical Resolution* of the detector and the selected wavelength range, recording a 3D-field can produce an enormous amount of data. This not only requires special data compression

procedures (see **Data / Raw Data Compression**), but also makes it impossible to control photodiode array detectors via conventional serial interfaces. Dionex PDAs are therefore connected to the PC via powerful special connectors and separate interface boards. This connection even allows online representation of the 3D-field within a ➢*Control Panel*.

Existing 3D-fields can be viewed and evaluated in different ➢*Presentation Modes*. This is via the partial method Peak Purity Analysis (PPA).

3D-Field: Presentation Modes

The ➢*3D-Field* represents the relation between the three values retention time (*t*), wavelength (λ), and absorption (A). For presenting these three-dimensional figures, two presentation modes have proved to be useful: the ISO plot and the 3D-plot presentation. Toggling between the two modes is via the **Decoration** dialog of the window.

Presentation Mode:	Description:
ISO Plot	In the area formed by *t* and λ, lines with equivalent absorption are shown in the same color. The resolution increases with the number of drawn lines (levels). The ISO plot can be viewed online, i.e., in real time.
3D-Plot:	A combination of perspective projection and iso-line plot. The iso-lines are moved to the third dimension, depending on the absorption degree. A grid containing all retention time and wavelength values is placed over the created profile.

***Note**:* As more computing resources are required for the 3D-plot presentation mode than for the ISO plot presentation, the representation on the screen will require more time. In addition, copying a 3D-plot to the clipboard or printing requires more time.

3D-Plot

See ➢*3D-Field: Presentation Modes*

A-Groups

See ➢*Access Groups*

A/D Converter (Technical Data)

The A/D Converter serves to convert electrical detector voltages into digital data for further processing in the Dionex Chromatography Management System.

The A/D converter functions on the basis of the auto ranging principle, i.e. it has 8 different measuring ranges in steps of 2, which are set by a 32-bit microprocessor, depending on the signal. The processor enables smooth transitions between the individual measuring ranges, by comparing and correcting with a calibrated power source. Non-linearity at the switch points and maladjustment by aging components and potentiometers are thus excluded.

Due to the fine measuring range graduation and the refined analog technology, sensitivity is less than 1mV at a dynamic ratio of 24bit; resolution and linearity is 16 bit over the entire measuring range.

The A/D converter can record up to 16 channels simultaneously at a sampling rate of 100 Hz. That means that from a continuous signal, a maximum of 100 values is recorded per second (sampling rate). The output voltage range of the detector is irrelevant; the A/D converter automatically adjusts to it. The A/D converter is designed for input voltages ranging from -10V to +10V (output voltage of a detector is usually 1 or 2V at the integrator output, in exceptions, as in GC, it can be up to 10V).

In addition to the 16 analog inputs, the A/D Converter is supplied with digital (remote) inputs. These inputs are designed for input voltages between 0V and +5V (TTL level). They enable reactions to external events (e.g. inject signal).

For further information, see

Device Communication / A/D Converter

Installation of the A/D Converter

Caution: Wrong polarity (remote inputs) and input voltages beyond the valid range will destroy the board!

Access Groups (A-Groups)

An A-group comprises various Dionex Chromatography Management System users. The membership in a specific A-group determines which objects (server, ➢*Timebases*, ➢*Data Sources*, and directories) can be accessed. Each user can be a member of several A-groups.

For example, the A-group **All** could consist of the users "A," "B," "C," "X," "Y," and "Z," while the group **Specials** consists of the users "A," "B," and "C."

The more A-groups are defined, the more specific the  **Access Control** (see **Installation** section) can be handled in the Dionex Chromatography Management System. Creating A- and P-groups is performed by the administrator with the ➢*CmUser* program (CmUser.EXE).

As soon as the A-groups are created via the CmUser program, it is possible to determine where the groups have access. The administrator also performs this task:

a) For datasources, directories, and sequences, access is defined in the ➢*Client* program of the Dionex Chromatography Management System, and for

b) For servers, and timebases, access is defined in ➢*Server Configuration* program.

To define the access, select the object. Open the context menu or the **Edit** menu, then select the **Properties** dialog to define the user groups who are granted access.

If a user is a member of a specific A-group, certain privileges are assigned. These ➢*Privileges* are defined in privilege groups.

Account

Each user has an account that is checked each time the user logs on with enabled ➢*User Mode*. The administrator can determine via the ➢*CmUser* program whether a user's account shall be locked after a specified number of failed ➢*Logons*. This is to prevent penetration from the outside. In addition, a user account can be locked completely (Account locked). In both cases, the user can restart the Dionex Chromatography Management System client only when the administrator allows access to the account again.

Acquisition On/Off

The **Acquisition on** command activates data recording (➢*Raw Data*) from all selected ➢*Signals* or channels of a ➢*Timebase*. The type of data from each signal is determined via signal parameters.

Also, see ⇒*AcqOn/Off*.

Additional Functions

The ➢*Report Publisher* that is an add-on module to the Dionex Chromatography Management System provides 141 additional functions for creating user-defined formulas in the ➢*Printer Layout*. Information on the significance of the individual formulas is included in the Online Help of the Dionex Chromatography Management System only.

For an application example, see **How to ... Actions in the Printer Layout**  **Entering User-defined Formulas**.

For an overview of the available functions, see the following list (these topics are available in the Online Help only):

ABS	*EXACT*	*MATCH*	*SECOND*
ACOS	*EXP*	*MAX*	*SIGN*
ACOSH	*FACT*	*MID*	*SIN*
ADDRESS	*FALSE*	*MIDB*	*SINH*
AND	*FIND*	*MIN*	*SQRT*
ASC	*FINDB*	*MINUTE*	*STDEV*
ASIN	*FIXED*	*MOD*	*STDEVP*
ASINH	*FLOOR*	*MONTH*	*SUBSTITUTE*
ATAN	*HLOOKUP*	*N*	*SUM*
ATAN2	*HOUR*	*NA*	*SUMIF*
ATANH	*IF*	*NOT*	*SUMSQ*
AVERAGE	*INDEX*	*NOW*	*T*
CEILING	*INDIRECT*	*ODD*	*TAN*
CHAR	*INT*	*OFFSET*	*TANH*
CHOOSE	*ISBLANK*	*OR*	*TEXT*
CLEAN	*ISERR*	*PI*	*TIME*
CODE	*ISERROR*	*PRODUCT*	*TIMEVALUE*
COLUMN	*ISLOGICAL*	*PROPER*	*TODAY*
COLUMNS	*ISNA*	*RAND*	*TRIM*

CONCATENATE	*ISNONTEXT*	*REPLACE*	*TRUE*
COS	*ISNUMBER*	*REPLACEB*	*TRUNC*
COSH	*ISREF*	*REPT*	*TYPE*
COUNT	*ISTEXT*	*RIGHT*	*UPPER*
COUNTA	*LEFT*	*RIGHTB*	*VALUE*
COUNTIF	*LEFTB*	*ROUND*	*VAR*
DATE	*LEN*	*ROUNDDOWN*	*VARP*
DATEVALUE	*LENB*	*ROUNDUP*	*VLOOKUP*
DAY	*LN*	*ROW*	*WEEKDAY*
DAYS360	*LOG*	*ROWS*	*YEAR*
DBCS	*LOG10*	*SEARCH*	
ERROR.TYPE	*LOOKUP*	*SEARCHB*	
EVEN	*LOWER*		

AIA

AIA is the abbreviation for **Analytical Instrument Association**. This association of manufacturing and sales companies for chemical analysis instruments and software aims at developing guidelines for a standardized chromatography file format to facilitate the data exchange between laboratory systems produced by different manufacturers.

This refers especially to the independence from operating systems and the selected transfer type, but standardization efforts also involve operation, documentation, maintenance, and ➢*GLP* requirements.

The generally valid AIA export format for chromatography data is known as **ANDI** (**AN**alytical **D**ata **I**nterchange**/**Chromatography).

Since 1992, there are five data format categories (Category 1, ... 5). However, only the categories 1 and 2 are widely accepted so far.

Data formats of *category 1* comply with standard raw data, unit, and scaling guidelines, and include information where original data and corresponding methods are stored. This allows exact restoration of a chromatogram from raw data.

In addition to amount values and names for substance identification, data formats of *category 2* also transmit all calculated results, e.g. based on a chromatogram. The data can thus be managed in a database or a LIMS system.

Using the AIA format (ANDI) in the Dionex Chromatography Management

System

To export data from the Dionex Chromatography Management System, the ANDI format can be used. Select the **Export/Backup** command in the **File** menu of the Browser and open the corresponding dialog box with the **ANDI/Chromatography (AIA)** option.

It is also possible to export and print data simultaneously. Select the **Batch Report** command in the **File** menu of the Browser. The **Export** option opens the **Batch Setup** dialog. The AIA format is defined on the **AIA format (*.cdf)** tab.

You can also import AIA files into the Dionex Chromatography Management System. Select the **Import / Restore** command in the **File** menu and choose **ANDI/Chromatography AIA**. A dialog box is opened in which you may select the file you want to import.

AIA Peak Type

See ➢*Detection Code at Peak Start / End*

Align

Use the **Align** function to align two or more selected ➢*Controls* in the ➢*Layout Mode* (**left**, **right**, **top**, **bottom**) or to assign the same dimensions (**width**, **height**, **size**) to them.

The ➢*Control Frame* of the control that is selected first is used as reference for the aligned control(s).

Amount

The **Amount** peak table parameter defines the content of a component in a standard. For each component of the standard used for calibration, exactly one amount value is entered in the **Amount** column of the peak table in the ⇒*QNT Editor*.

Also, see ⇒*Amount*

Amount Deviation

The **Amount Deviation** peak table variable specifies the difference between the nominal ⇒*Amount* included in the **Amount** column of the peak table and the value actually determined via the area calculation (actual amount).

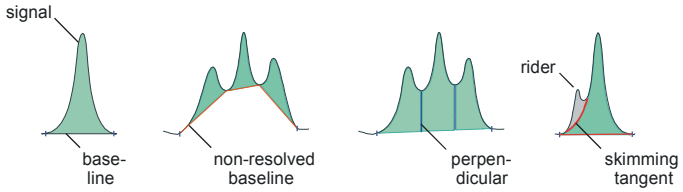
By default, the difference is expressed in absolute amount units (= **Absolute** parameter). Alternatively, input is possible in percent of the expected amount value (= **Relative** parameter).

Use this variable to check the quality of a calibration. The smaller the determined deviation, the closer the corresponding calibration point is to the calibration curve.

***Note**:* GynkoSoft users know this variable under the name **Amount Difference (Amnt Dif.)**.

Area

The **Area** peak result variable specifies the area between the signal curve, the baseline, and the perpendicular delimiters, if required. The size of the peak area is considerably influenced by the baseline (resolved or non-resolved).



Rider peaks have a separate area that is limited by a skimming tangent and the signal curve.

The peak area is computed via summation of trapezoids. The trapezoidal area between the two data points **(T1,A1)** and **(T2,A2)** is

Area = (T2-T1)*((A1+A2)/2).

After summation over the corresponding trapezoids of all data points, the baseline is subtracted. For the **(B_T1,B_A1)** and **(B_T2,B_A2)** baseline points at peak start and at peak end, the baseline area is computed as

Area = (B_T2-B_T1)*((B_A1+B_A2)/2).

The areas of the rider peaks are computed accordingly and subtracted from the corresponding main peaks.

The dimension of the area depends on the used detector type. For UV detectors, the dimension is usually specified in mAU * min (milliabsorbance minutes).

AS50 Sample Prep Commands (Overview)

The AS50 provides several functions for preparing the sample before injection. The Dionex Chromatography Management System can control these functions with commands programmed into a ➢*Program*. The standard AS50 supports six sample prep commands. If the AS50 is equipped with the Sample Preparation option, two additional commands are available.

Standard Sample Prep Commands

➢*Pipet*

➢*Mix*

➢*Delay*

➢*Flush*

➢*Needle Height*

Sample Preparation Option Commands

➢*Dilute*

➢*Dispense*

Aspect Ratio

Signals or chromatograms that are assigned an aspect ratio value, are displaced by the parallel projection of the y and z-axes in x direction.

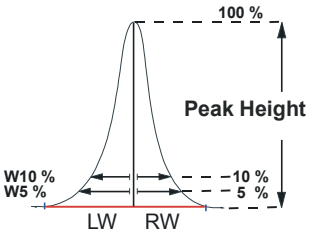
Asymmetry

The **Asymmetry** peak result variable is a measure for the peak fronting or tailing. With identical analysis conditions (identical solvent, identical column type, etc.), the **Asymmetry** can be used to evaluate the column quality.

Theoretically, peaks correspond to a symmetrical Gauss distribution. As any insufficient separation results in a deviation from this ideal, the reasons for any distinct asymmetry should be analyzed and eliminated

The parameter has no dimension and is defined differently, depending on whether using the US/ EU or AIA standard:

Asymmetry	**Calculation**
US/EU standard	A = (RW5% + LW5%) / (2 x LW5%)
AIA standard	A = RW10% / LW10%
With:	
RW5% LW5% RW10/%, LW10%	➢*Right* and ➢*Left* peak width in 5% and 10% of the peak height.



For ideal peaks, Asymmetry is A = 1. For realistic, tailing peaks, however, A is between 1.2 and 5. Values higher than 5 often produce imprecise quantitative results.

If the Asymmetry is calculated in 10% of the peak height, this value is referred to as ➢*Skewness*.

Select the column in the report, choose the **Column Properties** command from the context menu, and select the variable in the selection box. Press the **Parameter** button to define whether the calculation is based on the EU or US standard.

Atlas Electrolytic Suppressor (AES)

See ➢*Suppressor*

Audit Trail

An audit trail is a daily sample protocol that is kept independently by the system. It contains all ➢*GLP* (Good Laboratory Practice) relevant operations, such as current and future commands, events, and error messages.

For further information, see:

Audit Trail (in the **Hardware and Software Chromatography Components** section).

Protocol Data

Auto Autoscale

Use the **Auto Autoscale** option to automate the performance of the ➢*Autoscale* function.

During data acquisition, this option adjusts the scaling of the signal axis exactly to the size of the current chromatogram whenever the signal leaves the signal plot in y direction.

Autosampler

Autosamplers allow automating routine analysis. Depending on the autosampler type and model, a number of samples can be prepared and then processed (injected) in automatic ➢*Batch Processing*.

A distinction is made between the following two states:

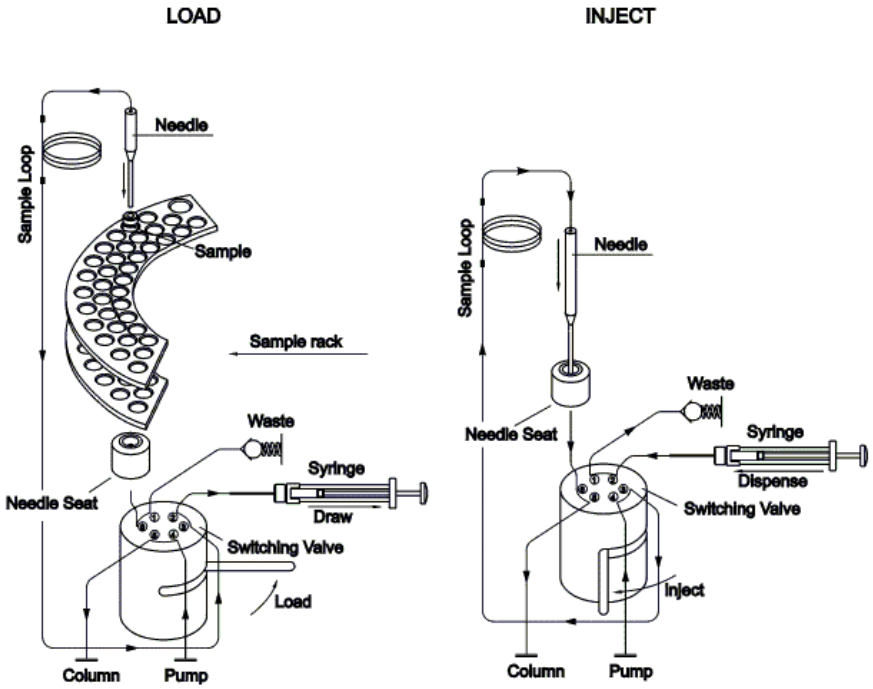
Loading the Sample

The fluidic input and output are directly connected. The solvent flow delivered by the pump is via the sampler to the column. In a second cycle, the volume to be injected is drawn from a sample vial into the sample loop using a syringe.

Injecting the Sample

To inject the sample, the needle is lowered into the needle seat (Gina 50, Gina 160, and ASI-100/ASI-100T) or the inject port (AS50). Via a switched valve, the solvent flow is directed from the pump via the sample loop and the needle seat or via the inject port to the column. Residues in the syringe are dispensed into the waste.

Example for a load/inject process (here: the Dionex ASI-100 sampler):



The Dionex Autosamplers Gina 50, Gina 160, ASI-100/ASI-100T, and AS50 function on this basis. Apart from the standard model, a coolable version (Gina 50T) and a model with integrated derivatization or method program (Gina 160) are available. (With the ASI-100/ASI-100T samplers, derivatization and method programming is possible with the standard version.)

For further information, see **Dionex Autosamplers**

Autoscale

Each time when performed, the **Autoscale** command adjusts the scaling of the signal plot exactly to the displayed window section (e.g. the height of a peak). The adjustment depends on the method.

For instance, the difference between maximum and minimum value of the largest peak fills 80% of the signal axis in the online mode and 100% in the PPA representation.

Select the ➢*Auto Autoscale* option to perform **Autoscale** automatically.

Autozero

The **Autozero** command resets physical or ➢*Virtual Signals* to zero. The subsequently measured data is interpreted and displayed in relation to the new zero point. In the chromatogram, this can normally be recognized by a sharp increase of the absorption value.

☞ ***Tip***: For detectors switched in series, the command must be entered separately for each detector.

Also, see ⇒*Autozero*

Average

The **Average** parameter allows averaging signals. This is possible for digital signals the detector sends to the server PC (as with the Dionex Detectors UVD 170S and UVD 340S) as well as for analog signals recorded via the ➢*A/D Converter* card.

The Dionex A/D converter records each analog signal with a frequency of 100Hz. This corresponds to a ⇒*Step* of 0.01 second or a ➢*Sampling Rate* of 100 data points per second. When increasing the step or decreasing the sampling rate, less data points than theoretically possible are stored.

Also, see ⇒*Average*

Averaged Baseline

The **Averaged Baseline** is a baseline that is valid throughout the entire chromatogram. The baseline can be defined for individual chromatograms.

For details, see **How to ...: Actions in the Chromatogram Defining an Averaged Baseline**.

Backup

The **Backup** command allows storing data for data security. For a description of the procedure see **How to ...: Actions in the Browser Creating Backup Files**.

The Dionex Chromatography Management System stores data in databases and other files organized in a hierarchical directory structure. There are many cross-links between the included objects.

For problem-oriented data archiving, it is necessary to know how the individual objects are linked with each other. As conventional backup and archiving programs do not offer this support, the Dionex Chromatography Management System has its own backup program. This integrated backup program offers the following functions:

- Archiving all objects displayed in the Browser (samples, sequences, files, entire directory trees, etc.) together with all linked files (➢*Raw Data*, Audit Trail (**Protocol Data**), history, preferred ➢*Report Definition File* (RDF), etc.)
- Selective restoration of objects stored via backup
- Compressing the stored data
- Dividing the backup files on several media (e.g. diskettes or ZIP media)
- Optionally deleting original files after the successful backup
- Generating corresponding entries in the ➢*History*

Backup files are located outside the ➢*Datasource*. Therefore, backup files cannot be stored within the directory structure of the datasources. They have no file history and the user management does not protect them.

Use the ➢*Restore* command (see **How to ...: Actions in the Browser Restoring Backup Files**) to restore backup files that were created via the **Backup** function.

Bandwidth

The bandwidth is the nm range at which the chromatogram is recorded. In general, this corresponds to the ➢*Optical Resolution*.

The bandwidth can be selected by averaging several single photodiode signals. This process is known as **Diode or Wavelength Bunching**. Averaging is performed symmetrically to the selected wavelength. Thus, at a bandwidth of 31nm and a wavelength of 255nm, the signals of all photodiodes in the range of 240 to 270nm are averaged.

Also, see ⇒*Bandwidth*

Baseline

The line drawn from peak start to peak end for calculating the peak area is called baseline.

***Note**:* In colloquial language, the chromatogram section between two peaks is also referred to as baseline.

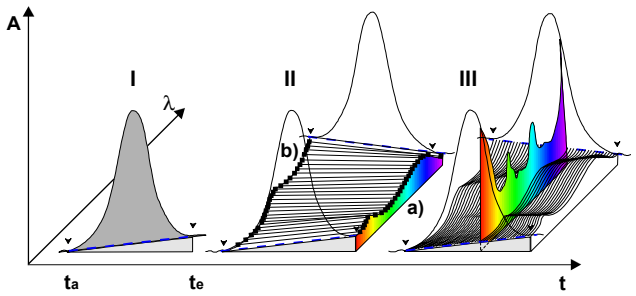
Baseline Correction

Automatically correcting a spectrum by a calculated baseline spectrum allows comparing individual spectra even under different conditions. Especially the spectra of a rider peak can thus be presented more precisely as, in general, a large "underground portion" must be considered, which must be attributed to the larger main peak.

When displaying the spectra plot (**Show Spectra**), it is always corrected by the baseline spectrum, in the PPA method baseline correction is performed only after activating the corresponding option.

Establishing a Baseline Spectrum

Based on the peak recognition algorithm, the Dionex Chromatography Management System establishes the start and end of peaks for the ➢*Reference Channel* and marks these points by positioning peak delimiters (ta and te). The ➢*Baseline* (**I**) is drawn between the two delimiters.



This is performed for all detected wavelengths. The absorption values at all wavelengths measured at the time ta and te result in the baseline spectrum of peak start and peak end (**II**, **a** and **b**). Between these two spectra, the Dionex Chromatography Management System performs an interpolation and thus calculates a separate baseline spectrum for each peak data point. Outside the peak limits, the 3D-field is by definition zero.

Each spectrum measured at any given time t can now be corrected by a calculated baseline spectrum (**III**).

Baseline Correction with Manual Re-Integration

Manual shifting of peak delimiters necessarily affects the baseline spectrum. After each manipulation, there is an automatic re-interpolation and re-calculation of new baseline spectra.

Depending on the modification to the peak delimiters this will change the spectrum (e.g. Spectra Plot).

☞ ***Tip***: A baseline correction can only be performed for the spectra of those peaks that are part of the integrated reference channel!

Near the detection limit, activating the baseline correction often results in considerable smoothing of the ➢*PPI* and ➢*Match Curve*, as the spectral baseline portion is eliminated.

In principle, the PPA report is baseline corrected.

If a spectrum is included in a spectra library from the Spectra Plot via the Windows clipboard, it is always baseline corrected.

If a spectrum is included in a spectra library from the PPA method via the Windows clipboard, the baseline correction is activated or deactivated via the **BL-Correction** option.

Baseline Point

The **Baseline Point** detection parameter defines a baseline point at the indicated time.

Also, see ⇒*Baseline Point*

For details on how to apply detection parameters, see **How to ...: Actions in the QNT Editor Modifying Detection Parameters**.

Baseline Value at Peak End

This peak result variable gives the *baseline* signal value of the peak end (in contrast to the **Signal Value at Peak End** variable which gives the actual signal value of the signal curve).

Baseline Value at Peak Start

This peak variable gives the *baseline* signal value at the peak start (in contrast to the variable **Signal Value at Peak Start** which gives the actual signal value of the signal curve).

Base Peak

In a ➢*Mass Spectrum*, the mass peak with the highest intensity is called base peak. It serves as reference point (base peak = 100 %) for representing relative intensities.

Batch Processing

Repeating a processing step several times is referred to as batch processing (also called **batch** or **online batch**). In chromatography, this means automatically processing or analyzing several samples in a defined order.

For further details, see **Samples and Sequences / Online Batch**.

Note: The automatic offline batch performed in the **GynkoSoft** data system for the recalculation of results is no longer required in the Dionex Chromatography Management System, as each modification of a quantification method results in an immediate recalculation of all involved variables. It is not necessary to recalculate data, as the displayed data is *always* up to date.

Binary-Coded Decimal Code ("BCD")

➢*Autosamplers* controllable via binary code (BCD-capable Autosamplers) can inform the data system, from which sampler position injection was performed. This requires connecting the remote inputs with the sampler outputs (e.g. Remote Inputs of the ➢*A/D Converter*).

For details on how to proceed, refer to the configuration of the **Remote Inject** ➢*Device Driver* in the ➢*Server Configuration* program (F1-key).

Blank Run Sample

A **blank run** is a chromatogram where no sample is injected but the solvent absorption (= baseline) is recorded.

In the sample list, blank samples are labeled with the sample type Blank and marked by the following symbol  . The optionally available **Blank** parameter of the ⇒*Inject* command forces an injection for blank run samples via **Inject**. Usually no injection is made for these samples (default: **Skip**). Blank samples are therefore treated in the ➢*Program* like normal integration samples.

Blank samples are stored together with the sequence. After a baseline or ➢*Blank Run Subtraction* is performed, it can be undone at any time.

Also, see ➢*Matrix Blank Sample*

Blank Run Subtraction

If the ➢*Raw Data* of a signal (channel or 3D-field) is corrected by the raw data of a comparable ➢*Blank Run* sample, this is called blank run subtraction. The chromatogram of the blank sample is subtracted point by point from the current chromatogram.

With a ➢*Matrix Blank Sample*, however, the peak areas are determined first before being subtracted from the corresponding peak areas of all samples in the sequence.

Tips: Blank run subtraction should be performed if peak detection is disturbed due to a strongly ascending chromatogram (e.g. gradient elution).

As both the normal and the blank run sample are saved, the subtraction can be undone or restored at any time.

With a special interpolation procedure, the subtraction of two 3D-fields functions even if the recording conditions are not identical (e.g. different wavelength range or optical resolution). However, this procedure should only be used in exceptional cases.

Branch

In the current ➢*Program*, use the **Branch** command to branch into a different program or to start a program via a command button from the ➢*Control Panel*.

Also, see ⇒*Branch*

Browser

The Browser of the Dionex Chromatography Management System enables setting up, deleting and moving ➢*Datasources*, subordinate directories and files.

It shows samples, methods, and programs as well as further details of a ➢*Sequence*. The functions and the structure are similar to the Windows Explorer. Open the individual files by double-clicking.

Caution: Functions and structure are similar to the Windows Explorer. However, do not confuse the Browser window with the Windows Explorer! Do use the Windows Explorer for operations within datasources of the Dionex Chromatography Management System!

For further details, see **Browser**

Bunch Width

To enhance the ➢*Signal to Noise Ratio* of a ➢*Photodiode Array Detector* the signals of several photodiodes can be averaged (or bunched). Bunch Width describes the sample bandwidth of a bunch of photodiodes.

Also, see ⇒*Bunch Width*.

c0

See ➢*Offset c0*

c1

See ➢*Slope c1*

c2

See ➢*Curve c2*

Calibration Functions, Calibration Coefficients

In each calibration, a mathematical ratio is established between the ⇒*Amount* of a standard sample f(A) and the corresponding area value (A). Depending on the location of the ➢*Calibration Points*, the ratio can be linear, a parabola or exponential. By selecting a ⇒*Calibration Type*, the user can evaluate, to which shape the calibration point should be assigned. The corresponding mathematical functions are called calibration functions.

Linear (Lin)	$f(A) = c1 \, x \, A$	min. 1 calib. point
Linear with offset (LOff)	$f(A) = c0 + c1 \, x \, A$	min. 2 calib. points
Quadratic (Quad)	$f(A) = c1 \, x \, A + c2 \, x \, A^2$	min. 2 calib. points
Quadratic with offset (QOff)	$f(A) = c0 + c1 \, x \, A + c2 \, x \, A^2$	min. 3 calib. points
Exponential (Exp)	$f(A) = c0 \, x \, A^{c1}$	min. 2 calib. points

The slope of the straight line (linear) or the shape of the curve (non-linear) is described by the value of the corresponding calibration coefficient c0, c1, and c2. The coefficients are calculated by simply replacing known amount and area values in the corresponding calibration function (standard sample). If c0, c1, and c2 are known, amounts of an unknown sample can also be calculated.

For further details, see **Theory of Calibration / Calibration Principle**

Calibration Mode

The calibration mode determines which standards are used for calibrating a specific sample of a sequence.

Also, see ⇒*Calibration Mode*

The mode is selected on the **General** page in the ⇒*QNT Editor*.

Calibration Point, Calibration Level, Replicates

If the corresponding peak area is determined for the known amount of a standard sample, the point resulting from both values in an x, y-diagram is referred to as calibration point.

If the corresponding peak area is determined several times for the same ⇒*Amount*, different area values are received depending on the precision. Thus, a larger number of calibration points is obtained. Calibration points based on the same concentration are referred to as replicates of the same concentration level.

Calibration points of different levels are obtained when area values are determined for various amounts of a standard. This can be via ➢*Dilution Series* or variation of the injection volume. From the calibration points, the data system calculates the calibration coefficients of the ➢*Calibration Function* selected by the user.

For further information, see the following topics in the **Theory of Calibration** section:

Calibration (Overview)

Calibration Principle

as well as **How to ...: Actions in the QNT Editor** **Weighting and Averaging Calibration Points** in the **Creating a Peak Table** section.

Calibration Type

The **Calibration Type** peak table parameter describes the mathematical model function (➢*Calibration Function*) based on which the data system calculates the calibration curve by inserting the calibration coefficients c0, c1 and c2.

Also, see ⇒*Calibration Type*

For details on the available calibration types, see **Theory of Calibration**:

Calibration Types (Linear)

Calibration Types (Non-linear)

Also, see **How to ...: Actions in the QNT Editor** **Weighting and Averaging of Calibration Points**.

Calibration Variables

Numerical calibration values are referred to as **calibration variables**. They can be included in a separate column in any table created by the Dionex Chromatography Management System. The following variables are calculated:

⇒*Calibration Type*
➢*Coefficient of Determination*
➢*Correlation Coefficient*
➢*DOF-Adjusted Coefficient of Determination*
➢*Curve c2*
➢*Number of Calibration Points*
➢*Number of Disabled Calibration Points*
➢*Offset c0*
➢*Relative Standard Deviation*
➢*RF Value*
➢*Slope c1*
➢*Standard Deviation*
➢*Variance Coefficient*
➢*Variance*
➢*Weights*

Capacity Factor (k´)

The peak result variable **k´** refers to the capacity factor, i.e. the ratio of the net retention time to the ⇒*Dead Time* T_o:

$k' = (T - T_o) / T_o$

T_o achieve a reasonable compromise between retention and required analysis time, k´ should be a value between 1 and 5.

Calculation is only possible if the dead time of the system was entered in the ⇒*QNT Editor* on the  **General** sheet.

To may either be measured at the inert peak, or calculated as the quotient of dead volume and flow.

If $T_o = 0$, k´ is not calculated.

Select the column in the report, choose the **Column Properties** command from the context menu, and select the variable in the selection box. Press the **Parameter** button to define the dead time required for the calculation.

Cascade

The **Cascade** command of the **Window** menu allows arranging the open windows one behind the other. This provides an overview on the currently open windows and allows you to quickly change to the desired window.

Channel

If a detector delivers more than one ➢*Signal*, as a multi-channel UV detector, the single signals are referred to as channels.

Check Commands

Various checks are available in the Dionex Chromatography Management System:

Syntax Check

A syntax check is automatically performed for each ➢*Program*. The syntax check verifies that a program complies with the program syntax. For example, the syntax check may detect the following:

Exceeded value ranges

- Incorrect punctuation
- Misspellings

Red coloring indicates any detected errors.

Semantics Check

The semantics check verifies the (chromatographic) meaning of a program. This includes for example the following checks:

- Is the sum of all partial flows 100%?
- Does the program contain an ⇒*Inject* command at the time t = 0.000?
- Are the **Inject**/⇒*AcqOn/Off* commands listed in the correct order?
- Is the minimum difference between the emission and the excitation value observed?
- Is the last command an ⇒*End* command? (Absolutely necessary)

The semantics check can be performed via the **Check** command in the PGM editor or the **Check** button in the **Properties** of a command button. Detected errors are indicated in a dialog box.

Ready Check

The ➢*Ready Check* allows you the check whether the connected instruments are ready to operate, e.g. to process a sample batch. The following items are checked:

- Is the instrument switched on?
- Are all instruments connected correctly?
- Is the lamp switched on?
- Are all required files available?
- Is there sufficient storage capacity?

You can perform a ready check via the **Ready Check** button in the **Batch** dialog box. In addition, a ready check is automatically performed for each online command. If there is a problem, an error message or warning will be displayed.

The semantics check usually includes the syntax check. In addition, the ready check includes the semantics check.

Check Derivative

See ⇒*Check Derivative*

Chromatogram Overlay

See ➢*Overlay*

Chromatographic Methods

All instructions and parameters regarding the chromatographic treatment, i.e. the analysis and the processing of a sample, are referred to as chromatographic methods. Depending on the included information, the following distinction is made:

Chromatographic method	Description
➢*Program* (part of the PGM file)	Commands and instructions enabling automation of the analysis.
Quantification methods (QNT)	All parameters required for qualitative peak identification and for quantitative area determination.

The data is stored in the ➢*Sequence Directory* or is copied there by the data system.

Chromatography Server

See ➢*Server*

Client

Workstations that can start the Dionex Chromatography Management System are called clients. The client provides a user interface that allows accessing chromatography data and ➢*Datasources* as well as appropriately representing their contents.

To control or monitor a chromatography system from a client PC, the client must be connected to the Chromatography ➢*Server* Normally, this connection is established when opening a ➢*Control Panel* and connecting to the desired ➢*Timebase*. As soon as there is a connection, the user has access to the devices installed on the server.

To manage database access, the Dionex Chromatography Management System uses the capability of modern **Operating Systems** to share resources, i.e. a client can access all files or datasources for which sharing was issued on a different workstation.

In addition, monitoring and controlling a system is only possible via the client. To do this, the client must establish a connection to a (chromatography) ➢*Server*.

In combination with a **Network**, this allows operating a system and online representation of the system status and the current chromatogram course from any client! Synchronous control of a system via several clients is not possible.

CmUser and CmSecure (User Management)

For the user management of the Dionex Chromatography Management System, two separate programs are available to the Administrator: the **CmUser** program (CmUser.EXE) for creating the ➢*User Database* and managing the actual users and the **CmSecure** program (CmSecure.EXE) for activating the User Mode. Both programs are located in the CmUser directory of the Setup and are **not** automatically copied to the program directory.

The CmUser program is password-protected and can only be opened by the Administrator or persons with a similar function.

Tip: Authorized persons should copy the CmUser directory to a floppy disk to enable on-site changes to user management. This directory also contains an Online Help file (**CmUser_E.HLP**) describing all steps and options of user management.

The main task of the CmUser program is the administration of *Users*, *Privileges,* and *Access Groups*. The following operations are possible:

- Creating and editing access groups (➢*Access Groups*)
- Creating and editing ➢*Privileges* (privilege groups or P-Groups)
- Creating and editing new users in the Dionex Chromatography Management System. The user's name and title, the ➢*Logon* and signature➢ *Passwords*, and the reaction on a failed logon can be defined.

The CmSecure program allows enabling and disabling the User Mode on client of the Dionex Chromatography Management System. In addition, the user database containing the status of each user and his/her rights is selected in the CmSecure program. Starting the Dionex Chromatography Management System requires a password when the ➢*User Mode* is enabled. Signing

sequences electronically (see: ➢*Electronic Signature*) is possible with enabled User Mode only.

Caution: Activate the **Compatibility Mode** (via the **Datasource Properties** command in the CmUser **File** menu) to allow ➢*Clients* of previous versions (version 6.01 and earlier) of the Dionex Chromatography Management System to logon to the system.

Coefficient of Determination

This variable allows you to view the **Coefficient of Determination**, i.e. the deviation of the measured data points from the calibration curve. The coefficient of determination can have value between 0 and 1. A coefficient of 1 indicates that all calibration points are exactly on the calibration curve. The coefficient of determination is calculated as follows:

$$r^2 = 1 - \frac{\sum_{i=1}^{N} W_i * (Y_i - F(X_i))^2}{\sum_{i=1}^{N} W_i * (Y_i - \overline{Y})^2}$$

With:

N	Number of standard samples participating in the calibration
i	Index for standard samples
Wi	Weight factor of the standard sample no. i
F(x)	Model function of the calibration
Xi	X-value of the standard sample no. i
Yi	Y-value of the standard sample no. i
$\overline{Y}$	Average of all Y-values.

Tip: If a linear calibration function leads through the origin, the coefficient of determination is identical to the ➢*Correlation Coefficient*.

Also, see ➢*DOF-Adjusted Coefficient of Determination*

Column Mode (DX-120)

Column mode enables switching of flow from one column set to another in a DX-120 Ion Chromatograph equipped with the dual-column option. When the column is switched, the eluent flow is also switched. For example, when

column A is selected, flow is from eluent reservoir A through column A. If a command switches the flow to column B, flow is then from eluent reservoir B through column B. Also, see ➢*Eluent Mode*

The ColumnAB command is used to switch the flow from one column set to the other. The command can be included in a ➢*Program*, executed directly from the Commands dialog box (select **Command** from the Control menu), or linked to a ➢*Control* on the control panel. To link the command to a control, place an edit box or switch control on the control panel (see ➢*Layout Toolbar*). Then, link the control to the **ColumnAB** object property. For details, see **How to ...: Actions in the Control Panel Linking a Control to a Device**.

To enable Column mode:

1. Open the **Server Configuration**.
2. Select the DX-120 under the timebase.
3. Double-click to open the Properties dialog box (or right-click and select Properties).
4. Select the **Mode** tab, and then the **Column** option.

Column Temperature

The **Column Temperature** command determines the nominal temperature of the column thermostat (**column oven**).

After defining the nominal temperature, the thermostat is set as quickly as possible to the new temperature (device-dependent). A linear interpolation between the actual value and the nominal value is performed.

It is also possible to enter several temperature commands (➢*PGM File*). In this case, the result is a ➢*Step Profile* instead of a linear interpolation between two values!

☞ ***Tip***: As with all instrument parameters, the Dionex Chromatography Management System attempts to represent the actual temperature on the screen. It depends on the connected column thermostat whether this is possible.

Comment

The Dionex Chromatography Management System allows entering a comment at different places.

- The ⇒*Comment* column allows you to enter any comment in addition to the sample name.
- The **Comment** column in the Peak Table of the ⇒*QNT Editor* allows you to enter comments regarding the sample.
- Comments are often needed in ➢*Program*. To enter a comment in the PGM file, enter a semicolon (;) in front of the comment text. The text is then given in green.
- A **Comment** column is also available in spectra libraries where you may enter any comment on the individual spectra.
- The **General** tab of the ➢*Datasource* **Properties** (to be opened via the Properties command of the context menu) allows you to specify that all modifications are logged in the ➢*History*. If the **Comment required** option is enabled, a dialog box opens whenever you save a modification and prompts you to comment the respective change.

If required, the Dionex Chromatography Management System automatically enters a comment at two places in the QNT editor:

- If the peak table is created automatically (via the **Autogenerate Peak Table** command), the Comment column of the peak table shows the following entry:
  - **Autogenerated** (if **Enumerate peaks of current chromatogram** is selected) or
  - **Autogenerated. Spectrum: *Reference spectrum name*, Match: *Match Factor*** (if **Use spectra library screening results** is selected).
- In the **Calibration Comment** column on the **Calibration** tab, the Dionex Chromatography Management System issues commands regarding the calibration. Usually, this comment will be **OK**. However, it may also indicate a calibration error or inconsistencies in calibration.

You may output the respective comments via the corresponding variables of the individual ⇒*Report Categories* in the Report and in the ➢*Printer Layout*.

Concentration

The **Concentration** peak result variable describes the quotient of the calculated ⇒*Amount* and the injection ⇒*Volume*. The value thus specifies the amount of a substance contained in a micro liter (µl) of the injected volume.

☞ ***Tip***: This variable is especially meaningful if an absolute amount value (e.g. 15.00 µg) is entered in the amount column of the

peak table instead of a concentration value (e.g. 1.0 µg/µl).

In this case, the value is divided by the injected volume (e.g. 20 µl), which results in comparable absolute amount values, always normalized to 1 µl (e.g. 15 µg/20 µl = 0.75 µg per µl).

Connect

Execute the **Connect to Timebase** command to connect a user PC (➢*Client*) with a ➢*Timebase* (➢*Chromatography Server*). In a network installation, a connection can thus be established between the current client and any server within the network.

Perform the command **Connect Device** to connect a device with the server to enable remote control. The command checks whether the specified device is actually connected. It then activates the instrument. For all installed instruments, the **Connect** command is automatically executed when the program is started.

***Note**:* For safety and ➢*GLP* reasons, the instrument keyboard is locked on most instruments that are connected via the **Connect** command. This means that in the **Connect** status, the instrument is operated by remote control exclusively. Input on the instrument is possible again after the **Disconnect** command.

Also, see ⇒*Connect/Disconnect*

Contents (Button)

The tab dialog box **Contents** in Online Help shows the contents list. Click a **book** icon to see further topics of a chapter. Click a **document** icon to open a specific help topic.

Continue

The **Continue** command cancels the ⇒*Hold* and ⇒*StopFlow* commands. An interrupted sample batch is continued as well as an interrupted pump flow.

Also, see ⇒*Continue*

Control

Elements that can be fitted with a ➢*Control Frame* by pressing the left mouse button in the ➢*Layout Mode* are referred to as **Controls**.

The Dionex Chromatography Management System provides various standard controls via the ➢*Layout Toolbar*. These can be used by authorized persons to create a new ➢*Control Panel* in the layout mode.

If a control is later placed on the area of another control, it is subordinate to the first control, i.e. modifications to the reference control below, such as the font or the function Autosize, will also affect the new control.

Use the Shift key to select several controls.

Control Frame

The control frame marks the outline of a ➢*Control*. By drawing the control frame, the control can be moved, enlarged, or reduced in size.

Control Panel

In online control, the control and display elements combined in one window are referred to as Control Panel. The control and display elements allow controlling and/or monitoring a ➢*Timebase*. The timebase that can be controlled is defined when creating the control panel. The assignment can be changed via the **Connect to Timebase** command of the **Control** menu and can be saved by closing the window.

The user interface of a control panel can be adapted to the requirements of the individual user via the design tools of the ➢*Layout Toolbar*. Provided you have the corresponding authorization, it is also possible to generate a completely new control panel. In order to create or alter a control panel, change to the ➢*Layout Mode*.

Each new control panel is saved as a PAN file (*.pan) and is then available to the user. New users open the default control panels of the Dionex Chromatography Management System that are easy to use.

Also, see

How to ...: Actions in the Control Panel.

Correlation Coefficient (Linear)

The linear **Correlation Coefficient** is an indication for the "linear dependence" in the amount/area ratio.

If all data points are located on a straight line, the correlation coefficient is exactly 1 (or 100%). If the data points are scattered very much, the coefficient approximates 0.

In contrast to the ➢*Coefficient of Determination*, the correlation coefficient is only an indicator for the linear dependence. This means that e.g. in a quadratic calibration function, the correlation coefficient may be very bad due to the curve shape, although all data points are located on or close to the calculated curve. In this case, the coefficient of determination will be near 0 or 100%.

The mathematical description of the correlation coefficient is as follows:

$$CorrCoeff = \frac{\sum_{i=1}^{N} W_i * (X_i - \overline{X}) * (Y_i - \overline{Y})}{\sqrt{\left(\sum_{i=1}^{N} W_i * (X_i - \overline{X})^2\right) * \left(\sum_{i=1}^{N} W_i * (Y_i - \overline{Y})^2\right)}}$$

With:		
	N	Number of standard samples involved in the calibration,
	i	Index for standard samples,
	Wi	Weight factor of the standard sample no. i
	Xi	X-value of the standard sample no. i
	$\overline{X}$	Average value of all x-values
	Yi	Y-value of the standard sample no. i
	$\overline{Y}$	Average value of all y-values

☞ ***Tip***: If a linear calibration function leads through the origin, the correlation coefficient is identical to the ➢*Coefficient of Determination*.

Cumulated Workload

The cumulated workload is an indication of the wear and tear of the pump. The Dionex pump **P 580** allows you to display the cumulated workload in megajoule (MJ). For information how to display this information, see **How to ...: Device Control Viewing Leak Sensor and Workload Status**.

Curve (c2)

The **Curve (c2)** calibration variable gives the curve value of the used ➢*Calibration Function*.

This value is available only for the functions **Quadratic** and **Quadratic with Offset**.

Cut Segment Volume (AS50 Command)

The **Cut Segment Volume** AS50 ➢*Autosampler* command determines the volume of sample discarded from each end of the aspirated sample. The middle portion of the sample is positioned in the loop and injected. The Cut Volume is used only for partial-loop injections. To perform a partial-loop injection from a limited amount of sample, specify a Cut Volume of 0. For full-loop injections, the Cut Volume is ignored. See ➢*Injection Types* for details.

Cycle Time (AS50 Command)

The **Cycle Time** AS50 ➢*Autosampler* command determines the time between injections. To set a uniform time between injections, specify a cycle time in minutes (1 to 999). When a cycle time is specified, the autosampler delays sample injection until the specified time has elapsed since the previous injection. If the cycle time is set to 0, the time between injections is determined by the commands in the ➢*Program* specified for each sample injection in a ➢*Sequence*. Specifying a cycle time allows a uniform time interval between injections, regardless of time differences in sample preparation and timed steps among program files.

Data Collection Rate

The data collection rate (or sampling rate) is the rate at which the data system collects digital data points from the detector, expressed as points per second or hertz (Hz).

In general, each peak should be defined by at least 20 data points. For chromatograms with co-eluting peaks or low peak-to-noise ratios, 40 points per peak is better. If you expect all of the peaks to be relatively wide, use a slow data collection rate; if any peaks of interest are less than a few seconds wide, set a fast data collection rate.

If the data collection is too slow, the starts and ends of peaks will not be precisely determined. If the data collection rate is too fast, data files will occupy more disk space and take longer to process than necessary.

In addition to the data collection rate, a ⇒*Step* value is also set. The default step value is the reciprocal of the data collection rate. For example, if you set a data collection rate of 5 Hz, the step value is automatically set to 0.2. In general, the automatically selected step value is preferred. It is possible to specify a step value that is independent from the data collection rate, but only advanced users should do this. Refer to the detector operator's manual for guidelines.

Datasource

The term datasource is used for a database that is registered on a Dionex Chromatography Management System ➢*Client*. Setting up (registering) a datasource is performed in the ➢*Browser*. The user specifies the format and the location of the database. For details, see **How to ...: Actions in the Browser Setting up a Datasource**.

During the initial installation of the Dionex Chromatography Management System, a local default datasource is created on each Client PC. In network operation, the datasource name is composed of the computer name and the addendum **LOCAL** (<**PC-NAME_LOCAL**>). In a local station not included in a network, the name stated in the operating system below **Control Panel / Network / Identification** is used. If no identification is entered, the datasource is named **PC-NAME_LOCAL**.

Normally, Dionex Chromatography Management System data is stored in an Access database, i.e. in an mdb (**Microsoft Data Base**) container. The default datasource is also based on an Access database. The ➢*ODBC Capability* of the data system also allows using various other formats (dBASE, SQL, Oracle

etc.). Independently of the chosen format, data of single samples (➢*Sample Data*) is saved as well as data of sequences (➢*Sequence Data*).

Datasources can be saved on a local hard disk or any other mass storage device.

The **Directory** command allows creating individual subdirectories below a datasource. The directories are used for saving ➢*Sequences* and corresponding data and programs.

Network Datasource

If the datasource is located on a centralized network PC, the database is accessible by all clients that are granted the appropriate access rights by the system administrator. If the datasource is stored on a local hard disk, it is up to the corresponding client to decide whether the datasource can be accessed via the Windows **File Sharing**. The Dionex Chromatography Management System also offers the possibility to lock datasources, directories, or sequences.

For further details on datasources, see **Data** **Datasource**

Non-Availability of the Network Datasource

In many companies and organizations, the database server is shut down during the daily backup. As with a network breakdown (see ➢*Network Failure Protection*), the network datasource will not be available during this time. In this case, it is known, however, when the datasource will not be available. The Dionex Chromatography Management System should be disconnected before to ensure data integrity. When the database is available again, the Dionex Chromatography Management System automatically connects to the database and writes back any data that were acquired during the breakdown.

Also, see **How to ...: Actions in the Browser** **Network Failure/Non-Availability**

***Note**:* "Old" GynkoSoft data has the required database structure. The Dionex Chromatography Management System is therefore capable of handling this data as "real" Dionex Chromatography Management System data. The user simply establishes a connection (**Connect**) to the data stored under **Drive ...**.

Data Smoothing

See ➢*Smoothing*

DC Mode

The basic operating mode of an electrochemical detector is the DC mode (**direct current**).

When applying a fixed potential between reference and working electrode, a proportional current is observed depending on the concentration of an oxidable or reducible substance.

For optimum results, the potential must be adjusted to the substance to be detected. This is performed in the ➢*SCAN Mode*.

If modifications occur during the analysis, e.g. due to separating processes, the detector should be operated in the ➢*PULSE Mode*.

DC Voltage

The **DC Voltage** command for the ED40, ED50, and ED50A electrochemical detectors sets the fixed potential applied to the working electrode, in the range of -2.04V to +2.04V.

Dead Time

The Dead Time To is defined as the time required for the peak maximum of an unretained substance to reach the detector from the point of injection.

Also, see ⇒*Dead Time*

Delay (AS50 Sample Prep Command)

The **Delay** ➢*Sample Prep Command* specifies a number of minutes to pause before proceeding to the next step in a sample preparation sequence.

Delay Time

The time needed by a substance to travel from the detector cell of one detector to the detector cell of a second detector is referred to as Delay Time. It can be entered on the  **General** tab of the ⇒*QNT Editor*.

See ⇒*Delay Time*.

DELTA (Signal Property)

The Dionex Chromatography Management System is capable of recording and evaluating signals or output variables supplied by a detector (e.g. UV/VIS channel 1, Temperature, Pressure, %A, Flow rate, etc.).

Instead of the actual value (in mAU, Volt, °C, ml, etc.), the changes of a variable in a specific period can be calculated. This is possible via the signal property DELTA.

This option is especially useful when creating complex ⇒*Trigger* conditions. A peak can thus not only be recognized by the height of its absorption signal within a chromatogram, but also by a sharp increase of the signal, for example.

For information on how to express this type of trigger condition, see **How to ...: Device Control Trigger Commands**.

***Note**:* The calculation of the first derivative is once per second, independently of the ➢*Sampling Rate* or the ⇒*Step* that is used for the data acquisition.

Demo Mode

Demo Mode lets you simulate data acquisition by loading a pre-recorded demo file and then displaying the data from the demo file in the ➢*Control Panel's* signal plot. The demo file is "read back" as though the data were being acquired in real time.

For information on how to simulate data acquisition see **How to ...: Actions in the Control Panel Using/Recording Demo Data**

Detect Negative Peaks

The **Detect Negative Peaks** detection parameter determines whether negative peaks are recognized apart from positive peaks.

Also, see ⇒*Detect Negative Peaks*

For information on how to apply detection parameters, see **How to ...: Actions in the QNT Editor Modifying Detection Parameters**.

Detection Code at Peak Start / End (AIA Peak Type)

This peak result variable indicates how the peak start is classified. In principle, this corresponds to the ⇒*Peak Type* classification used in the Dionex Chromatography Management System (CMS). The classification described below complies with the ➢*AIA* convention.

The following AIA peak types are evaluated:

AIA Peak Type	Description	Dionex CMS Peak Type
B (baseline peak)	The peak starts on the baseline.	**BM**, **bM**
VD (vertical drop)	The peak starts with a perpendicular line dropped to the baseline.	**MB**, **M**
PT (pretangent skim)	The peak is interpreted as a rider.	**Ru** or **Rd**

Device Driver

Each controllable instrument has its own device driver that is activated when the Dionex Chromatography Management System is started. The device driver translates the user's PC instructions (via "mouse click") into device-specific digital commands that are then converted in "real control commands" after the data is transferred to the instrument. In the opposite direction, the signals of all instruments (readings, status information etc.) is converted so that they can be read by the Dionex Chromatography Management System and can be displayed on the screen.

Device drivers are also capable of monitoring regularly inquired or automatically given device parameters in a target/actual value comparison. Unexpected events can be corrected or displayed (in an error message). Full support for all instrument functions by the device driver can only be guaranteed for Dionex instruments. Support for third party instruments may be limited. If the functionality of the driver can be modified via parameters (e.g. determining the shared A/D channels, relays or remote inputs), this is performed in the **Server Configuration**.

The names of the device drivers are derived from the corresponding instrument. The extension **CDD** means "Chromatographic Device Driver." For example, the device driver for the ➢*A/D Converter* is **SADCONV.CDD**, for the Dionex M480 pump the driver is **M480.CDD**.

During the installation of the Dionex Chromatography Management System, all device drivers are saved to the BIN directory and receive a version ID that can

be viewed via the **Properties** command in the context menu, e.g. in the Explorer.

In special cases, the generic device driver can be used to create a user-defined device driver (for details, see **Generic Device Driver**).

Digital Input

See ➢*Remote Input*

Dilute (AS50 Sample Prep Command)

The **Dilute** ➢*Sample Prep Command* dilutes a sample with a specified volume of reagent. This command can be used only when the AS50 Sample Preparation option is installed.

- **Concentrate Source** is the vial that contains the concentrated sample.
- **Concentrate Volume** is the amount of concentrated sample to be diluted.
- **Diluent Source** is the reservoir that contains the diluent.
- **Diluent Volume** is the amount of diluent to be used.
- **Destination** is the vial in which the concentrated sample and diluent are dispensed.

Dilution Factor

The ⇒*Sample Variable* **Dilution Factor** is a correction factor for diluting consecutive calibration samples.

See ⇒*Dil. Factor* (dilution factor)

Dilution Series

A dilution series ("concentration series") consists of several samples with different concentrations. The samples were generated from a common original sample. Alternatively, varying the injection volume can also generate a dilution series.

Preparing a dilution series is especially useful when performing a multiple-point calibration. Instead of injecting standard samples of various concentrations, various volumes are injected from a standard sample (principle: the double injection volume contains exactly the double amount of each component).

The corresponding amount is calculated as follows:

$$Amount = Am._{(Peak-Tab.)} * \frac{Inj.Vol._{unknown\,Amount}}{Inj.Vol._{known\,Amount}} * \frac{Smp.\,Wght}{Dil.Factor}$$

⚠ ***Caution***: Note that the calculated amount values refer to the same standard sample. In the peak table, only one ⇒*Amount* value (column 1) must be entered for each substance contained in the standard.

Dimension of Amounts

This peak table parameter defines the physical dimension of the amount values (⇒*Amount*), i.e. either amount or concentration.

Also, see ⇒*Dimension of Amounts*

Diode Array Detector

See ➢*Photodiode Array Detector*

Disconnect

Execute the **Disconnect** command to separate a user PC (client) from a ➢*Timebase* or to operate an instrument locally. The specified instrument is no longer monitored by the data system, nor can it be operated via the data system, as the instrument keyboard lock of the ⇒*Connect* command is no longer valid.

Note: Use the **Connect** command to undo the operation.

Also, see ⇒*Connect/Disconnect*

Dispense

The **Dispense** command causes the ➢*Autosampler* to dispense a specific quantity (volume) from the sample loop into a certain sample vial (⇒*Position*). The amount of time the sampler may take for this operation, is determined via the ➢*Duration* parameter.

After the operation is completed, the sampler sends the signal **Sampler.Ready** (in case of an ASI-100 / ASI-100T sampler or ➢*Ready* for a GINA50/GINA160 sampler) back to the data system. The time interval between the **Dispense** command and the response signal **Sampler.Ready (or Sucked)** can vary depending on the instrument.

Also, see ⇒*Dispense*

Dispense (AS50 Sample Prep Command)

The **Dispense** ➢*Sample Prep Command* moves a volume of reagent from a reservoir to a vial. This command can be used only when the AS50 Sample Preparation option is installed. **Source** is the reservoir from which reagent is dispensed. **Volume** is the amount of reagent to dispense and **Destination** is the vial in which reagent is dispensed.

DOF-Adjusted Coefficient of Determination

The calibration variable **DOF-Adjusted Coefficient of Determination** allows to return the coefficient of determination corrected by the degree of freedom. The calculation is as follows:

$$r_{DOF-adj}^{\ 2} = 1 - \frac{(N-1)*\sum_{i=1}^{N} W_i*(Y_i - F(X_i))^2}{(N-m-1)*\sum_{i=1}^{N} W_i*(Y_i - \overline{Y})^2}$$

With:		
	N	Number of standard samples involved in the calibration
	m	Number of degrees of freedom (= coefficients to be determined according to the ⇒*Calibration Type*: LIN: *m* = 1; LOFF: *m* = 2; QUAD: *m* = 2; QUOFF: *m* = 3 and EXP: *m* = 2),
	i	Index for standard samples
	Wi	Weight factor of the standard sample no. i
	F(x)	Model function of the calibration
	Xi	X-value of the standard sample no. i
	Yi	Y-value of the standard sample no. i and
	$\overline{Y}$	Average of all Y-values.

Also, see ➢*Coefficient of Determination*

Dongle

A dongle is an adapter that is placed on the parallel PC interface. The free end of the adapter is designed as a parallel interface connector; thus, it provides the parallel interface functions.

Similar to the ➢*PAL Plug-In Board*, the dongle serves to store the serial number of a Dionex Chromatography Management System station. Each station has its own serial number.

Only if the serial number of the dongle and the ➢*Key Code* stored in the Dionex Chromatography Management System match, can the Dionex Chromatography Management System be operated correctly. Otherwise, it will run in ➢*Demo Mode* only.

If there is neither PAL, dongle, nor license server (or if the key code is incorrect), the Dionex Chromatography Management System can be operated only in demo mode.

For further details, see **Installation Software Protection** and **How to ...: Actions in the Server Configuration Selecting the Copy Protection Location and Entering the Key Code**

Drag & Drop

Instead of respective menu options, you can use the **Drag & Drop** function to copy, move, and print any element. The function is available in the online and offline modules, and is most useful when editing lists.

Press the mouse button and keep it pressed to move the selected element to its new position. To move an object, use the left mouse button, to copy use the right mouse button.

Draw

The **Draw** command (**Draw** for the ASI-100/ASI-100T, **Suck** for the GINA 50/GINA 160) induces the ➢*Autosampler* to draw a specific injection ⇒*Volume* from a certain sample vial (⇒*Sample Position*). The amount of time this operation is allowed to take is determined via the ➢*Duration* parameter.

When the operation is completed, the autosampler sends the signal **Sampler.Ready** (in case of an ASI-100/ASI-100T sampler, ➢*Ready* for a GINA 50/GINA 160 sampler) back to the data system. The time interval between the command **Draw** (or **Suck**) and the response **Sampler.Ready** (or **Sucked**) can vary depending on the instrument type.

Also, see ⇒*Draw*

DS3 Detection Stabilizer

A temperature-controlled chamber that houses a conductivity cell and an eluent heat exchanger.

The DS3 Temperature command can be used to set the temperature of the DS3. The command can be executed directly from the ➢*Control Panel* or linked to a ➢*Control*. To link the command to a control, place a string display, gauge slider, or edit box control on the control panel (see ➢*Layout Toolbar*). Then, link the control to the object property, **DS3_Temperature.** For details, see **How to ...:** Actions in the Control Panel **Linking a Control to a Device**.

Tip: The DS4, which is installed in the DX-120 Ion Chromatograph, is identical in function to the DS3. The only difference is the connections required for installation in the DX-120.

Duration

Relay On/Off

Closing or opening duration in seconds [sec]. Specifying the duration is optional. The relay on/off duration for the same relay may not overlap! Some ➢*Device Drivers* support trigger contacts that are treated as two (dependent) relays R1 and R2. Switching on R1 will switch off R2 and vice versa. Thus, you can control a trigger contact with only one Relay On command. However, you can also ignore the second relay R2 and control the trigger contact via the ⇒*Relay On/Off* commands of relay R1.

Autosampler

The **Duration** parameter indicates the minimum time that the ➢*Autosampler* may take to perform ⇒*Draw* or ⇒*Dispense* operations. To prevent evaporation of the sample load, not more than 10µl per second should be sucked or dispensed. Otherwise, the gas bubbles resulting from an insufficient **Suck** duration may considerably impair measuring precision.

Sound

Duration defines the time in seconds of the tone reproduction for the ⇒*Sound* command.

DX-LAN

The local-area network (LAN) that connects Dionex modules to the PC on which the Dionex Chromatography Management System is installed (for details, see **DX-LAN**).

Electronic Signature

According to the "21 CFR Part 11" rules and regulations published by the FDA in 1997 electronic signature means " a computer data compilation of any symbol or series of symbols executed, adopted, or authorized by an individual to be the legally binding equivalent of the individual's handwritten signature.

In the Dionex Chromatography Management System, electronic signature allows you to sign the results from your ➢*Raw Data* that is important within the scope of quality assurance and ➢*GLP*. With enabled ➢*User Mode*, you can sign and save ➢*Sequence* reports that have been accepted as correct so that your results can be completely verified and understood.

Electronic signature includes three steps:

- Submit
- Review
- Approve

Typically, the report will be signed and **submitted** by the user who created it. Having **reviewed** the report, e.g. the laboratory manager will sign it again. Finally, the quality assurance manager can **approve** the results.

Note: Electronic signature requires the User Mode to be enabled and is available for user databases only that were created with a ➢*CmUser* program version 6.10 or higher. Update your database if an error message notifies you that electronic signature will not be possible.

For information on how to sign reports electronically, see: **How to ...: Actions in the Browser** **Signing Sequences Electronically** as well as the CmUser Online Help (CmUser_E.HLP).

Eluent Generator (EG40)

The EG40 eluent generator can generate high-purity acid or base eluents on-line at the point of use, using only deionized water as the carrier. The EG40 consists of a high-precision programmable current source (power supply), a ➢*DX-LAN* automation interface, a high-pressure gas removal device, and a disposable eluent generator cartridge (EluGen).

The EG40 is configured in a ➢*Timebase* as part of the IC pump (for example, a GP50 or IP25).

The Dionex Chromatography Management System provides the following EG40 control functions:

- Control of the generated eluent concentration (from 0.0 to 100 mM)
- Monitoring of the ions remaining in the EluGen cartridge
- Monitoring of the EluGen cartridge expiration date

Also, see: **How to ...: Device Control**:

Controlling the Eluent Generator Concentration

Monitoring the Eluent Generator Cartridge Lifetime

Eluent Mode (DX-120)

Eluent mode enables switching of flow from one eluent to another in a DX-120 Ion Chromatograph equipped with the dual-column option. In this mode, the column-switching valve is disabled. The selected eluent always flows to the column that was selected when Eluent mode was enabled. Also, see ➢*Column Mode*

The EluentAB command is used to switch the flow from one eluent reservoir to the other. The command can be included in a ➢*Program*, executed directly from the Commands dialog box (select **Command** from the Control menu), or linked to a ➢*Control* on the control panel. To link the command to a control, place an edit box or switch control on the ➢*Control Panel*) (see ➢*Layout Toolbar*). Then, link the control to the **EluentAB** object property. For details, see **How to ...: Actions in the Control Panel Linking a Control to a Device**.

To enable Eluent mode:

1. Open the ➢*Server Configuration* program.
2. Select the DX-120 under the ➢*Timebase*.
3. Double-click to open the Properties dialog box (or right-click and select Properties).
4. Select the Mode tab page and select the **Eluent** option.

Emergency Program

The Dionex Chromatography Management System differentiates between three types of errors:

- Fatal Error (**Abort** - batch is aborted)
- Serious Error (**Error** - batch continues - error is corrected as far as possible)
- Error (**Warning** - batch continues - a warning is issued)
- Minor Error (**Ignore** - batch continues - only logged in the audit trail)

For the first error types, an emergency program can be defined. Instead of aborting the batch, the emergency program is started automatically.

The retention time continues while the emergency program is active and the times are interpreted as offset. Data acquisition and audit trail will continue as well. Upon termination of the emergency program, an **End of Sample** entry is made in the audit trail.

For emergency program examples, see **How to ...: Actions in the PGM Editor**  **Creating an Emergency Program**.

Emission

If a substance is fluorescent, it emits light at a specific wavelength range. The fluorescence is measured via a fluorescence detector that is set to the respective emission wavelength maximum. This emission wavelength is entered via the **Emission** parameter.

 ***Note:*** The excitation wavelength of the fluorescence detector is entered via the ➢*Excitation* parameter.

Excitation

To induce a substance to fluoresce, the irradiating light must be of higher energy than the emitted light. Therefore, the selected excitation wavelength must be lower than the emission wavelength. To enable the analyzed substance to absorb as much as possible of the irradiated energy, the highest absorption maximum below the emission wavelength should be selected as the excitation wavelength. This excitation wavelength is entered via the **Excitation** parameter.

 ***Note:*** The emission wavelength of the fluorescence detector is entered via the ➢*Emission* parameter.

F1 Key

Use the F1 key to open context-sensitive Online Help, i.e. the displayed help text refers to the current cursor position.

Filter

The Dionex Chromatography Management System distinguishes three types of filters:

Data Acquisition Filters

These filters can be set via the ➢*Control Panel* if the device driver of the detector supports this option.

Data Reprocessing Filters

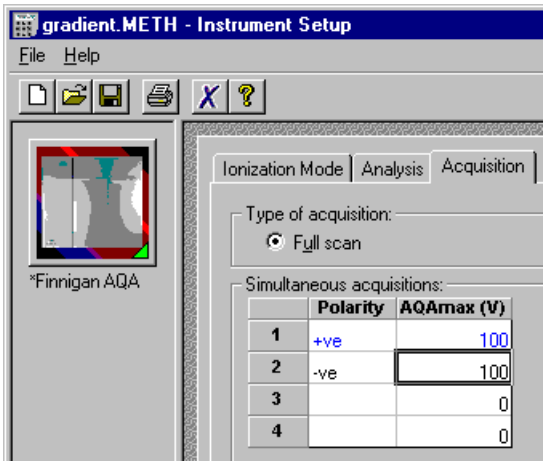
Often, ➢*Smoothing* filters are used to improve the ➢*Signal to Noise Ratio*. They allow smoothing chromatograms that have already been acquired. The following smoothing filters are available:

- Moving Average (Boxcar)
- Olympic
- Savitzky-Golay
- Gaussian

Data Display Filters

1. **MS Filter:** In case of ➢*Mass Spectra,* you can define the ionization polarity and the ionization voltage for the mass spectrum plot.

   If, in ➢*Full-Scan* mode, several ionization settings are used, you may enter an MS filter index in the mass spectra plot of the control panel to display those mass spectra of the entire signal (➢*TIC*) that correspond to a specified group of settings. For example: The index 1 corresponds to the first line in the Simultaneous acquisitions table (= TICF_1 - in the following example: polarity "+ve", maximum voltage 100 V):



The numbers of the settings (1 to 4) are also called filter index.

2. **Audit Trail Filters:** In the control panel, Report, and ➢*Printer Layout* you may specify the filter level for displaying messages. This is to avoid that the Audit Trail (see **Basic Operation / Control Panel** **Audit Trail**) includes messages that are not relevant for you and thus becomes unnecessarily long. Errors, warnings, and system messages are always given. However, commands are displayed only from the specified level on (color code in the control panel):

   Errors and Warnings: no commands

   Normal: green

   Advanced: yellow ("normal" and "advanced" commands are displayed)

   Expert: red ("expert" and "advanced" commands are displayed)

Find (Button)

The **Find** tab in the Online Help window allows you to find specific words, terms, or text included in Online Help. All help texts of the Dionex Chromatography Management System are searched.

Flow Gradient

Alterations to the ⇒*Flow* within one chromatogram are referred to as flow gradient. The gradient can be generated manually or program-controlled.

Note: Pumps that are controlled *serially* will deliver a specific flow rate via command. As it is not possible to enter an unlimited number of these commands in very short intervals, this type of flow gradient will have small steps. Pumps with voltage, frequency, or pulse width control can continually change the delivery rate. There are virtually no steps.

Flow Rate

In general, the **Flow Rate** indicates the total volume (in [ml/min]) delivered by the chromatography pump. It is composed of the sum of all ⇒*Partial Flows* (%A+%B+%C+%D=100%).

Normal flow rates are in the range 0.5 to 10 ml/min. Flow rates deviating from this range are achieved by using micro pumps (0.1 - 0.5 ml/min) or especially equipped pumps (as from 10ml/min). For gas chromatographs, the amount of mobile gas phase is also called flow rate.

Caution: As there are pressures up to 400bar in the chromatography column and as solvent mixtures are subject to volume compression (e.g. methanol/water), the delivered volume in ➢*High-Pressure Gradient Systems* does not correspond to the volume transported via the column. However, the number of delivered and transported solvent particles is not changed by this fact.

Also, see ⇒*Flow*

Flush (AS50 Sample Prep Command)

The **Flush** ➢*Sample Prep Command* flushes the inject port with a specified volume of flush fluid. During the flush cycle, the needle moves to the waste port and expels any fluid. The needle then moves to the inject port and delivers a volume of fluid for flushing the inject port. If the injection valve is set to the Load position, the loop is also flushed. The needle then moves to the flush port and delivers a volume of flush fluid, which washes the outside of the needle.

Flush Volume (AS50 Command)

The **Flush Volume** AS50 ➢*Autosampler* command determines the volume of fluid used to flush the inject port. The flush cycle is performed either before or after each injection, depending on the option selected.

Formula for Amount Calculation

The formula calculates the substance amount in an analysis sample. The prerequisite is that all necessary ➢*Calibration Coefficients* as well as the peak areas of the unknown sample were determined.

$$Amount_p = a_p(x_p) * Resp.Fact._p * ISTD - Fact * \frac{Dil.\ Factor_n}{Smp.\ Wght_n}$$

p	Peak number
a_p	Calibration function for peak p calculated in the calibration.
X_p	Determined area of peak p
$Resp.Fact_p$	Scaling factor that can be entered peak-specifically, e.g. serving as a compensation for the differing absorption behavior.
ISTD Fact.	Correction factor for internal/external standard method. For the external standard, this factor equals 1.
Dil.Fact.	Corresponding parameter from the sample list.
Smp.Wght.	As sample-specific factors, they always refer to all peaks!
n	Sample number

Formula for Amount Calculation (Rel. to ISTD)

The function calculates the substance amount in an unknown sample relative to the added ➢*Internal Standard*. The prerequisite is that all peak areas of the sample were determined (including that of the internal standard).

$$\frac{Amount_{Peak}}{Amount_{ISTD}} = Am._{p.rel} = a_p * \frac{Area_{Peak}}{Area_{IS}} * Resp.Fact._p * \frac{Dil.Fact._n}{Smp.\ Wght._n}$$

p	Peak number
a_p	Calibration function for peak p calculated in the calibration.
X_p	Determined area of peak p
$Resp.Fact_p$	Scaling factor that can be entered peak-specifically, e.g. serving as a regression function for the differing absorption behavior.
ISTD	Name of the internal standard
Dil.Fact.	Corresponding parameter from the sample list.
Smp.Wght.	As a sample-specific factor, Smp.Wght. always refers to all peaks!
n	Sample number

Fraction Collector

At the detector output, fractions can be collected for occasional preparative chromatography as well as for the exact determination of the separated substances in subsequent analytical procedures. A fraction collector is imperative if this is routine operation.

The fraction collector must collect the fractions depending on the incoming signal, i.e., fraction collector control is via extensive ➢*Programs*. If the absorption signal exceeds a specified threshold value, ⇒*Trigger* commands are used to close a relay and move to the next collecting tube.

Installing the **Fraction Collection Automation** driver in the ➢*Server Configuration* considerably shortens the respective program and thus facilitates fraction collector control. In addition, the ➢*Device Driver* of the respective fraction collector has to be installed in the server configuration. The Fraction Collection Automation driver compares to the ➢*Integrator Driver* that is required in addition to the respective pump driver for recording the pump pressure.

For information on how to control fraction collectors, see **How to ..: Device Control Controlling Fraction Collectors**.

Front Riders to Main Peaks

The **Front Riders to Main Peaks** detection parameter allows you to change rider peaks on the ascending edge of a peak into main peaks.

☞ ***Tip***: This parameter has priority over the ➢*Rider* peak type indicated in the peak table.

Also, see ⇒*Front Riders to Main Peaks*

For detailed information on how to apply the detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**

Fronting Sensitivity Factor

For information on this topic, see ➢*Tailing Sensitivity Factor*.

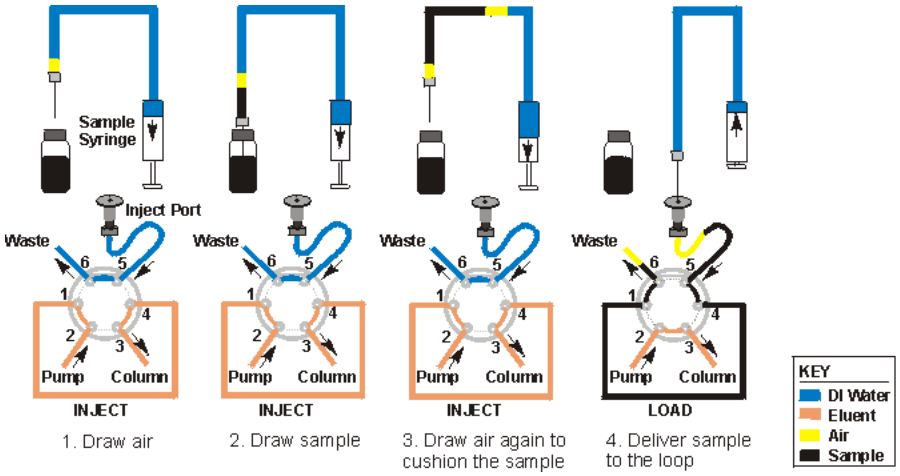
Full-Loop Injections (AS50 Sample Prep Command)

When performing a full-loop injection, the AS50 ➢*Autosampler* draws four times the loop volume from the sample vial and delivers it to the injection valve. The middle portion of the sample is positioned in the loop and injected.

Important: For very small loop sizes (less than 17 µl), 2.5 times the loop volume plus 25 µl is delivered to the valve.

The maximum loop size for full-loop injections is 300 ml. If a larger loop size is used, sample can contaminate the flush bottle because the sample volume drawn is greater than the sample transfer line volume of 1200 ml.

Full-Loop Injection Sequence



Full-Scale

The **Full-Scale** command sets the voltage for a full-scale analog output. For example, if 0.1V is selected and a recorder is connected to the detector's analog output, the recorder's full-scale response will be at 0.1V. For the AD20 detector, the full-scale voltage is fixed at 1V.

Full-Scan

Full-Scan is the ➢*Mass Spectrometer* method for recording ➢*TIC* chromatograms. Contrary to ➢*SIM* (Selected Ion Monitoring), this method records the entire ➢*Mass Spectrum* of each individual analyte.

In full-scan mode, you can extract ➢*Mass Traces* already during data acquisition (see **How to …: Actions Related to the aQa-MS Extracting Mass Traces Afterwards**).

Also, see: **Defining the Number of MS Channels**.

Full Size

The **Full Size** function undoes all previous **Zoom** operations. To undo only the last operation, use the **Unzoom** function.

In the signal plot, double-click in the ➢*Overview Window* to perform the **Full Size** function.

Gain

For the fluorescence spectrometers RF1002 and RF2000, the **Gain** signal parameter determines the factor with which the analog output signal is increased or reduced. **Gain** has therefore the same significance as the ➢*Range* parameter for other detectors.

***Note**:* The Dionex ➢*A/D Converter* ranges from -10V to +10V and thus covers virtually all detector output signals. It is possible to record signals directly, without considering the Gain parameter. If size adjustment is still necessary, this can be performed via the **Factor** parameter of the A/D converter.

GLP ("Good Laboratory Practice")

Good Laboratory Practice means the adherence to regulations on the organization and conditions of planning, performing, and monitoring laboratory work.

A special focus is the complete and clear listing of the complete data in an analysis process. In addition, regular checks of the instruments and the software are required.

GLP contributes to enhancing the quality of test data. In Germany, the GLP principles were introduced in 1983. In 1990, they became part of the chemical law (ChemG).

Gradient

Usually, gradients are used in HPLC/IC and GC to accelerate the separation of substance mixtures. Due to the different separation mechanisms in HPLC/IC on the one hand and GC on the other, different gradient types can be used.

In HPLC/IC, there are two different gradient types:

If the composition of the mobile phase changes, this is referred to as ➢*%-Gradient*. If the flow rate is altered, this is called a ➢*Flow Gradient*. The Dionex Chromatography Management System can generate flow and %-gradients. Both gradient types can be performed at the same time (!).

☞ ***Tips***: This results in non-linear partial flow alterations in the total flow. With ➢*High-Pressure Gradient Systems* with more than one pump it will result in non-linear partial flow alterations for each individual pump. Not all chromatography pumps support this option.

The chromatographic conditions for high-pressure and low-pressure gradients are not transferable due to the different properties in solvent compressibility and dead volume!

In GC, there are three different gradient types:

Usually, temperature gradients are used. In addition, flow or pressure gradients can be used with some GCs. With GC gradients, the flow (or the temperature, or the pressure) is usually increased during the chromatogram. Changing one of the three variables automatically changes the remaining two according to the equitation of state for ideal gases and the Hagen-Poisseuille law. Nevertheless, it is also possible in GC to run a temperature and a flow or pressure gradient simultaneously. In this case, the flow or pressure change which results from the temperature increase is considered for the flow and pressure settings, respectively.

Independently of the gradient types described above, the gradient forms can be different: Ramps and ➢*Step Gradients* are distinguished. In case of a ramp the solvent composition, for example, changes slowly until the desired composition is finally reached at the desired end. In case of a step gradient, however, the composition would be set immediately. (Depending on the column, the solvent change, and the flow, it may nevertheless take some time until the desired composition is reached on the column.)

Gradient Curves

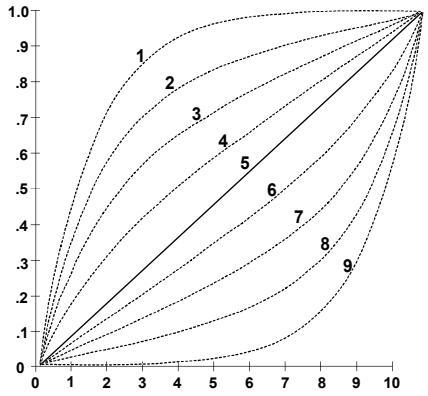
The Dionex pumps GP40, GP50, and GS50 let you specify linear or non-linear ➢*%-Gradient* profiles (gradient curves). ➢*Eluent Generators* can also deliver non-linear %-gradient profiles. Also, see ➢*Gradient Curves Equations* for the mathematical descriptions of the curve types.

Curve 5 (the default) is linear. Changes in composition of the delivered solvent over time are constant.

Curves 1 - 4 are convex upward. Convex curves cause rapid changes in solvent composition at the beginning of the gradient and slower changes at the end. Slope changes over time become extreme as curves go from 4 (least convex) to 1 (most convex).

Curves 6 - 9 are concave upward. Concave curves cause slower changes in solvent composition at the beginning of the gradient and rapid changes at the end. Slope changes over time become extreme as curves go from 6 (least concave) to 9 (most concave).

The figure below shows the solvent composition profiles of curves 1 through 9, for a change from 0 - 100% B over 10 minutes.



Gradient Curves Equations

The following equations describe the ➢*Gradient Curve* profiles generated by the Dionex gradient pumps GP40, GP50, and GS50, and by the eluent generator.

For convex gradients:

$$Ve = Vf + (1-k)(Vt-Vf)\left(1-2^{\frac{-10(Te-Tf)}{(Tt-Tf)}}\right)+\frac{k(Vt-Vf)(Te-Tf)}{(Tt-Tf)}$$

Where: k = 0, ¼, ½, ¾, 1 for curve numbers 1, 2, 3, 4, 5 respectively

For concave gradients:

$$Ve = Vf + (1-k)(Vt-Vf)\left(2^{\frac{-10(Tt-Te)}{(Tt-Tf)}}\right) + \frac{k(Vt-Vf)(Te-Tf)}{(Tt-Tf)}$$

Where: k = ¾, ½, ¼, 0 for curve numbers 6, 7, 8, 9 respectively

Ve	Current eluent value
Vf	Eluent value at the previous step time
Vt	Eluent value at the next step time
Te	Current elapsed time
Tf	Time at the beginning of the gradient step
Tt	Time at the ending of the gradient step
k	Parameter that is changed to produce different curve number results

Group (Peak Group)

Within a chromatogram, it is possible to group individual peaks and to calibrate and integrate them together. Assign a common name to these peaks in the **Group** peak table column in the ⇒*QNT Editor*. The peaks do not have to succeed each other directly but can be scattered at will.

Also, see ⇒*Group*

If a peak belongs to a user-defined group, the **Group** report peak variable indicates the group's name. In addition to the user-defined peak groups, two pre-defined groups are available:

1. The group of all unidentified peaks without explicit group entry (empty group)

2. The group of all identified peaks without explicit group entry (empty group)

All other peak groups must be defined on the **Peak Table** tab in the **QNT Editor**. For unidentified peaks, the group defined in the dialog **Unidentified Peaks** is indicated provided the peaks occurs in the corresponding time interval.

Height (Peak Height)

This peak result variable refers to the peak height in the maximum, i.e. at the retention time, relative to the baseline.

The height dimension depends on the detector type. For UV detectors the area is usually specified in mAU (milliabsorbance units).

Also, see ➢*Relative Height*

Help

See ➢*Online Help*

High-Pressure Gradient System

In a high-pressure gradient system, each partial flow is delivered via a separate pump into the mixing chamber against the pressure of the column. Differences in volume contraction and compressibility, as observed in most solvent mixtures, are not important during delivery but when mixing the solvents on the high-pressure side of the pump.

Unlike ➢*Low-Pressure Gradient Systems*, the delivered volume of each partial flow can be determined precisely in high-pressure gradient systems. The gradient profile is more precise and can be achieved with relatively simple pumps. However, the costs for the additional pump are disadvantageous.

In Dionex instruments, control of additional pumps ("slave") is usually by a main ("master") M480 pump. The new Dionex pump P 580 combines master and slave pump in one housing. Alternatively, several pumps e.g. 2x M300 can be controlled centrally via the data system and the pump control board.

⚠ ***Caution***: Due to solvent compressibility and differing dead volumes, the chromatographic conditions of high-pressure and low-pressure gradient systems are not interchangeable.

History

The History mode (or more exactly the File History Mode or Modification History Mode) completely documents any changes and operations performed in specific objects and files. Objects include samples, ➢*Sequences* or ➢*Datasources*, ➢*Control Panels*, ➢*Report Definition Files* (RDFs), ➢*PGM Files*, and/or ➢*QNT Files*, and of course modified chromatograms.

The History mode can be activated (or deactivated) individually for each datasource (see **Properties of a datasource / Enable Modification History**). If the **Comment required** option is activated, each user is prompted to enter a comment before saving the changed object (defined above).

Select a datasource, a directory, or a single object and choose the **Show History** command to view the changes that are already documented.

Entering and editing comments as well as enabling or disabling the History Mode requires the corresponding ➢*Privileges*.

Hit Criteria

If there are too many hits in a spectra comparison (see **How to ...: Actions in the UV Spectra and Mass Spectra** **Starting a UV Spectra Search**) due to the selected comparison function (see ⇒*Check Derivative*) or ⇒*Match Criterion*, this list can be limited by adding the following selection criteria:

Comparison Conditions	Additional Limitations
Standard of comparison	Number of extrema
Minimum match degree	Retention time deviation
Comparison function	Solvent composition (*)
Wavelength range	➢*PGM File* name (*)
Comparison of the largest relative maximum	

Only spectra fulfilling the corresponding criterion will be admitted into the selection.

All fields accepting alphanumeric input (*), can be searched with a so-called regular expression, which may contain the wildcards '?' and '*' also used in MS-DOS.

Example: If ***y?ene** is entered as name filter, the hydrocarbons pyrene, chrysene and perylene would be hits, but not anthracene. The hit criteria can be used to comfortably generate sub-libraries. If using these filters, without comparing spectra, the hit list contains the spectra fulfilling the hit criteria. The partial quantity can be stored as a separate library.

Caution: Please note that a distinction is made between upper and lower case letters in the case of alphanumeric input. When using a capital letter in the filter expression, hits must also contain a capital letter at exactly the same position. When using lower case letters, the corresponding hit may contain lowercase and uppercase letters.

Hold

In the Hold mode, no more data is acquired, the pump continues delivery with the current solvent composition, and processing of the batch samples is stopped before the next sample.

Also, see ⇒*Hold*

Holmium Oxide Filter

Recent Dionex UV/photodiode array detectors (the two-channel detector UVD170S and the ➢*Photodiode Array Detectors* UVD340S and PDA-100) feature holmium oxide filters.

For the UVD170S and UVD340S detectors, the holmium oxide filter allows calibrating UV/VIS spectra recorded with the detector due to the typical absorption spectrum of holmium oxide.

For the PDA-100 detector, the holmium oxide filter is used to verify wavelength accuracy.

Note: It is also possible to fit older UVD170S/340S instruments with holmium oxide filters. Please contact Dionex Service.

Index (Button)

The **Index** tab dialog box contains the alphabetical index list of Online Help terms that are available in the Dionex Chromatography Management System. Enter the initial letter of the topic and choose **Display** to view help information on this topic.

Industry Minute

An industry minute (also referred to as decimal minute) has 100 units instead of 60 seconds.

"2.500" (industry minutes) therefore means "2 minutes, 30 seconds," and "2.100" means "2 minutes, 6 seconds" etc.

Inhibit Integration

The **Inhibit Integration** detection parameter serves to shut off certain chromatogram areas

Also, see ⇒*Inhibit Integration*.

For information on how to apply detection parameters, see

How to ...: Actions in the QNT Editor  **Defining Detection Parameters**.

Inject Command

The Inject command defines the start of a chromatogram and thus the time when the sample is brought into the high-pressure cycle of the system. By definition, the time of the first Inject command is set to zero.

In a dialog box, you define the sample vial position in the ➢*Autosampler* (⇒*Position*) and the quantity of the substance (⇒*Volume*) to be injected. When a hand-operated valve is used for injection, this information is used for documentation purposes.

Also, see ⇒*Inject Command*

Injection Time

The **Inj. Time** column in the peak table shows the day, month, year, hour, minute, and second when the sample was injected (Also, see ➢*Time*). This

column cannot be edited. The Dionex Chromatography Management System enters the injection time of the sample in the corresponding column of the sample list. For samples with the ⇒*Status* (sample status) "M" the time of the last injection is entered.

The kind of entry (empty or time value) indicates whether and when the sample was processed.

Also, see ⇒*Inj. Date / Time* (Time of Injection)

Injection Types (AS50 Autosampler)

The type of injection performed by the AS50 ➢*Autosampler* is selected automatically, depending on the settings of other variables:

- A full-loop injection is performed when the ⇒*Inj. Vol.* (injection volume) is greater than the ➢*Loop Volume* (see ➢*Full-Loop Injections*).
- A partial-loop injection is performed when the injection volume is less than the loop volume and the ➢*Cut Segment Volume* is greater than 0 (see ➢*Partial-Loop Injections*).
- A partial-loop, limited-sample injection is performed when the injection volume is less than the loop volume and the cut segment volume is 0 (see ➢*Partial-Loop, Limited-Sample Injections*).

☞ ***Tip***: Partial-loop, and partial-loop, limited-sample injections are available only when the injection valve is installed in the AS50 autosampler compartment, or in the AS50 chromatography or thermal compartment.

Injection Volume *(Volume)*

The ⇒*Sample Variable* **Inj. Vol.** is in micro liters (µl). In automatic operation, the installed ➢*Device Driver* converts this value into a volume readable by the ➢*Autosampler*, and then the value is sent to the autosampler.

By entering different injection volumes, a ➢*Dilution Series* can be created in case of a multiple-point calibration (see ➢*Single-Point and Multiple-Point Calibration*).

Also, see ⇒*Inj. Vol.* (injection volume) and ⇒*Volume* (command).

Installation Qualification (IQ)

As defined in cooperation with EURACHEM, Installation Qualification (=IQ) is "the process of installing an instrument up to and including its response to the initial start of operation" [P. Bedson and M. Sargent, Accred. Qual. Assur. (1996) 1, 265-274].

An important task of Installation Qualification is to ensure that the instrument and its individual components are supplied as ordered (i.e. according to the specification agreed on by the customer and the manufacturer). In addition, the correct installation in the selected environment is checked. Finally, the IQ must be formally documented.

For Dionex hardware, the IQ is performed in accordance with this definition and the Dionex **Installation Qualification, Operational Qualification, Performance Qualification** SOP. For an "instrument" of the Dionex Chromatography Management System, the IQ can be started via the **Chromeleon IQ** and **Check Installation commands** of the **Qualification** menu in the Browser. The IQ checks the system information, the data system status, as well as all installed files. Examine the report for possible installation errors.

 ***Note***: This may result in warnings stating that previous versions of the system files and the ODBC files already existed before the Dionex Chromatography Management System was installed. However, as these warning are not critical they can be ignored.

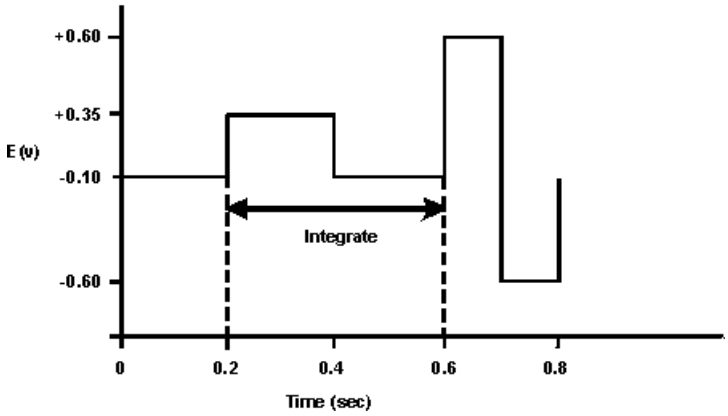
Use the **Save**, **Save as** or **Print** commands of the **File** menu to formally document the IQ of the Dionex Chromatography Management System from within the indicated report (dialog box **CHK.Setup.log - Editor**)

For further information on the Installation Qualification, see *CHROMELEON Installation Qualification* in the Online Help.

Integrated Amperometry Mode

In addition to the ➢*DC Amperometry Mode*, Dionex electrochemical detectors can be operated in Integrated Amperometry mode. Integrated amperometry detection employs a repeating ➢*Waveform*. The cell current is ➢*integrated* during a specific section of the waveform. It is a more general technique than ➢*Pulsed Amperometric Detection* in that pulsed amperometry employs a repeating sequence of three potentials, while integrated amperometry can be any waveform.

With the integrated amperometry waveform shown below, the current is integrated twice - first, while the potential is swept across the metal oxide formation wave, and then during the reverse sweep across the oxide reduction wave. Without the presence of analyte molecules, the net charge is around zero. Positive and negative cleaning pulses are added to the waveform following the integration period.



Integration Parameters

In the Dionex Chromatography Management System, these parameters are referred to as **Detection Parameters**. For an overview, see ⇒*Detection Parameters*.

Integration Period

In Integrated Amperometry detection, the integration period is the time during the ➢*Waveform* in which data is recorded. The integration period is also referred to as analysis or sample time.

Integration Type

The **Integration Type** peak table parameter indicates which peak property is to be used for the calculation of quantitative results.

Also, see ⇒*Integration Type*.

Integrator Driver

The Dionex Chromatography Management System does not directly process analog signals that are received via a Sharable Device (e.g. the ➢*A/D Converter* or the ➢*UCI-100 Universal Chromatography Interface*). Recording these analog signals (e.g. from gas chromatographs or pumps) via the channels of the A/D board requires the Integrator Driver (also, see ➢*Device Driver*) that assigns the individual channels of the sharable device.

The advantage is that you do not have to rewrite all ➢*PGM Files* concerned if you plan to connect a device to a different channel. Instead, only change the A/D port assignment in the integrator driver. This also allows you to distribute the channels of a ➢*Sharable Device* to several ➢*Timebase*, thus, eliminating the need to have e.g. one individual A/D converter for each timebase.

The integrator driver allows you, for example, to record the pump pressure in order to check whether signal variations in the chromatogram are caused by pump pressure variations. Also, see **How to ...**: **Device Control** **Recording the Pump Pressure.**

Intercept

See ➢*Offset (c0)*

Internal Standard ("ISTD")

An internal standard is a substance that is added both to standard and unknown samples. The internal standard should have a similar retention time behavior as the analyzed substances, but it should be easily separated from them.

As a rule, the amount of injected internal standard is constant, i.e. all samples receive precisely the required amount of internal standard so that identical amounts reach the column when injecting the same volumes. In the case of a ➢*Dilution Series*, the internal standard must be pipetted after the dilution! The dilution can therefore not be simulated by variation of the injection volume but must be actually performed.

***Note**:* With an appropriate ➢*Autosampler* (e.g. Dionex ASI-100), pipetting can be performed automatically. The quantitative accuracy thus reached is one level above the standard method **External**. The methods with internal standard also compensate

minor injection inaccuracies, as the internal standard is equally affected by a possible loss or excess.

Substances serving as an internal standard are labeled as such in the **Standard** column of the peak table. Depending on the type of internal calibration, they receive the label **Internal/External; Peak** or **Internal; Peak**.

"Internal/External" Principle

All substances contained in a sample are calibrated as usual with known standard substances (including the internal standard). As the same amount of ISTD is contained in all samples of a sequence, a uniform value for the ISTD should result. If this is not the case, this is an indication for an error during sample processing (provided that the same amount of the internal standard is actually contained in all samples). The results of the remaining substances of this sample can then be relativized.

"Internal" Principle

Instead of absolute areas and amounts, calculation is based on area and amount ratios. Calculation of all substance amounts is relative to the internal standard. By forming the ratio, inaccuracies in sample processing (from adding the ISTD) can be eliminated (**const. Internal standard**).

Due to the high experimental expenses, this type of calibration is rarely used (the internal standard must be added with a pipette to each sample, in the case of a dilution series this must be after the dilution).

Exceptions (= Variable Internal Standard)

The method itself or the properties of the internal standard make it impossible to add the same amount of ISTD to all samples. To solve this problem, the Dionex Chromatography Management System offers the **Use sample amount as reference (Variable)** option (see F8 box of the **Standard** column in the peak table).

In this case (irrelevant whether **Internal/External** or **Internal**), the amount of the internal standard is entered in the ⇒*Amount* column of the sample list, not in the ⇒*ISTD Amount* column of the peak table. For each sample, the amount of internal standard can thus be entered separately.

Also, see ⇒*Standard*

IQ

See ➢*Installation Qualification (IQ)*

ISTD

See ➢*Internal Standard ("ISTD")*

Isocratic

A solvent flow of constant composition is called isocratic. It is irrelevant whether it is a pure solvent or a solvent mixture of constant composition.

ISO Plot

See ➢*3D-Field: Presentation Modes*

Jump to Another Help Topic

As soon as the mouse cursor is positioned on a link term, it changes into a pointing hand. All link terms are displayed in green.

Terms underlined by a dotted line (e.g. ➢*F1 Key*) are links to additional information in a pop-up; terms underlined by a single line are links to a new help topic.

Key Code

The range of functions available for the individual stations of the Dionex Chromatography Management System is determined during installation by a key code.

A 12-digit or a 24-digit number serves as key code that makes available specific functions and options. Each station of the Dionex Chromatography Management System has a ➢*Dongle* or a ➢*PAL Plug-In Board* and can only be operated if the serial number coded there matches the key code.

If a user expands the scope of functions of the Dionex Chromatography Management System by acquiring the corresponding licenses, s/he receives a new key code. The extended scope of functions is made available immediately upon entering the new code.

The key code is entered via the **About** box in the Help menu or via the ➢*Server Configuration* program. Valid characters are numbers, letters, spaces, and hyphens. Input is not case-sensitive.

For further details, see **Installation** **Software Protection** and **How to ...: Actions in the Server Configuration** **Selecting the Copy Protection Location and Entering the Key Code**

Kovats Index

The Kovats Index serves for achieving a uniform scaling of the ⇒*Retention Time*. Define the Kovats Index on the **Peak Table** tab of the ⇒*QNT Editor*.

Also, see ⇒*Kovats Index*

Lamp On/Off

This command switches the lamp of an optical detector on and off. UV/VIS detectors often have a separate lamp for each range (deuterium/halogen). To activate both lamps, the command must be entered and executed twice. However, it is also possible to switch both lamps simultaneously or to switch on the second one automatically when the first lamp reaches a certain value.

Also, see ⇒*Lamp On/Off*

Layout Mode

For some elements of the Dionex Chromatography Management System, a special Layout Mode is available that allows designing them according to your requirements:

- ➢*Control Panel*
- ➢*Printer Layout* (printout) and
- Report (screen table)
- ➢*History* report

Control Panel

Choose the **Layout Mode** command in the **Edit** menu or context menu to change from the online mode to the layout mode. In the Layout mode, you can create new control panels or modify the appearance and the functions of existing ones. Running online processes will be continued. However, controlling the system is not possible in this mode.

Click an icon on the layout toolbar to add a new control to the control panel by a simple mouse click. The pointer function of the ➢*Layout Toolbar* enables the selection of a ➢*Control* (display and control elements). Selected controls are indicated by a ➢*Control Frame* and can be modified in size, shape, and function.

For detailed instructions on how to modify a control panel, see **How to ...: Actions in the Control Panel Modifying a Control Panel**.

Note: Creating a new or modifying an existing control panel can only be performed, if the user has the corresponding access rights.

Printer Layout

In the Printer Layout, you can enable and disable the Layout Mode via the **Layout Mode** command of the **Edit** menu. Inserting, modifying, and copying the different Printer Layout elements is possible only if the Layout Mode is enabled.
With enabled Layout Mode, an additional field for entering text is given in the upper report section. Input is similar to MS Excel.

Report

In the Report, the **Layout Mode** command of the **Table** menu allows enabling and disabling the Layout Mode. With enabled Layout Mode, an additional text field for entering the desired values is given in the upper report section.

History Report

A special Layout Mode is available in the ➢*History* Report. If Detail columns are available, you can enable this Layout Mode via the Layout tab of the **History Report Properties** dialog box.
A shortened report is displayed in which you can easily define the layout.

Layout Toolbar

The layout toolbar contains icons of all default ➢*Controls* and display elements of the ➢*Control Panel* that are available in the ➢*Layout Mode*. The layout toolbar is only accessible in the layout mode.

Click an icon to position the selected default control within the current control panel. The display of the layout toolbar can be enabled/disabled via the **Toolbars** command from the **View** menu.

The following default controls are available (links available in the Online Help only; for further details, see the respective Online Help topics)


Pointer (selecting, moving ...)


Check Box


Color Box

String Display


Gauge Indicator


Command Button


Online Signal Plot


Group Box


Slider


Lamp


Switch


Entry Field (Edit Field)


Audit Trail


Gradient Control


3D-Plot


Rack Control (➢*Rack*)


Mass Spectrum

Left Limit

Normally, peak integration is performed automatically. However, it is possible to limit or extend integration on the left, right or on both sides. This is by entering a left and/or a right integration limit in the peak table.

Also, see ⇒*Left/Right Limit*

Left Width

If a perpendicular line is dropped to the baseline from the peak maximum, the ➢*Width* of the peak is divided in a left and a right section. The two sections are referred to as **left width** and **right width** and can be expressed as separate peak result variables.

The Dionex Chromatography Management System also determines the left and right peak width at 5, 10, and 50% of the peak height. As pointed out under the glossary term ➢*Width*, height is very important for the calculation of the peak width. This also applies to the calculation of the left and right peak widths.

The abbreviations for the left and right peak widths are **LW** and **RW**.

To display the left peak width in the report, please proceed as follows: Select the column in the report, choose the command **Column Properties** from the context menu and select the **Left Width** variable in the selection box. Press the **Parameter** button to determine at which peak height to determine the peak width.

License Server

If installations include a large number of computers, a License Server is optionally available for Dionex Chromatography Management System that can manage the licenses of the Dionex Chromatography Management System. With this type of installation, it would not make sense to equip all ➢*Client* PCs with ➢*Dongles* or ➢*PAL Plug-In Boards* and to enter the corresponding ➢*Key Codes*.

If no PAL, dongle, or License Server is specified, the Dionex Chromatography Management System can be operated in ➢*Demo Mode*, only.

For information on how to install the License Server, see **Installation Instructions for Different Devices** **Installing the License Server**

For further information, see **Installation** **Software Protection** and **How to ...: Actions in the Server Configuration** **Selecting the Copy Protection Location and Entering the Key Code**.

LIMS

LIMS is the abbreviation for **Laboratory Information Management System**. LIMS receives electronic tasks, ensures that they are processed, and makes the results available in a defined format.

In the chromatography system, this can mean that the samples to be analyzed are read via bar code, before the samples are included in a sequence and are processed one after another. The results are saved in a default format (e.g. AIA). The sequence is generated by the data system if the required information is supplied in a defined format.

In the Dionex Chromatography Management System, reading this type of data is via the defined format of a ➢*Worklist*.

Lock Baseline

By activating this parameter, it is possible to keep the baseline on the prescribed level.

Also, see ⇒*Lock Baseline*

For information on how to apply detection parameters, see **How to ...: Actions in the QNT Editor** **Modifying Detection Parameters**.

Log

The **Log** command allows you to document the values of variables in the Audit Trail at any time. This option is especially useful to log information that is not periodically retrieved.

The command is also available directly in the **Command** dialog box of the **Control** menu.

Also, see ⇒*Log*

Logon

The **Logon** dialog ensures access to the respective program. Access is permitted for authorized users only who are identified via a ➢*Password* in the logon dialog.

In the Dionex Chromatography Management System, access to the ➢*CmUser* program is always via the logon dialog. Opening a Dionex Chromatography Management System client requires a logon with a password only if the ➢*User Mode* is enabled.

Loop Volume

Loop Volume is the sample loop volume obtained from the value entered in the Plumbing Configuration screen on the AS50 ➢*Autosampler* front control panel.

Low-Pressure Gradient System

In low-pressure gradient systems, the same pump delivers all partial flows.

Simple systems generate the required solvent mixing ratio in the mixing chamber. Then, the mixture is sucked from the chamber and carried to the column. The solvent composition is controlled via different valve closing times in the feed lines of the individual components. As the mixing chamber volume represents a dead volume, producing the correct mixing ratio on the column is delayed.

Systems that are more complex mix the individual partial flow during the suction period in the piston. This requires the calculation of how much volume can be sucked (the value is not constant as delivery is not always against the same external pressure, i.e. small volumes are pumped if the external pressure is high, larger volumes are delivered if the external pressure is low). Also, it is necessary to calculate the time of how long each valve must be opened for the individual partial flows to reach the exact mixing ratio.

Despite these mechanical and electronic procedures, the gradient profile produced by low-pressure gradient systems is less precise than ➢*High-Pressure Gradient Systems*, however, it is the less expensive alternative.

⚠ ***Caution***: Due to solvent compressibility and differing dead volumes, the chromatographic conditions of high-pressure and low-pressure gradient systems are not interchangeable.

Manipulations

Minor changes during the integration of single chromatograms are called **Manipulations**. For information on how to perform manipulations, see: **How to ...: Actions in the Chromatogram** **Manual Re-Integration**. The **Save Manipulations** and **Delete Manipulations** commands of the **Edit** menu allow accepting or rejecting these manipulations.

Mark

The **Mark** command sends a positive pulse to the detector's analog output as an event marker. The pulse is 10% of the full-scale analog output. A mark is typically used to indicate a sample injection.

Mass Defect

The mass defect is the difference between the calculated mass and the nominal mass (integer). Summing the masses of all the components of the compound uses calculated mass. The masses of the elements come from the periodic table, with the mass of ^{12}C being exactly 12.0000000 amu. Most of the other elements have masses close to their nominal elemental mass (the difference between the integer and the actual mass is the mass defect):

^{1}H 1.007825 amu

^{12}C 12.00000 amu

^{13}C 13.00335 amu

^{14}N 14.00307 amu

^{16}O 15.99940 amu

^{19}F 18.99840 amu

So, when you want the mass of a compound you can calculate as follows:

Formula	Nominal Mass [amu]	Actual Mass [amu]	Defect [amu]
$C_5H_{10}O_5$	5(12) + 10(1) + 5(16) = 150	5(12.00) + 10 (1.008) + 5(15.999) = 150.075	0.075
$C_{50}H_{102}$	50(12) + 102(1) = 702	5(12.00) + 102(1.008) = 702.8	0.8

Therefore, as you get to larger compounds with more atoms in it, you will sum all the "defects" of the individual atoms together and the difference can get to be substantial, especially if you display the mass as an integer. In the examples above, the first would be displayed as an integer 150 amu either way. In the second example, the actual mass in integer format would be 703 amu that is a whole mass unit from the nominal mass of 702 amu.

If you have organic compounds with nitrogens and hydrogens in them and the only other element is carbon you end up with a positive mass defect. Since many hydrocarbon compounds have a lot of hydrogen, it can be a very large defect.

If you have in addition a substantial amount of oxygen, its negative mass defect can offset the nitrogen and hydrogen and the mass defect will not be as large. That is why the user sets the type and magnitude of the mass defect depending upon what kind or class of compounds he is working with. The

correction for mass defect is generally set as x mmu per 100 amu where mmu is **m**illi**m**ass **u**nit or one thousandth of a mass unit.

So if the correction is set to **100 mmu/100 amu** (it is usually set from 30 to 120 mmu/100 amu) the correction for the examples above would be:

Correction Factor [amu]	Corrected Mass [amu]	In Integer Format
150 (0,100/100) = 0.15	150.075 - 0.15 = 149.925	150 amu
702 (0,100/100) = 0.7	702.8 - 0.7 = 702.1	702 amu

Thus, the correction factor just works to "modify" the data so that people used to working with integer masses for their elements in a compound end up with what they expected.

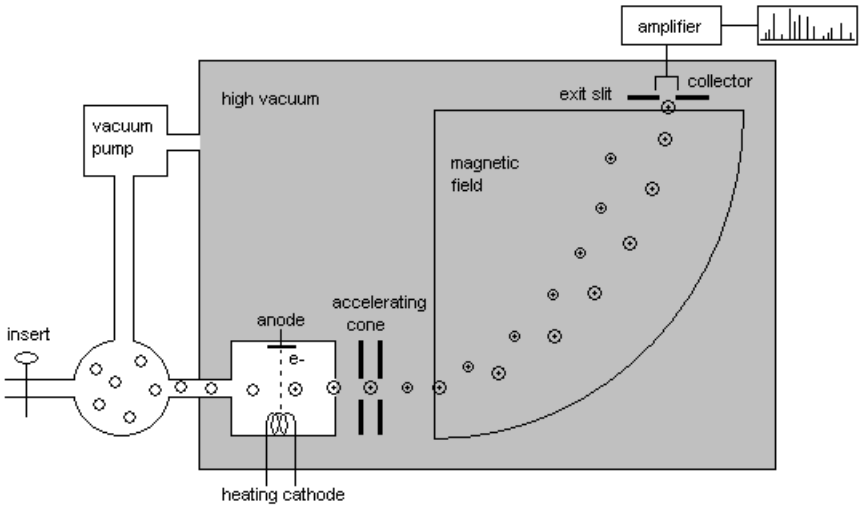
Mass Spectrometer

Mass spectrometer were originally developed as stand-alone instrumentation to analyze the structure of unknown, mostly organic compounds. In combination with chromatographic separation procedures, however, they also allow the qualitative and quantitative analysis of complex mixtures of substances. While the GC/MS coupling has long been part of the standard equipment in analytical laboratories, HPLC-MS is not yet that widely spread because of its problematic coupling. However, acceptance is steadily growing as the HPLC/MS coupling has been decisively enhanced during the past years. Besides, with the MS Detector another detector allowing qualitative statements on individual substances of a chromatogram is available in addition to the ➢*Photodiode Array Detector*

Mass spectrometry includes four steps:

- Sample loading (neutral molecules)
- Ionization of individual molecules
- Ion separation according to their masses
- Ion registration in form of a ➢*Mass Spectrum*

Different processes can be used for ionizing and separating ions with different masses. The following image illustrates ionization by means of an electron impact and the subsequent mass separation by means of a vertical magnetic field:



The ions that are created via the electron impact are first accelerated by means of the cones and then separated according to their mass in the magnetic field. Due to the varying intensity of the magnetic field (or the accelerating voltage), ions of different masses are directed through the exit slit into the collector and registered. In this way, mass spectrometers perform a mass scan similar to the wavelength scanning of many photodiode array detectors.

For information on how to record and process MS Data with the Dionex Chromatography Management System, see

How to ...: Actions Related to the aQa-MS.

Mass Spectrum

An MS detector (➢*Mass Spectrometer*) allows recording of a mass spectrum at any time t of a chromatogram. The two-dimensional view of a chromatogram (retention time and intensity) is extended by a third dimension (mass). In addition to the information on retention time *(t)* and intensity *(I)* information, each of the recorded data points also includes information on the masses *(m)* detected in the mass spectrometer.

Mass spectra usually include a great number of narrow peaks. To distinguish them from the comparatively wide chromatogram peaks they are called mass peaks.

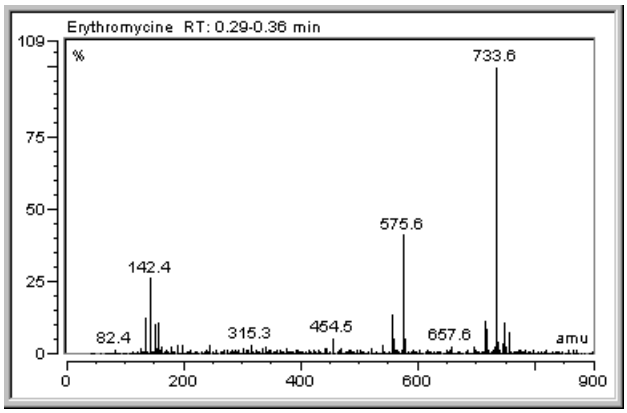
The Dionex Chromatography Management System allows viewing in the report the mass spectrum of a peak or the mass spectrum at any time of the chromatogram. During data acquisition, you can view the current mass spectrum in the control panel.

In addition, you may aggregate single mass spectra, thus, enhancing their ➢*Signal to Noise Ratio* (see **How to ...: Actions in the QNT Editor** **Processing Mass Spectra**).

To view recorded mass spectra in the Mass Spectra Plot press the

button on the **Method** toolbar.

Mass spectra are generally represented via their relative intensities. The base peak, i.e., the mass peak with highest intensity, is used as reference point. Thus, its relative intensity is always 100 %.



The base peak in the above example is the mass peak at 733.6 amu. The time when the mass spectrum was recorded is indicated as well. The mass spectra in the example were aggregated to the displayed total mass spectrum between 0.29 and 0.35 min.

Mass Trace

Contrary to original ➢*TIC* or ➢*SIM* chromatograms that are recorded during data acquisition, a mass trace is a MS chromatogram for a specific mass area. Mass traces can be extracted from a ➢*Mass Spectrum* and saved as a new channel. This is possible online during data acquisition but can be done later as well.

Also, see **How to ...: Actions Related to the aQa-MS**

Extracting Mass Traces Online

Extracting Mass Traces Afterwards

Defining the Number of MS Channels.

Match Criterion

The match criterion defines the mathematical method of comparison for the curve shape (= standardized (!) spectra).

Also, see ⇒*Match Criterion*

Match Factor

The match factor is an indicator of the similarity between two chromatograms. It varies from 0 (=no match) to 1000 (=perfect match).

The match factor is calculated as soon as two spectra are compared with each other in a spectra search (**Library Search** command or on the **Spectra Library Screening** tab of the ⇒*QNT Editor*). This command is possible in windows or partial methods capable of displaying a spectrum (see: **Spectra Library** and **PPA: Peak Purity Analysis**). The displayed spectrum is used as the basis. It is calculated by averaging all spectra recorded for one peak.

The result of the spectra search is the **Hit List**. It lists all spectra that have a certain similarity with the original spectrum. The match value in the **Match** column indicates how much they correspond.

Note: Within the method PPA, the match can be indicated as a curve. Please note that instead of determining the similarity of two independent spectra, the spectra of the same peak (at different wavelengths) are compared with each other here (see ➢*Peak Purity Match Factor*)!

Matrix Blank Sample

The sample matrix can considerably influence the sample analysis. To consider this, the matrix of the standard samples should be the same or at least similar. In addition, matrix blank samples can be used to filter out the influence of the sample matrix in the individual samples.

Select the sample type **Matrix** for the respective blank sample. Matrix blank samples are marked by the symbol  . The different peak areas (or peak heights, if these were used for quantification) are determined for this sample as well. The Dionex Chromatography Management System automatically subtracts the peak areas (or peak heights) of the matrix blank sample from the corresponding peak areas (peak heights) of all sequence samples. The resulting areas (heights) are then used for all further calculations (e.g. for the calibration).

 ***Note***: Thus, matrix blank values are treated differently from "normal" ➢*Blank Run Samples* for which the chromatogram is subtracted point by point from that of the current sample.

If more than one matrix blank sample was recorded in the sequence, the respective peak areas (peak heights) are averaged and the resulting value is subtracted from the corresponding peak areas (peak heights) of the other samples.

 ***Tip***: Matrix blank samples are subtracted only if they are evaluated in the same QNT method. Otherwise, they will not be taken into account.

Maximum Area Reject

The **Maximum Area Reject** parameter defines the maximum peak area up to which a peak is rejected. Peaks with a peak area below the defined value are not identified.

Also, see ⇒*Maximum Area Reject*

For detailed information on how to use the detection parameters, see **How to ...: Actions in the QNT Editor**  **Defining Detection Parameters**

Maximum Height Reject

The **Maximum Height Reject** parameter defines the maximum peak height up to which a peak is rejected. Peaks with a peak height below the defined value are not identified. (Determination of the height is always relatively to the baseline).

Also, see ⇒*Maximum Height Reject*

Maximum Peak Height *(MaxHght)*

Positive peak identification is via the ⇒*Minimum Height* parameter. *All* peaks above this height value are identified.

Also, see ⇒*Maximum Height Reject*

Maximum Rider Ratio

If one or several peaks (h1 to h4) is above the ➢*Rider Threshold* in a series of non-resolved peaks, the Dionex Chromatography Management System determines via the **Maximum Rider Ratio** detection parameter whether it is classified as a peak or a ➢*Rider*.

Caution: The ⇒*Peak Type* peak table classification criterion has priority! The criterion indicated here is valid for Peak Type = AUTO only!

Also, see ⇒*Maximum Rider Ratio*

Maximum Width

The **Maximum Width** detection parameter defines the maximum width above which peaks are ignored during peak detection.

Also, see ⇒*Maximum Width*

For detailed information on how to use the detection parameters, see **How to ...: Actions in the QNT Editor Modifying Detection Parameters**.

Message

The Message command allows the user to enter reminders for things to do or to consider when executing a ➢*Program*. The message is then displayed on the screen. The user must confirm the message by clicking **OK** before the program is continued.

Also, see ⇒*Message*

Minimum Area

The **Minimum Area** detection parameter is used as a minimum criterion determining the area threshold, below which peaks are ignored during peak detection or integration.

Also, see ⇒*Minimum Area*

For detailed information on how to use the detection parameters, see **How to ...: Actions in the QNT Editor** **Modifying Detection Parameters**.

Minimum Height

The **Minimum Height** detection parameter is used as a height threshold, below which peaks are ignored. The peak height is measured relative to the baseline (a).

Also, see ⇒*Minimum Height*

For detailed information on how to use the detection parameters, see **How to ...: Actions in the QNT Editor** **Modifying Detection Parameters**.

Minimum Width

The **Minimum Width** detection parameter is used as a minimum criterion, defining the minimum width, below which peaks are ignored during peak detection.

Also, see ⇒*Minimum Width*

For detailed information on how to use the detection parameters, see **How to ...: Actions in the QNT Editor** **Modifying Detection Parameters**.

Mix (AS50 Sample Prep Command)

The **Mix** ➢*Sample Prep Command* mixes the contents of a vial by repeatedly drawing and expelling a volume of the vial contents. **Vial** is the vial to be mixed. **Volume** is the amount of the vial contents to draw and expel, and **Cycles** is the number of times to draw and expel the specified volume.

Modem Cable (1:1 RS Cable)

Modem cables are frequently used standard cables for connecting instruments to a PC. The cable assignment is as follows (Also, see: ➢*Pin Assignment*):

Instrument			PC	
9-pin male connector	25-pin male connector		25-pin female connector	9-pin female connector
2	3	----------	3	2
3	2	----------	2	3
5	7	----------	7	5
If there is an additional hardware handshake, the following assignments are also required:				
7	4	----------	4	7
8	5	----------	5	8

Modem cables are also called 1:1-RS cables.

Dionex part number 8914.014: (25-pin - 9-pin, 5m)

8914.0128: (25-pin - 25-pin, 5m)

☞ ***Tip***: Do not confuse non-crossover modem cables (= 1:1 RS cables) with crossover ➢*Null Modem Cables*!

For information on additional or other connections, refer to the installation instructions for the respective instrument for details (Also, see: **Installing and Controlling Third-Party Instruments**).

Moduleware

The instrument control firmware installed on all modules connected to the ➢*DX-LAN*. Moduleware sends status information and data to the Dionex

Chromatography Management System and receives control parameters from the Dionex Chromatography Management System.

"Monitor Only" Mode

If a user establishes a connection to the local server via a control panel, the user can control the instruments connected to a ➢*Timebase* via the controls on the control panel (control mode).

If a second user accesses the same timebase, this user only receives the **monitor only** status. In this case, the control panel displays all current values and states, but changing any values, e.g. the flow rate, is not possible. This prevents several users from simultaneously controlling the same timebase. If one user accesses a timebase on the network, the **monitor only** status is assigned.

Changing from Monitor Mode to Control Mode

Changing between the two modes is by activating or deactivating the function **Monitor Only** in the **Control** menu. If the user A takes over the control of the local timebase B, user B is automatically assigned the **monitor only** status.

Organizing Access Options

If the ➢*User Mode* feature is activated, the privileges assigned to a user define, whether this user has the monitor only status, control access or whether changing between the two modes is possible.

If access control is disabled, each user has all privileges at all times. Objects that are members of an ➢*Access Group* will not be visible.

Independently of this, access can be generally limited directly on the server or on the timebase. Only if monitoring and/or controlling a server or a timebase is explicitly enabled in the ➢*Server Configuration* program, individual users have control and/or monitoring access (via the network). This does not apply to users accessing their own local servers.

Move to Background

Use the **Move to Background** function to move a selected object to the background.

Move to Front

Use the function **Move to Front** to move a selected object to the foreground.

Multi-Tasking

Multitasking refers to simultaneous operations of several programs on a PC. Unlike earlier Windows versions (3.1; 3.11), allocation of processing time under Windows 98 and Windows NT/2000 is no longer between programs (cooperative), but is monitored and controlled externally (preemptive). This guarantees that each application (process) is automatically continued after a specific time. A single process cannot claim the entire processing time at the expense of other processes.

Caution: The key combination **Alt-Ctrl-Del** interrupts Multitasking in Windows 98. All running processes are stopped. The device control of the Dionex Chromatography Management System is interrupted. **Do not use the key combination Alt-Ctrl-Del in Windows 98 during a running batch or during data acquisition. Otherwise, data overrun and communication problems with the controlled instruments will result.** This does not apply to the operating system Windows NT.

Multi-Threading

Multi-threading allows simultaneous execution of two or more application parts as separate processes.

If, for example, many control commands are communicated simultaneously to a chromatography system, a certain amount of time is required for this. Before, it was not possible to continue work during this time, regardless of whether the operation took a split second or longer.

Multi-threading allows simultaneous execution of this type of operation (**Threads**). This is possible because each operation is internally separated into many small steps that are executed with a time lag, without being noticed by the user.

Thus, the user can perform other tasks, e.g. manually re-integrating a chromatogram despite the comprehensive communication of control commands.

Name

The user enters the **Name** for the substance in the peak table. The name is available as peak result variable.

Needle

The **NeedleUp** command allows lifting the sample needle. Then the internal sample valve is switched (see the example for a load/inject process in the ➢*Autosampler* section).

Also, see ⇒*NeedleUp*

Needle Height (AS50 Sample Prep Command)

The **Needle Height** ➢*Sample Prep Command* positions the tip of the needle at the specified height (in mm) above the bottom of the vial. A value of 0 is closest to the bottom of the vial; a value of 46 is closest to the top. This height is used for subsequent sample preparation steps (mixing, pipetting, and dispensing) until another Needle Height command is given.

☞ ***Tip***: The Needle Height value is not used for sample injections. Instead, the ➢*Sample Needle Height* command determines the position of the needle at injection.

Network Failure Protection

Often it is useful to store important data on central data server PCs. In case the network connection is interrupted or the central data server PC crashes, data acquisition should continue, nevertheless. For this purpose, all data that are relevant for the server of the Dionex Chromatography Management System are stored locally on the server's hard disc. If the network connection is interrupted,

the ➢*Server* will continue to process these sequences, nevertheless. Therefore, all data that may be relevant for the server must be mirrored locally before the sequence is started.

An interruption of the network connection is logged in the Audit Trail (**Protocol Data**). The server continues to process the ➢*Batch* using the last conditions. All data are saved locally. The mirrored data are filed in the TEMP directory of Windows the position of which can be influenced by the environment variables **TMP** or **TEMP**. However, ensure that a local drive is used. A network share or a RAM disc is unsuitable. Thus, they would ruin the actual object and aim of such a protection.

In order to ensure that Windows and all other applications work properly after the network recovery we recommend rebooting your PC. With the restart, the locally saved data are automatically written back to the network datasource. Again, this is logged in the audit trail.

In addition to the network-failure protection, a ➢*Power-Failure Protection* is available.

***Tip**:* The network-failure protection is available for **Windows NT and Windows 2000 only**! It is disabled on Windows 98 because these systems are unstable under network failure conditions.

If there is a network failure while ACCESS databases are accessed, the datasource (mdb file) of the Dionex Chromatography Management System could be damaged. Therefore, we recommend using MS SQL or ORACLE servers as central database to protect your data even in case of a network failure.

Also, see **How to ...: Actions in the Browser Network Failure / Non-Availability**

Nice Size

Use the function **Nice Size** to optimize the size of one or more controls. The ➢*Control Frame* is adjusted so that the ➢*Control* including the caption is just visible.

(Signal) **Noise**

The **Signal Noise** parameter indicates the signal noise within a chromatogram calculated by the Dionex Chromatography Management System. The value

serves as the basis for the ➢*Signal to Noise Ratio* determined from the raw data at the start of the data acquisition.

Determining the Signal Noise (according to the default)

All datapoints recorded during the first 10 seconds of a chromatogram form the basis for determining the noise value. The Dionex Chromatography Management System calculates a regression line using the method of least squares, then determines the maximum distance of two datapoints above *and* below the line. (When calculating the regression line, all datapoints are weighted with their corresponding step unless the step is equidistant.) Adding both values supplies the first noise value.

The same procedure is used for the last 10 seconds of a chromatogram; it supplies a further noise value.

The lower value is given under **Noise** and used as ➢*Sensitivity*.

Signal Noise in User-defined Range (Input of Parameters)

You can also determine the signal noise for a specific range of the chromatogram. Select a range without any peaks in the window **Report Properties Column** (after double-clicking the column to edit or the window **Add Report Column** via **Add** from the **Table** menu). Select the **Signal Noise** variable of the **Chromatogram** Category. Open the **Parameter Input for "Signal Noise"** via the **Parameter** button and enter the desired range under **Specific Range**.

⚠ ***Caution***: To define the **determination**, **identification**, and **detection** limit via the signal to noise ratio, the noise of the user-defined range must always be used! If not, the determination, identification, and detection limits might be miscalculated.

Normalization (Overview)

In the linear range, the height of a spectrum recorded at the time t is always proportional to the current substance concentration in the flow cell. An objective comparison of two spectra is therefore only possible if the concentration is identical.

As this condition is rarely fulfilled, and as it is not possible to convert a spectrum recorded at a specific concentration to another concentration, the height of one spectrum must be scaled to the height of the other. This is called normalization. The following factors must be considered:

- The base area portion must be considered - especially in trace analysis (see ➢*Baseline Correction*).
- The noise portion depends on the wavelength and the solvent. Thus, at 200nm, not only the lamp energy of a deuterium lamp is considerably lower than at 250nm, but also the absorption of common solvents is especially high.
- Normalization should be performed where little influence on the above factors is expected and where a relative absorption maximum of the substances to be compared is observed.

Normalization can therefore be performed by the ➢*Absolute Maximum*, by the ➢*Relative Maximum* or by a fixed ➢*Wavelength*.

***Note**:* Chromatograms and peaks can also be compared. They are referred to as normalized chromatograms, areas, or amounts.

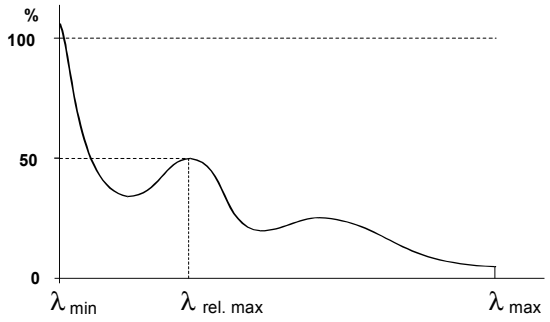
Normalization (Absolute Maximum)

The absolute maximum of the spectrum is determined. The absorption maximum is chosen as reference point and it receives the absolute height **1** (=100%).

Also, see ➢*Normalization (Overview)*

Normalization (Relative Maximum)

The relative maximum of the spectrum is determined. This will be the greatest λ-peak of the spectrum. After normalization, this peak has the height **0.5** (50%). This prevents normalization with incomplete maxima on spectrum margins.



☞ ***Tip***: Note that spectrum maxima can exceed the 100% line on the margin of the spectrum, due to the definition!

Also, see ➢*Normalization (Overview)*

Normalization (Fixed Wavelength)

Normalization with a fixed wavelength is analogous to normalization at a relative maximum.

Instead of the relative maximum, the user can choose the wavelength of the absorption value, which seems suited best for normalization.

☞ ***Tips***: Note that spectrum maxima on the margin of the spectrum can exceed 100%, due to the definition!

If you use the wavelength of the absolute maximum for the normalization, it is possible that this wavelength is on the margin of the spectrum. Often, this will be on a flank. On flanks, wavelength fluctuations will have stronger effects, so that the results there are somewhat less precise. This is especially true for detectors that have an optical bandwidth higher than 5nm.

Also, see ➢*Normalization (Overview)*

Null Modem Cable (RS232)

Null modem cables are frequently used (crossover) standard cables for connecting instruments to the PC. The cable assignment is as follows: (Also, see ➢*Pin Assignment*):

Instrument			**PC**	
9-pin female connector	25-pin female connector		25-pin female connector	9-pin female connector
2	3	----------	2	3
3	2	----------	3	2
5	7	----------	7	5

If there is an additional hardware handshake, the following assignments are also required:

4	7	----------	6	6
6	6	----------	7	4

7	4	----------	5	8
8	5	----------	4	7

Tip: Do not confuse crossover null modem cables with non-crossover ➢*Modem Cables* (1:1 RS cables)!

To order null modem cables from Dionex, use the following part numbers:

9-pin to 9-pin:

- Dionex part no. 8914.0129 for RS cable RU, 2.5m
- Dionex part no. 8914.0130 for RS cable RU, 5m
- Dionex part no. 8914.0131 for RS cable RU, 10m

25-pin - 9-pin:

- Dionex part no. 8914.0103A for RS cable RU, 2.5m
- Dionex part no. 8914.0120 for RS cable RU, 5m
- Dionex part no. 8914.0121 for RS cable RU, 10m

If necessary, use an adapter to connect the cable to a 25-pin socket. These null modem cables have been slightly modified to ensure data transmission even with enabled hardware handshake. However, the above hardware handshake is not realized.

For information on additional or other connections, refer to the installation instructions for the respective instrument for details (Also, see: **Installing and Controlling Third-Party Instruments**).

Number (No.)

The **Number** variable is the successive number assigned to a peak during peak detection. The peak number can be output as peak result variable.

If the values in this column are not successive but contain gaps, the missing peaks fell victim to one of the inhibition criteria, e.g. **Relative Area Threshold** or **Report Unidentified Peaks = OFF**.

Number of Calibration Points

The **Number of Calibration Points** calibration variable gives the number of values that are used for the calibration.

The ➢*Number of Disabled Calibration Points* can be displayed separately.

Number of Disabled Calibration Points

The **Number of disabled calibration points** calibration variable indicates the number of values that were not considered in the calibration.

The ➢*Number of Calibration Points* can be displayed separately.

ODBC (Open DataBase Connectivity)

ODBC is the name of a standard database interface that allows accessing various databases (e.g. SQL server, dBASE or ORACLE) via an ODBC driver.

Offset

Signals or chromatograms with an assigned offset value (in %) are offset vertically by this value in percent of the window size. Valid entries are from 0 to 50.

Offset (c0)

The **Offset (c0)** calibration variable gives the offset value of the used ➢*Calibration Function*.

As a y intercept is available for the **Linear with Offset** (= LOff), **Quadratic with Offset** (= QOff), and **Exponential** (= Exp) functions only, no output is possible for the **Linear** (= Lin) and **Quadratic** (= Quad) functions.

Offset Level

The **Offset Level** command (also called zero position) offsets the detector's analog output signal as a percentage of the full-scale voltage. Offsetting the output allows an attached recording device to plot the signal if it becomes negative.

Offset Volume

The ➢*Eluent Generator* **Offset Volume** option specifies the loop volume between the pump outlet and the injection valve. Because the EG40 is located between the pump and the injection valve, the eluent concentration gradient produced by the EG40 reaches the column more quickly than the ➢*%-Gradient* produced by the pump. The Dionex Chromatography Management System uses the offset volume to calculate a time delay in starting the EG40. The delay synchronizes EG40 and gradient pump operation.

The default offset volume of 400 µL is used for most systems. The actual offset volume may be different, however, depending on the system configuration. To change the value, start the ➢*Server Configuration* program and double-click the pump entry in the list of devices for the ➢*Timebase*. The pump's configuration properties open. Select the **Eluent Generator** tab.

The offset volume has no effect during isocratic operation and can be set to 0.00 µL.

Online Help

The **Online Help** of the Dionex Chromatography Management System offers help information in any situation on the screen.

- Press the **Help** button on the toolbar to view **help information on a specific item on the screen**.
- Press the F1 key to see **context-sensitive help information for a specific situation**. A description of the selected menu bar, (tab) dialog box, or the activated control will appear.
- Select **Index** in the **Help** menu to view **the table of contents of Online Help**. Select **Using Help** to see more details on working with Online Help.

Operational Qualification (OQ)

According to the definition formulated together with EUROACHEM Operational Qualification is "the process of demonstrating that an instrument will function according to its operational specification in the selected environment" [P. Bedson and M. Sargent, Accred. Qual. Assur. (1996) 1, 265-274]

The purpose of OQ is to prove and document that your analytical system functions according to its operating specification while your specific environmental conditions are taken into account. Normally OQ is performed following the installation of new devices or following a repair or system service.

The **Qualification** menu that is available in the Browser of the Dionex Chromatography Management System offers the menu items **Instruments OQ** *OQ Setup* (for details, see OQ Setup in the Online Help). Select **Instruments OQ** to perform the operational qualification. Select **OQ Setup** to generate those templates required for performing the operational qualification. Normally this is only necessary after a new installation or when the configuration has been modified.

The individual report pages of the **Instrument OQ** correspond to the pages ➢*Performance Qualification* for instruments. However, the limits valid for OQ are stricter than those that are used for PQ.

It is also possible to check the Operational Qualification of the Dionex Chromatography Management System. Select **CHROMELEON OQ** in the **Qualification** menu.

Tip: For further details regarding the Operational Qualification please refer to the Operation Manual **Operational Qualification / Performance Qualification** that can be ordered from your Dionex Service.

Optical Resolution (Spectral Resolution)

The difference between two detectable wavelengths [in nm] that can only just be separated is referred to as optical resolution of a photodiode array detector. It is determined by two factors:

- ➢*Photodiode Resolution*
- Quality of grating required for spectral dispersion (**optical bandwidth**)

The values for the optical resolution of conventional detectors are approx. 2 - 6nm (Dionex Detector UVD340S: 1.9nm (UV range), Dionex PDA-100 Detector: 1.0nm).

Caution: The optical resolution is only one criterion for the quality of a detector. The combination of optical resolution and signal to noise ratio leads to a meaningful detector comparison. In this connection, it is also important that the ratio between the individual factors is balanced. This correlation becomes clear when taking the example of benzene in the 230 - 265nm range. A fine structure ("benzene finger") is only recognizable if the number of photodiodes, the imaging optics, and the ➢*Signal to Noise Ratio* are in a sensible performance relation to each other.

Optimum Integration Path

A chromatogram recorded at a fixed wavelength usually does not have an optimum ➢*Signal to Noise Ratio* for all included peaks. The selected wavelength represents a compromise that allows "seeing" all substances.

It would be ideal to detect Peak 1 at 230nm, peak 2 at 254nm, peak 3 at 320nm etc.

This is enabled by performing ➢*Wavelength Switches* (if the wavelength switch points are known) or recording a ➢*3D-Field* using the ➢*Photodiode Array Technology* with subsequent determination of the optimum integration path.

Definition

The optimum integration path is characterized by

- An optimized signal to noise ratio,
- Minimum overlay of neighboring peaks, and/or
- Optimum linearity.

This means that the integration path must pass through the absorption maximum of a peak, without being influenced by another peak. As the precision of the recording is greater in relative maxima and minima than in steep spectra flanks (this is especially true for large optical bandwidths of a detector), selecting the largest *relative absorption maximum* is recommended, and not the absolute maximum. In addition, the absolute maximum of UV spectra is frequently located in the low UV range, i.e. near 200nm. In this range, the sensitivity of the detector usually decreases, while interferences such as solvent absorption or humidity increase.

When dealing with large substance quantities, as in preparative chemistry, total absorption should be below 2 AU. For optimum precision, select a *relative spectra extremum* for the recording.

If the complete chromatographic separation of two peaks is not possible, it makes sense to record each channel at a point where the other peak has its absorption minimum, or ideally, is inhibited entirely.

Implementation

The Dionex Chromatography Management System automatically calculates the course of the optimum integration path and can display the path in the ➢*3D-Field*. The transition between two wavelengths is exactly between the peak end of one and the peak start of the other peak. For neighboring peaks, the peak end, peak start, and switch time therefore coincide.

The result, i.e., the switch times at which the **Wavelength** signal parameter is changed, can be included in a ➢*Program* via the command: **Extract: Opt.Int.Path to clipboard**.

For details, see **How to ...: Actions in the Peak Purity Analysis (PPA) window Selecting the Optimum Integration Path**.

OQ

See ➢*Operational Qualification (OQ)*

Origin

See **How to ...: Actions in the QNT Editor** **Selecting the Calibration Function** in the **Creating a Peak Table** section.

Original Size

See ➢*Full Size*

Overlay

An **Overlay** is a chromatogram that is displayed in addition to the current chromatogram, i.e., it overlays the current chromatogram. Overlays are often used to compare chromatograms. For chromatogram comparison several chromatograms can be overlaid at several positions in the Dionex Chromatography Management System:

Control Panel

Overlaying chromatograms is possible already during data acquisition. During data acquisition, the **Chromatogram Overlay** command that is available in the context menu of an online signal plot of a ➢*Control Panel* allows displaying a chromatogram that was acquired earlier in addition to the currently recorded channels.

QNT Editor and Report

The **Add Overlay** command of the **File** menu in the **Report** or in the ⇒*QNT Editor* allows overlaying any chromatograms after data acquisition.

Printer Layout

In the printout, too, you can plot overlaid chromatograms using the **Overlay** tab of the **Chromatogram Decoration** (to be accessible via the **Chromatogram Properties** command in the context menu of a chromatogram) in the ➢*Printer Layout*. In each plot, the comparison chromatogram can be taken from an already processed sample of the current sequence or any other sequence.

Also, see **Performing a Chromatogram Comparison**

Overview Window

When zooming, an overview window is displayed in the upper right corner of the signal plot. The overview window shows the entire chromatogram and indicates the currently enlarged section.

P-Groups

See ➢*Privilege*

PAL Plug-In Board

A PAL is a PC plug-in board that is placed on another board such as the ➢*A/D Converter* or the pump control board or is inserted in the PC as a separate board.

As the ➢*Dongle*, the PAL plug-in board serves to store the serial number of a station of the Dionex Chromatography Management System. Each station has its own serial number.

Only if the serial number of the PAL plug-in board or the dongle and the ➢*Key Code* stored in the Dionex Chromatography Management System match, can the Dionex Chromatography Management System be operated correctly.

If neither PAL, nor dongle nor license server is specified, the Dionex Chromatography Management System can only be operated in the demo mode.

For further details, see **Installation Software Protection** and **How to ...: Actions in the Server Configuration Selecting the Copy Protection Location and Entering the Key Code**.

Panel

See ➢*Control Panel*

Partial Flows

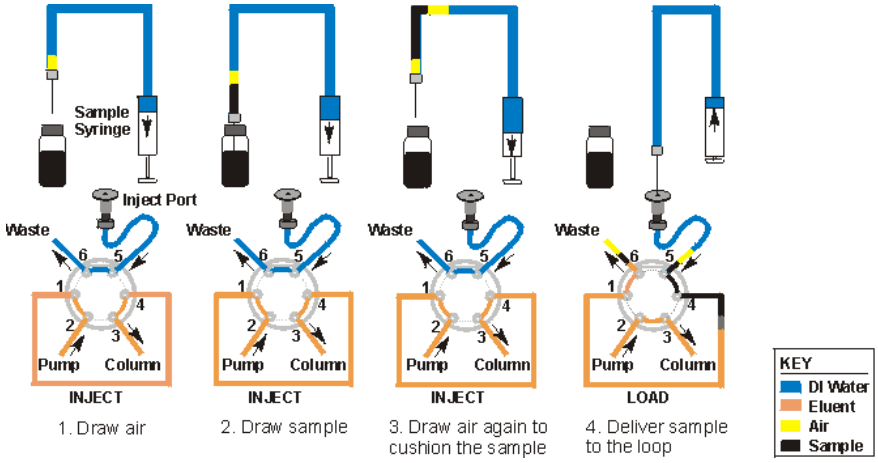
See ➢*%B, %C, %D*

Partial-Loop Injections (AS50 Autosampler)

When performing a partial-loop injection, the AS50 autosampler draws from the sample vial the volume to be injected, plus two times the ➢*Cut Volume*.

Tip: Partial-loop injections are possible only when the injection valve is installed in the autosampler compartment or in a chromatography or thermal compartment. If the injection valve is installed externally (for example in a DX-120), only full-loop injections can be performed.

Partial-Loop Injection Sequence

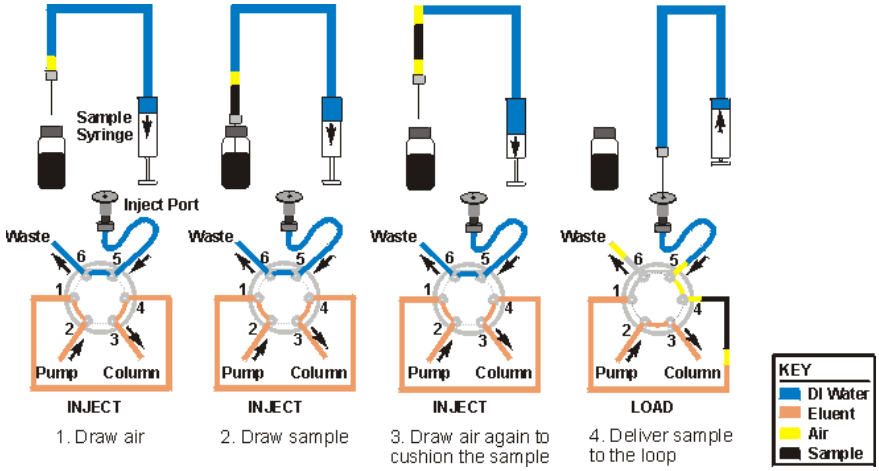


Partial-Loop, Limited-Sample Injections (AS50 Autosampler)

When performing a partial-loop, limited-sample injection, the AS50 autosampler draws from the sample vial only the volume to be injected.

Tip: Partial-loop, limited-sample injections are possible only when the injection valve is installed in the autosampler compartment or in a chromatography or thermal compartment. If the injection valve is installed externally (for example in a DX-120), only full-loop injections can be performed.

Partial-Loop, Limited-Sample Injection Sequence



Password

Passwords protect the access to specific software or areas thereof. The Dionex Chromatography Management System requires passwords in different situations:

Opening the ➢*CmUser* program always requires a password. The administrator allocates a password upon creation of the user database.

With enabled ➢*User Mode*, the client of the Dionex Chromatography Management System can only be opened upon input of the correct password. The administrator allocates each user an individual password in the CmUser program. However, having entered the currently valid password, the user can change this password later.

Signing sequences electronically (see: ➢*Electronic Signature*) requires a password as well. Each user has his/her own password that allows transmitting, checking, and approving the signature according to his/her privileges. This password, too, is allocated by the administrator in the CmUser program and can be changed later by the user. Signing sequence electronically is possible with enabled User Mode only.

Peak Group Start / Peak Group End

The two detection parameters **Peak Group Start** and **Peak Group End** allow identification of several successive peaks as one peak group. A peak group that has been defined in such a way is treated as one single peak.

Also, see ⇒*Peak Group Start/End*

For information on how to apply detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Peak Name

The **Peak Name** peak table column in the ⇒*QNT Editor* is used to enter the name of the substance detected at the time t. The peak name can be indicated as separate peak variable in the report.

Also, see ⇒*Name (Peak Name)*

Peak Number (No.)

See ➢*Number (No.)*

Peak Purity

See the following topics:

➢*PPA (Peak Purity Analysis)*

➢*PPI (Peak Purity Index)*

➢*PPA Report*

Peak Purity End Wavelength (PPWlEnd)

In combination with the Peak Purity Start Wavelength detection parameter, **Peak Purity End Wavelength** limits the wavelength range for peak purity calculations.

Also, see ⇒*Peak Purity Start/End Wavelength*.

For information on how to apply detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Peak Purity Match Factor

The Match Factor expresses the similarity of two curves. A peak purity match factor can be expressed for both, UV spectra and mass spectra.

With UV spectra, the match factor (= UV match factor) refers to the correlation between the spectrum in the peak maximum and the spectra in the ascending and descending flanks. Ideally, none of the spectra between peak start and peak end deviates from the spectrum in the peak maximum. They correspond to 100%, i.e., the match value is 1000. For ➢*Mass Spectra*, the distance between the single masses and the relative height of the different mass peaks are taken into account. Similar to UV spectra, a match factor of 1000 indicates a perfect match. However, the MS match factor is far more selective than the UV match factor.

⚠ ***Caution***: The calculation of the match factor is more inaccurate on the peak margins due to the poorer ➢*Signal to Noise Ratio*. Using the ⇒*Peak Purity Threshold* detection parameter, the selection of the UV and mass spectra can be limited to a sensible peak height in the ⇒*QNT Editor*.

If the match factor of a peak is included in a report column, the value will be averaged from all determined match values of the peak. The UV match factor is always baseline-corrected (see ➢*Baseline Correction*), as this portion usually cannot be neglected; it would falsify the result.

With mass spectra, you may define in the QNT editor whether to subtract background mass spectra and which ones. This also defines whether the match factor shall be output baseline-corrected.

For details, see **How to …: Actions in the Chromatogram Subtracting MS Background Spectra**.

The deviation of the averaged single match values can be included in the ➢*PPA Report* as the ➢*Peak Purity: Relative Standard Deviation of the Match Factor (RSD Match)*.

Peak Purity: Relative Standard Deviation of the Match Factor (RSD Match)

The relative standard deviation of the ➢*Peak Purity Match Factor* indicates its homogeneity over the entire course of the peak.

Calculation is analogous to the ➢*Relative Standard Deviation of the PPI (RSD PPI)*. Instead of the PPI values, the corresponding match values are used. The relative standard deviation of the match factor (RSD Match) in percent results when the standard deviation is divided by the average of all match values (Match Ø), and the result is multiplied by 100%.

$$RSD\,(Match) = \frac{SD}{Match\ \varnothing} * 100\%$$

Peak Purity Start Wavelength (PPWlStart)

In combination with Peak Purity End Wavelength, the **Peak Purity Start Wavelength** detection parameter limits the wavelength range for the peak purity calculations.

Also, see ⇒*Peak Purity Start/End Wavelength*.

For information on how to apply detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Peak Purity Threshold (PPTrshold)

The **Peak Purity Threshold** detection parameter determines the threshold for the signal height above which spectra comparison is performed. The parameter is important for the Peak Purity Analysis (PPA) and the Peak Ratio.

Peak Purity Analysis (PPA)

In the PPA, the parameter defines the signal height above the baseline, from which the UV or ➢*Mass Spectra* are extracted for calculating the ➢*PPI (Peak Purity Index)* or the ➢*Peak Purity Match Factor*.

Peak Ratio

For the Peak Ratio, the **PPTrshold** parameter defines the signal height above which the ratio of two UV or MS channels shall be calculated.

Also, see ⇒*Peak Purity Threshold*

For information on how to apply detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Peak Shoulder Threshold

The **Peak Shoulder Threshold** parameter defines a threshold value for peak shoulder recognition.

Also, see ⇒*Peak Shoulder Threshold*

For detailed information on how to use the detection parameters, see **How to ...: Actions in the QNT Editor Defining Detection Parameters**.

Peak Slice

The **Peak Slice** detection parameter determines from which width (= time span) several successive data points are interpreted as peak or as noise.

Note: This parameter should always be considered in combination with the ⇒*Sensitivity*!

Also, see ⇒*Peak Slice*

For detailed information on how to use the detection parameters, see **How to ...: Actions in the QNT Editor Modifying Detection Parameters**.

Peak Start Time

This peak result variable refers to the peak start in minutes. The peak start is determined via the left peak delimiter.

Peak Stop Time

This peak result variable refers to the peak end in minutes. The peak end is determined via the right peak delimiter.

Peak Summary

A Peak Summary lists peak and sample variables of any required samples in a table. Generally, it includes samples of one sequence. A Summary can also be created based on a ➢*Query*.

For details, see

Peak Summary Report

Peak Table

The peak table is part of the ⇒*QNT Editor*. The QNT editor allows defining parameters for the identification and calibration of peaks.

For details, see

QNT Editor / Peak Table

Peak Type

See ➢*Type*

Peak Width

See ➢*Width*

Performance Qualification (PQ)

As defined in cooperation with EURACHEM, Performance Qualification is "the process of demonstrating that an instrument consistently performs according to a specification appropriate for its routine use" [P. Bedson and M. Sargent, Accred. Qual. Assur. (1996) 1, 265-274].

The task of PQ is both to ensure and to document that your system functions as required by your special (routine) operation. The frequency and the scope of the Performance Qualification depend on the special requirements in your laboratory. This can be specified in internal instructions or in a SOP. The parameters should be similar to the normal routine operation. In addition to the Performance Qualification the ➢*Operational Qualification* as well as the ➢*Installation Qualification* is an important factor for validating instruments and software.

The **Qualification** menu in the Browser of the Dionex Chromatography Management System offers the menu items **Instruments PQ** and *PQ Setup* (for details, see the PQ Setup in the Online Help). Select **Instruments PQ** to perform the performance qualification. Select **PQ Setup** to generate those templates required for performing the performance qualification. Normally this is only necessary after a new installation or when the configuration was modified.

The Dionex Chromatography Management System CD supplies a datasource with a master template in the directory PQ\Templates\PQ. This template is designed for the Performance Qualification in a standard HPLC configuration. In addition to various sequences, the template contains a PQ report template with the following sheets:

SPECIFICATION: The sheet **SPECIFICATION** allows you to enter the system specifications (instruments, fluidics, and limits).

INJ_REPRO_AND_RET_REPRO and **ASI_REPRO_AND_RET_REPRO**, respectively: The sheet **INJ_REPRO_AND_RET_REPRO** allows checking the reproducibility of the injector and the retention time. If the result is within the specified limits, the **Result** column indicates **OK**.

INJ_CARRY_OVER: The sheet **INJ_CARRY_OVER** supplies a measure for the carry over in your system. If the result is within the specified limits, the **Result** column indicates **OK**.

INJ_LINEARITY: The sheet **INJ_LINEARITY** supplies a measure for the linearity of injection volume and peak area.

PUMP_GRADIENT: The sheet **PUMP_GRADIENT** serves to check gradient precision. The limits of the **Specification** sheet are included. If the values are within the specified limits, the last column (**Result**) indicates **OK**. The **Result** column of all tests' then indicates **Test passed**.

PUMP_3_GRADIENT: The sheet **PUMP_3_GRADIENT** serves for checking the gradient reproducibility (with 3 repetitions in this example). The limits of the **Specification** sheet are included. If the values are within the specified limits, the last column (**Result**) indicates **OK**. The **Result of all tests** column then indicates **Test passed**.

DET_NOISE_AND_DRIFT: The sheet **DET_NOISE_AND_DRIFT** serves to check whether noise and drift in your system correspond to the limits on the **SPECIFICATION** sheet. If the values are within the specified limits, **OK** is indicated under **Results**.

DET_WAVELENGTH: The sheet **DET_WAVELENGTH** supplies a measure for the wavelength precision of the corresponding detector.

DET_LINEARITY: The sheet **DET_LINEARITY** serves for checking the detector linearity. From five different injections at different concentrations, the correlation coefficient (supplied in %) between the peak height and the concentration is determined. If the value is above the specified limit, **Test passed** is returned as the result.

RF_DET_NOISE and **RF_DET_WAVE**: These sheets evaluate the noise and the wavelength precision of the fluorescence detector.

Audit Trail: The sheet **Audit Trail** shows the protocol data (Audit Trail) for the analyzed sample.

Caution: **Do not edit report sheets**, even if editing is possible! The Dionex Chromatography Management System automatically reads the corresponding values. Within the report, individual data sheets are very often accessed via references. If you insert or delete lines and columns, these references will be lost. Thus, the calculations will be wrong!

The report **must** be printed as **Batch Report** from the browser to ensure that, in the report, the data are read in and processed correctly. Select the sequence for which the report shall be printed**. Make sure that no sample is selected**. Select **Batch Report** in the **File** menu and start printing by clicking **Ok**.

Tip: Enter the actual concentrations of the used standards in the amount columns of the QNT file for evaluating the detector linearity.

For further details on the Performance Qualification, see the Operating Manual **Operational Qualification / Performance Qualification** Operating Manual available from Dionex service.

PGM File

The PGM file (also called control file) can include up to three parts that correspond to the different views of the PGM editor:

- The actual ➢*Program* (**Commands** view in the PGM editor)
- The instruments method for the ➢*Mass Spectrometer* (**Finnigan AQA** view in the PGM editor - only with PGM files for a timebase including MS)
- Extractions and data smoothing steps that are performed after the data acquisition (**Post-acquisition steps** view in the PGM editor)

The **Program Wizard** allows easy creation of the PGM file (especially of the program). All user inputs are automatically converted into uniform command syntax so that it is readable by the data system. This allows even new users to quickly create functioning programs.

Having terminated the Program Wizard, the user needs to enter the mass spectrometer method and the **Post acquisition steps** on the corresponding pages of the PGM editor.

Photodiode Array Detector

A photodiode array detector is a special multi-channel ➢*UV Detector*. For further information, see

➢*Photodiode Array Detectors (Main Features)*

➢*Photodiode Array Detectors (Functionality)*

Highest optical resolution and at the same time high sensitivity are decisive factors for the quality of a photodiode array detector. For further information, please refer to ➢*Optical Resolution (Spectral Resolution)*.

Main Features

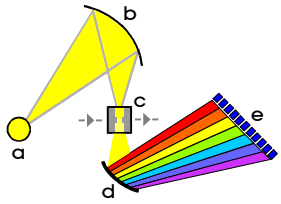
➢*Photodiode Array Detectors* (PDAs) feature high sensitivity and a large linearity range, they are relatively independent from temperature fluctuations, and can be used for gradient elution (%-gradient). The simultaneous detection of all wavelengths at the time t is made possible by:

- Peak Purity Analysis
- Peak identification via Spectra Library
- Determination of optimum integration path for later wavelength alterations
- Normalization of spectra
- Quantification of non-resolved peaks

The measuring range of the PDA-100 detector is from 190 to 800nm. The measuring range of the UVD 340S detector is from 200 to 355nm in the UV range, and from 357 to 600nm in the visible range.

Functionality

Unlike conventional (1 or 2-channel) ➢*UV Detectors*, multi-channel detectors (PDAs) send the entire spectrum of the light source (a), in focused form (b), through the flow cell (c). Thus, absorption not only causes the intensity of a single wavelength to change, but that of all wavelength portions of the entire spectrum. After that, the white light is dispersed spectrally using a grating (d). The resulting spectrum is measured by adjoining photodiodes (e) almost synchronously.



Dionex detectors store this information analog to a UV channel via the signal ➢*3D-Field*. Apart from the quality of the optics and the grating, the number and size of the photodiodes determine the ➢*Optical Resolution* of the detector.

Caution: The optical resolution cannot be considered by itself, but must be seen in connection with the achieved signal to noise ratio!

Photodiode (Pixel) Resolution

The bandwidth of wavelengths on an individual photodiode is referred to as photodiode or pixel resolution.

If 150 photodiodes are available in the UV range (200 - 350nm), the photodiode resolution is 150nm / 150 photodiodes = 1nm per photodiode.

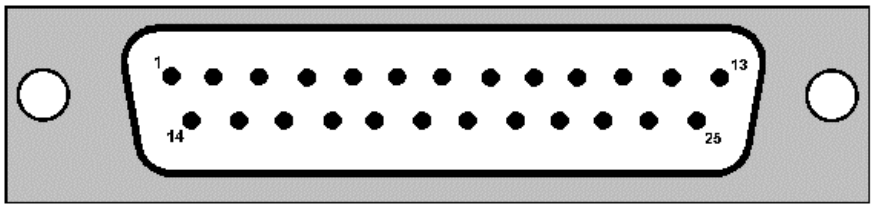
Photodiode resolution and the optics (mirror, slit, grating, optical bandwidth) determine the ➢*Optical Resolution* of the UV detector.

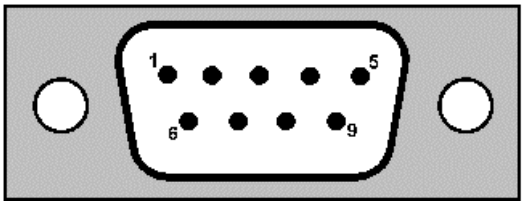
Pin Assignment

Usually 9-pin or 25-pin ➢*Modem Cables* or ➢*Null Modem Cables* are used for instrument connections. The pin assignments are as follows (only the most important pins are mentioned):

25-pin	9-pin	Abb.	Description
2	3	TxD	Transmitted data
3	2	RxD	Received data
4	7	RTS	Request to send
5	8	CTS	Clear to send
6	6	DSR	Data set ready
7	5	GND	Signal ground/common return
8	1	DCD	Received line signal detector
20	4	DTR	Data terminal ready

The pin numbering (order for plug) is as follows:





Should other connectors be required, see the installation instruction for the respective instrument for details (also, see **Installing and Controlling Third-Party Instruments**).

Pipet (AS50 Sample Prep Command)

The **Pipet** ➢*Sample Prep Command* moves a volume of sample from one vial to another. **Source** is the vial from which to pick up the sample volume, **Volume** is the amount of sample to be pipetted, and **Destination** is the vial in which to add the sample volume.

Polarity (Analog Output)

The **Polarity** command switches the polarity (+/-) of the analog output signal on Dionex detectors. For example, if components are appearing as negative peaks instead of positive, use this command to switch the analog output polarity from **+** to **-**.

Power-Failure Protection

The Dionex Chromatography Management System recognizes during the load sequence of the data system whether online ➢*Batch Processing* was interrupted by a power failure.

This is possible, because the date and the time are entered in the sequence editor whenever processing of a new sample is started. The Dionex Chromatography Management System checks whether all "started" samples (labeled with date and time) were completed, e.g. whether they reached the status **F** (finished). If this is not the case, the **Power-Failure Handling** allows you to define (via the **Error Handling** command of the **Batch** menu) how to continue processing:

- Continue with the interrupted sample
- Continue with the next sample
- Reprocess the entire online batch
- Abort the batch
- Prompt the user what to do

In addition, you can define a ➢*PGM File* which shall be started after booting the server (see **How to ...: Actions in the PGM Editor Creating a Power-Failure Program**).

In addition to this power-failure protection, a ➢*Network Failure Protection* is available in your Dionex Chromatography Management System.

PPA (Peak Purity Analysis)

Peak purity analysis (PPA) is a partial method of the offline module. It consists of a graphical section and the ➢*PPA Report*.

For details, see **PPA: Peak Purity Analysis (Overview)**.

PPA Report

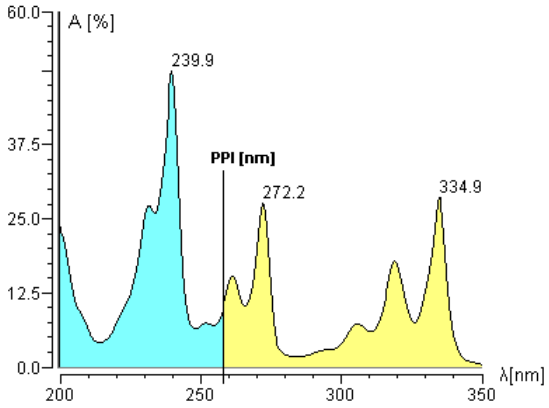
The PPA report represents the numerical addition to the partial method Peak Purity Analysis. In a table, this report combines variables characteristic for the peak purity analysis and variables freely selectable by the user.

Especially meaningful variables are:

- ➢*PPI (Peak Purity Index)*,
- ➢*Relative Standard Deviation (RSD PPI)*,
- ➢*Peak Purity Match Factor*, and
- ➢*Relative Standard Deviation of the Match Factor (RSD Match)*.

PPI (Peak Purity Index)

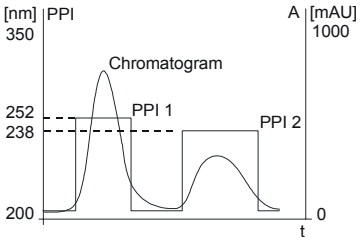
The peak purity index (PPI) represents the central wavelength of a spectrum. In simplified terms, this is the wavelength where the areas of the spectrum to the left and right are identical. The PPI is thus independent of the concentration.



A pure single peak should supply the same PPI value from peak start to peak end for each spectrum recorded in this range. The following conditions must be fulfilled:

- The baseline portion must be insignificant. If this is not the case, a ➢*Blank Run Subtraction* must be performed.
- During analysis, the solvent composition and thus the UV absorption of the solvent may not change significantly (special attention is required for gradient applications).
- Compared to the signal height, the drift must be very small.
- The Lambert-Beer Law must be valid for the entire range.

In the ideal case of a pure peak, entering individual PPI values results in a rectangle curve. The height of each single rectangle corresponds to the value of the central wavelength. The deviation from the rectangle shape can be expressed mathematically by the relative standard deviation of the PPI value.



Significant deviations from the rectangle shape indicate peak impurity. However, it is not necessarily correct to deduce from the rectangular shape that the peak is pure.

☞ ***Tip***: The calculation of the PPI value becomes inaccurate near peak limits due to the poorer ➢*Signal to Noise Ratio*. Using the ⇒*Peak Purity Threshold* detection parameter, the selection of spectra can be limited to a sensible peak height in the ⇒*QNT Editor*.

If the Peak Purity Index (PPI) is entered in a report column, this value is averaged from all determined PPI values of a peak.

The deviation of single PPI values from each other can be expressed as the ➢*Relative Standard Deviation (RSD PPI)* in the ➢*PPA Report*.

PPI: Relative Standard Deviation of the PPI (RSD PPI)

The relative standard deviation of the PPI expresses the degree of deviation of the computed individual PPI values from each other.

To determine this value, all PPI values of a peak are averaged (PPIØ) and are then squared (Q-Sum).

$$Q - Sum = \sum_{i=1}^{n} (PPI - PPI\varnothing)^2$$

The standard deviation (SD) is defined as the root that is extracted from the Q-sum divided by (n-1), with n being the number of data points.

$$SD = \sqrt{\frac{Q - Sum}{(n-1)}}$$

The relative standard deviation of the PPI (RSD (PPI)) in percent is obtained by dividing the standard deviation by the average of all PPI values (PPIØ), and by multiplying the result by 100%.

$$RSD(PPI) = \frac{SD}{PPI\varnothing} * 100\%$$

PQ

See ➢*Performance Qualification (PQ)*

Pressure Limits

Depending on solvent composition and the selected ⇒*Flow*, pressures of up to 450bar occur on the high-pressure side of a chromatography system. The Dionex Chromatography Management System is capable of monitoring the pressure value provided by the pump. The user can define upper and lower pressure limits. When one of the limits is exceeded, the Dionex Chromatography Management System stops the flow, displays an error message, and stops the sample batch, as necessary.

Also, see ⇒*Pressure Limits*

Printer Layout

The Printer Layout allows preparing your data for the printout. If the ➢*Layout Mode* is enabled, different elements can be added to the Printer Layout:

- Sheets (worksheets that can also include the following elements)
- Report Table
- Row(s)
- Column(s)
- Variable (individual variables)
- Chromatogram
- Calibration Plot (calibration curve)
- Spectra Plot (UV spectrum)
- Mass Spectra Plot (➢*Mass Spectrum*)
- 3DFIELD Plot (➢*3D-Field*)
- Chart (graphical display of the values of the individual cells/columns)

The Printer Layout is saved in the ⇒*Report Definition File (RDF)* together with the (screen) report. You can open the Printer Layout of the selected report definition file with the current sample data via the following button from the **Method** toolbar:

For information on how to design a report template, see **How to...: Actions in the Printer Layout**.

For information on how to print your results, see **How to: Actions in the Printer Layout Printing with a Report Template**.

Privilege

Most actions in the Dionex Chromatography Management System can be executed by the user only if he/she has the corresponding rights (privileges). The Dionex Chromatography Management System offers almost 100 different user privileges (e.g. Read Sequence, Copy Sample, Delete Sequence, etc.). Instead of assigning individual privileges to each user, the privileges are combined in P-groups (**Privilege Groups**). Thus, the P-Group membership defines the privileges of the respective user.

Each P-group defines a specific range of operations. These are divided in the areas **CM Server Control**, **Datasource**, **Sequence**, **Data Reduction**, **Reporting**, and **Miscellaneous**. The scope of functions available for one P-group increases with the number of privileges activated in the individual areas. (For further information on the user privileges, see the CmUser Online Help if this program is installed on your PC: **CmUser_E.HLP**)

Members of a specific P-group can use all privileges assigned to this group. Each user can be a member of one or several P-group(s). The names of the current members are listed in each P-group.

Creating a larger number of different P-groups allows defining access control in the Dionex Chromatography Management System more precisely. The privileges available for an individual user are defined by the combined privileges of all P-groups in which the user is a member.

Privileges (e.g. Delete Sequence) are assigned globally, i.e. a specific privilege is granted for all datasources the user can access. To restrict this access, ➢*Access Groups* (**Access Groups**) can be defined in addition to P-groups.

A-groups and P-groups are created by the administrator in the ➢*CmUser* program (CmUser.EXE).

Program

The control program (in short: program) is part of the ➢*PGM File* and is displayed in the **Commands** view of the PGM editor. It can be considered a "schedule" for the execution of different ⇒*Control Commands*. In this file, the user notes all commands to be executed before, during, and after analyzing a sample. This enables complete automation of the analysis including routine procedures before and after the analysis, e.g. conditioning a column or rinsing with various solvents.

Monitoring parameters or limits as well as triggering reactions to be performed at specific values, is also possible via the program.

A ➢*Wizard*, the  **Program Wizard** facilitates creating the basic structure of a program. The user input is converted automatically into a uniform syntax that is readable by the data system. This allows even new users to quickly create functioning programs.

For further details, see **Control** **Control Program** and **Program Syntax**.

Also, see ⇒*Program*

Note: The command syntax is different from the syntax of the GynkoSoft data system. When importing GynkoSoft PGM files, their syntax is automatically converted into the syntax of the Dionex Chromatography Management System.

Protocol Command

The **Protocol** command enables you to log specific events in the ➢*Audit Trail* while executing a ➢*PGM File*.

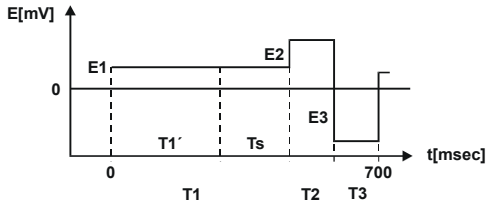
Unlike simple comments that are only part of the ➢*Program*, the **Protocol** text is included in the Audit Trail and is thus directly linked with the corresponding sample. The **Protocol** text can thus be used for commenting individual samples. Event-controlled execution of the command is also possible.

Also, see ⇒*Protocol*

Pulse Mode

In addition to the ➢*DC Mode*, most electrochemical detectors can be operated in the **Pulse Mode**. This method is also called PAD (pulsed amperometric detection) and is characterized by a series of potential changes. This method allows a continuous regeneration of the electrode surface (platinum or gold electrode).

A distinction is made between three different potentials (E1, E2, E3) and the period (T1, T2, T3) for which a potential is connected to the electrode. T1 + T2 + T3 form a cycle that is constantly repeated.



T1 = T1´ + Ts

Ts = Measurement time

T1` = Stabilisation (Delay) time

T2 = Cleaning

T3 = Conditioning

Data is recorded only during the second half of T1. The duration of Ts is either set directly or is determined by defining a delay T1´ (stabilizing phase).

The material of the working electrode largely determines the period and the height of the various potentials.

Quantification Method (QNT Method)

A quantification method includes all parameters that are used for the evaluation of a peak or the entire chromatogram. The QNT method serves as the basis of calculation for evaluating a sample and contains:

- All data for the assignment according to the order of elution within defined limits (time windows) (**identification**) and
- The parameters (calibration constants) that are part of the area/concentration (amount) conversion formulas as well as the calibration points required for the calculation.

Also, see: ⇒*QNT Editor*.

The **Method** column of the sample list (in the **Browser**) contains the name of a **Quantification Method** (also known as **QNT Method**).

Also, see ⇒*Quantification Method*

Query

The Dionex Chromatography Management System offers the possibility to efficiently search e.g., directories, sequences, samples, or comment lines for specific names or character strings:

- In the ➢*Browser* choose the **Query** command in the context menu or select **New / Query (using Wizard)** in the **File** menu. A wizard opens which facilitates entering the desired conditions.
- On the first page, define whether to perform the query in the currently open ➢*Datasource* or in a different one. In addition, define whether to find certain sequence properties and/or sample properties, and/or other result properties.
- Having pressed **Finish**, you can enter additional conditions to limit the query.

From the entered information, the Dionex Chromatography Management System generates an ➢*SQL* statement that can start a query within all ➢*ODBC*-capable databases.

For details on performing a query, see **How to ...: Actions in the Browser** **Performing a Query**.

The result of a query can be saved as a new sequence via the **Save as** command. QNT files and ➢*PGM Files* are copied; raw data is copied optionally. File names occurring more than once receive a consecutive number. The following symbol indicates the query sequence:

QNT Method

See ➢*Quantification Method (QNT Method)*

Rack

Many ➢*Autosamplers* offer a choice of racks to meet individual capacity and vial number requirements. For optimum operation, the currently used rack must be specified in the **Server Configuration**. This is performed when the corresponding device driver is installed.

The rack of the Dionex Autosampler **ASI-100** consists of three different colored segments. The following segment types are available:

Rack types	Description
Analytical:	Choose this option if you are using the default segment. The analytical segment can house up to 39 vials at 1.1 or 1.8 ml + 1 vial at 4 ml.
Semiprep:	Choose this option if you are using the semipreparative segment. The semiprep segment can house up to 21 vials at 4 ml each.
Mini:	Choose this option if you wish to analyze a large number of samples or if small sample volumes are available only. The mini segment can house up to 64 vials at 1.2 ml + 1 vial at 4 ml.
Eppendorf:	Choose this option, if you are using the rack for Eppendorf reaction vials. The Eppendorf segment can house up to 22 reaction vials at 1.5 or 2 ml + 1 vial at 4 ml.

If you are using a coolable rack (Dionex ASI-100T), you can determine the controllable temperature range. The range can be from +4°C to +45°C (39.2°F to 113°F), i.e. an exact set temperature can be observed only within this temperature range. The ASI-100T autosampler allows cooling the rack by 18K from ambient as well as heating the samples by up to 35K from ambient.

Range

For controllable detectors, the **Range** parameter determines the factor by which the analog output signal is amplified or reduced.

***Note**:* The Dionex ➢*A/D Converter* offers the measuring range -10V to +10V, thus it covers virtually all detector output signals. It is therefore possible to record the signal directly and to adjust the size via the **Factor** parameter of the A/D converter.

For the fluorescence detector RF1002 the term **Range** has a different meaning. Instead, the ➢*Gain* parameter is used.

Raw Data

Raw data refers to all analog and digital data points that are stored digitally on a PC. Raw data therefore only exists for signals or channels that were selected by the user before data acquisition.

The scope and precision of the stored raw data depends on the selected ➢*Sampling Rate* or ⇒*Step*.

For details, see **Data** **Raw Data Storage** and **Raw Data Compression**.

Ready (Signal)

After each autosampler operation (e.g., **Draw** for the ASI-100/ASI-100T samplers or **Suck** for the GINA 60/GINA 160 samplers), a ready signal command (**Sampler.Ready** for the ASI-100 sampler or **Sucked** for the GINA 50/GINA 160 samplers) is sent to the data system as confirmation. Other commands (e.g., **Dispense**) can only be executed after receipt of this signal.

The time interval between the sampler operation and the response **Sampler.Ready** (or **Sucked**) is the minimum value for the **Duration** command.

To execute two commands successively, ⇒*Wait* is entered after the first command in the ➢*Program*. The next command will then be executed immediately after the arrival of the **Sampler.Ready** (or **Sucked**) signals.

Ready Check

The Ready ➢*Check* command verifies whether performing the automatic batch is actually possible. The Ready Check allows you to check whether the instruments in the HPLC system are ready to operate (instruments are switched on, connected, lamp is switched on, etc.). In addition, this check verifies that all required files exist and that the storage capacity is sufficient.

As the batch list can be extended by further sequences during operation, the **Ready Check** command can also be performed during operation.

Reconnect

Use the **Reconnect** command to check the connection between the user PC and the timebase or the instrument and the data system. If there is no connection, the ⇒*Connect* command will be issued automatically.

Recorder Calibration

The **Recorder Calibration** commands allows calibration of the recorder's response to three detector analog output settings:

AU	Sets the analog output to AU, scaled from 0 to 1 V, based on the AU full-scale response selected by the ➢*Recorder Range* command.
Zero	Sets the analog output to 0 volts.
Full Scale	Sets the analog output to the full-scale setting (1V).

Recorder Range

The **Recorder Range** command sets the range of a full-scale recorder response in the signal units appropriate for the detector. For example, for conductivity detectors, the Recorder Range is given in microSiemens (µS). This command can be used to adjust the recorder output to accommodate larger or smaller peak heights.

Reference Bandwidth

The reference bandwidth can be selected separately for each channel. The 3D-field of a photodiode array detector also has its own reference bandwidth.

Analogous to the conventional ⇒*Bandwidth* of a channel, the reference bandwidth serves to average several photodiode signals of the ⇒*Reference Wavelength*.

Also, see ⇒*Reference Bandwidth*

Reference Channel

= Reference Channel for Baseline Correction

Performing an automatic ➢*Baseline Correction* requires a reference channel.

As a channel, either a physical channel can be used or a channel that was extracted from the 3D field and stored afterwards. The wavelength of the channel is variable, i.e., a channel recorded via ➢*Wavelength Switching* is also valid.

Which channel is actually used as reference channel in the PPA method depends on how the PPA window is opened.

If the PPA window is opened in the Browser by selecting the **Open ... 3DFIELD** command, the channel specified in the **File** menu under **Preferences** is used as reference channel.

If the PPA window is accessed from a different method, the currently displayed channel is used as reference channel.

The current reference channel can be included in the PPA chromatogram window via **Draw Reference Channel** (**Decoration** dialog box). The channel serves as a basis for the integration and peak detection.

Tip: Do not confuse the reference channel with the ⇒*Reference Wavelength* of the signals from a photodiode array detector.

Reference Peak

Reference peaks are references for calculating relative retention times for different substance peaks. The relative retention time can be indicated as absolute time difference (in minutes) or as percent quotient (retention time substance peak/retention time reference peak). In addition, the reference peaks can be used for calculating the ➢*Relative Peak Area* and the ➢*Relative Peak Height*.

You can specify the reference peaks in the QNT file on the **Peak Table** tab. Double click the **Ret. Time** column to open the **Retention Time for ...** dialog box (see ➢*Retention Time Interpretation*) or the corresponding peaks. Choose one of the options **Time distance to reference peak** or **Time ratio to reference peak** to select a **reference peak** for each substance peak via the selector arrow.

The retention time is re-calculated automatically when a different reference peak is selected. Only peaks with absolute retention times can be selected as reference peaks. It is not possible to delete reference peaks from the peak table.

Besides, the retention time can be entered directly in the entry field in the following format:

[<Reference Peak>] <Ret. Time> [<Unit>]

You are free to choose the order in which the fields are used. If no name is entered for the reference peak, the time is interpreted as absolute time, otherwise as relative time.

Either **min** or % can be selected as unit. If no entry is made, **min** is used. The unit determines whether the time given is the difference (**min**) or the ratio (**%**) to the time of the reference peak. For absolute times only **min** is permitted.

Note: Even if the retention time is then specified in **Absolute times**, the Dionex Chromatography Management System saves the selected reference peaks.

Reference Wavelength

For Dionex photodiode array detectors, the reference wavelength is used to correct absorption values of the wavelength(s) selected for analysis. If the absorption of the reference wavelength changes during the analysis, absorption values of the analysis wavelengths are adjusted up or down accordingly. The selected reference wavelength should be in a quiet area of the spectrum where little absorption occurs. Each change in the absorption then indicates substantially changed conditions, for example, a reduction of the lamp energy (lamp drift). Each change can be used to correct the absorption in the remaining wavelength range even during the analysis (the recorded signal is reduced or amplified accordingly, as necessary).

Reference wavelengths are especially useful for gradient analyses, because as the light intensity changes over time (due to the gradient), absorption values are adjusted, thus minimizing baseline drift.

The reference wavelength is freely selectable, not only for each channel of the detector, but also for a 3D-field. Because the absorption of the reference wavelength is stored, it is possible to undo a correction later. The reference wavelength can be changed later by extracting the absorption values of the "new" reference wavelength from the 3D-field and using them for correction.

Also, see ⇒*Reference Wavelength*

Relative Amount

This peak result variable refers to the amount portion of a peak relative to others. The peaks used as a reference are determined via the following options:

Option	Description
All Peaks:	Amount portion relative to the sum of all amount portions of all peaks (default setting).
All Peaks of the same Group	Amount portion relative to the sum of all amount portions in one group.
The corresponding ISTD Peak	Amount portion relative to the amount of the peak of the ➢*Internal Standard*.
The corresponding Reference Peak	Amount portion relative to the amount of a ➢*Reference Peak*.

Note: The values of the options 2 to 4 can considerably exceed 100 %.

Select the respective column in the report, choose the **Column Properties** command from the context menu, and select the variable in the selection box. Press the **Parameter** button to determine the peak to be used as reference.

Relative Area

The **Relative Area** peak variable is the portion of the peak area in the sum of all peak areas (total area).

Which peak areas form the total area, is determined by selecting one of the following options (The values of all **relative peak areas** always result in 100% for the options 1 to 3).

Option	Description
All detected Peaks	The areas of all detected peaks are used for the calculation (default setting).
All identified Peaks	Only the areas of identified peaks are used for the calculation.
All Peaks of the same Group	Only the peaks of one group are used for the calculation.
The corresponding ISTD Peak	The area of a peak is put in relation to the area of the ➢*Internal Standard* peak
The corresponding Reference Peak	The area of a peak is put in relation to a ➢*Reference Peak*.

Select a column in the report, choose the **Column Properties** command from the context menu, and select the variable in the selection box. Press the **Parameter** button to choose another option.

Relative Height

This peak variable refers to the peak height relative to the average height of a certain peak group or a specific peak. As with the ➢*Height* variable, the maximum (i.e. at the retention time) is measured, relative to the baseline. The dimension does not depend on the detector type.

The selection of the peak heights is possible via the following options:

Option	Description
All detected peaks	The relative peak height is indicated in relation to the

	average height of all detected peaks (default setting).
All identified peaks	The relative peak height is indicated in relation to the average height of all identified peaks.
All Peaks of the same group	The relative peak height is indicated in relation to the average height of all peaks in one group.
The corresponding ISTD peak	The relative peak height is indicated in relation to the height of the ➢*Internal Standard Peak*.
The corresponding reference peak	The relative peak height is indicated in relation to the height of a selected ➢*Reference Peak*.

Select the column in the report, choose **Column Properties** from the context menu, and select the variable in the selection box. Press the **Parameter** button to choose another option.

Relative Retention Time (Rel. Ret. Time)

The **Relative Retention Time** peak variable of the **Peak Results** category is the quotient of the peak retention time ⇒*Retention Time* (T ret.) and the retention time of the corresponding reference peak (T ret. Ref.) in percent.

Relative retention time = 100 x T ret.(Peak) / T ret.Ref.

The reference peak is specified in the peak table (see Online Help: *Retention Time Interpretation*).

The **Parameter** button offers the following options:

Reference Peak:	The relative retention time refers to the reference peak (default)
Fixed Peak:	The relative retention time refers to a user-defined peak. If so, enter the name of the reference peak as second parameter that can be selected from the list of identified peaks with the selector arrow.

Relative Standard Deviation

The **Relative Standard Deviation** is the standard deviation in relation to the size of the measured area values, i.e. the standard deviation is normalized. In contrast to absolute standard deviations, relative standard deviations can be compared (for area values around 1000 a standard deviation of 1 is minor, for values around 10, this is a major deviation). Usually, the relative standard deviation is expressed in percent.

The relative standard deviation (relStdDev) is calculated as follows from the absolute standard deviation (StdDev):

$$relStdDev = \frac{StdDev}{\overline{Y}}$$

With: $\overline{Y}$: Average value of all Y-values.

Relay

Relays are closing contacts that can be switched by the data system. Apart from the physical ("real") relays on the rear of various Dionex instruments, there are also virtual relays that can only be used within the data system. Virtual relays are mostly used for defined functions, such as moving the needle. Virtual relays are available if the respective instrument or function is installed.

Before using a "real" instrument relay, it must be installed in the **Server Configuration**, i.e. it must receive identification. This ID consists of the relay name and the relay number.

***Note**:* Some device drivers support trigger contacts, which function as two dependent relays. When the first relay is switched on, the second is switched off and vice versa.

Relay On/Off

The **Relay On (Off)** command closes (opens) a relay output (contact closure relay) for a defined time. Switching valves are also treated as contact closure relays.

The specified relay is opened or closed for a specified time in seconds. **Relay On** opens the relay upon completing a certain period (➢*Duration*), **Relay Off** closes the relay after completing the duration. If no duration is specified for **Relay On (Off)**, the relay remains closed (open) until the next relay command is given.

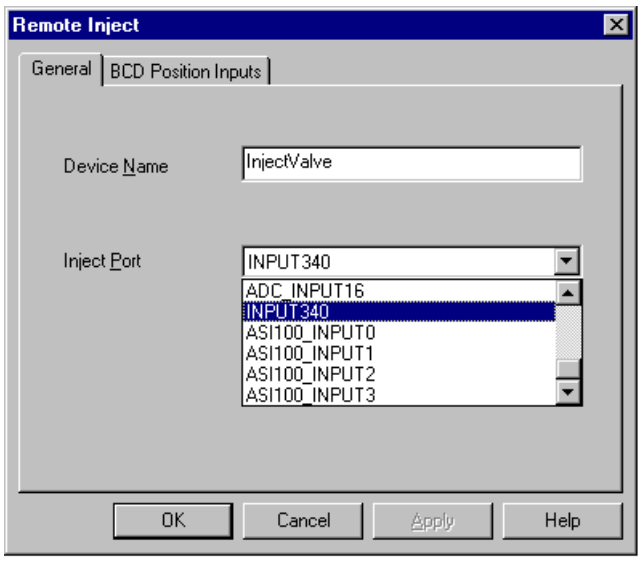
Also, see ⇒*Relay On/Off*

Remote Inject

The **Remote Inject** driver is required for non-controlled chromatography systems. Typically, non-controlled systems are GC systems or third-party HPLC systems for which no separate driver is available.

With controlled HPLC systems, the ➢*Autosampler* directly communicates the time of injection to the Dionex Chromatography Management System via an RS232 cable. This is not possible with non-controlled systems. The **Remote Inject** driver then serves to communicate the time of injection from the autosampler to the Dionex Chromatography Management System. Via a digital input (typically via the detector), the autosampler communicates the inject signal to the Dionex Chromatography Management System. As soon as the signal is received, for example, the data acquisition (⇒*AcqOn/Off* can be started. With GC systems, the time of injection is communicated in the same way.

Choose for example the following setting if the inject output of the autosampler is connected to the input of the UVD:



Remote Input

To enable a reaction to external events (e.g. injection), several Dionex instruments and additional boards offer remote inputs. The remote inputs are suitable for input voltages between 0V and +5V (TTL level).

As the remote input level is kept at +5V by internal board resistors (pull-up resistance), a simple contact closure relay can be used as external signal source. This contact must be switched between GND and the respective remote input. If the contact is closed, the digital voltage is grounded. The relay

itself is under a low current of approximately 1mA. Opening the contact restores the initial state.

If the signal source itself is active (e.g., Dionex ➢*Photodiode Array Detector* UVD340S), the polarization of the remote input must be correct. Ground must be connected to ground, and the digital output must be connected to the remote input.

Installation is for the instrument that supplies the remote inputs. Determine clear installation names and numbers for the required remote inputs. The instrument determines the timebase to which the remote inputs are assigned. Only in the case of remote inputs of an ➢*A/D Converter*, the ➢*Timebase* must be specified in addition.

⚠ ***Caution***: Do not supply higher voltages (>5V) to the remote inputs, as this may result in a malfunction of the microprocessor system on the A/D board, in the destruction of the input modules or in further damage.

Example:

A hand-operated valve (injection valve) is connected to a **Remote Input** of the A/D converter. In the **Server Configuration**, a free input number, the name of the remote input signal (= INJECT), and the name of the timebase (e.g. SYS1) is entered below the A/D board. By switching the hand-operated valve (from the **Load** to the **Inject** position), the two contacts of the remote input are connected and grounded. This state is recognized as an Inject signal by the system and as the start of the chromatogram. When switching back the hand-operated valve, the original state is restored. The remote input is in the initial state again.

Replicate

In the case of multiple injections from a standard or sample vial, all samples following the first injection are called replicates. The name **Replicate** is used independently of the injected volume (see ⇒*Inj. Vol.* (injection volume))

Each replicate must be added to the sample list of the sequence as an independent sample! Document the injection from a single vial (identical sample position) in the ⇒*Replicate ID* column by entering the same number / the same text. When a new sequence is generated using the Sequence Wizard, the ⇒*Pos.* (sample position) is automatically entered as replicate ID.

Replicates of a standard sample with the same injection volume will produce ➢*Calibration Points* on the same level. Each alteration of the injection volume will generate calibration points of a new level.

Replot from Beginning

Enable the **Replot from beginning** option to automatically replot when the signal leaves the right-hand border of the signal plot. The current chromatogram is then replotted from the beginning. One unit scales the time axis to fit the chromatogram into the window. For example, if the first time axis was 2min, after 2min the window is enlarged by 2min to show 4min, after 4min it is enlarged by another 2min to show 6min, etc.

Report Definition File (RDF)

Report Definition Files (**RDFs**) have two functions: They serve to display and reprocess your results on the screen (**Report**) on the one hand and to prepare the printout (➢*Printer Layout*) on the other.

For details, see: ⇒*Report Definition File*.

Report Publisher

The **Report Publisher** is an add-on product to the Dionex Chromatography Management System. With its 141 ➢*Additional Functions* is provides considerable enhancements to report templates in the ➢*Printer Layout*.

Choose the **About** item in the **Help** menu to see whether this add-on is available on your system.

Report Publisher = On

This setting indicates that the Report Publisher is available on your system. After activating the edit line in the **Printer Layout**, you can enter the character **=** followed by the required formula. In addition, the **Insert ... Chart** command is available via the context menu. It allows the graphical representation of specific cell values.

For details on the available options, see **How to ...:**  **Actions in the Printer Layout**.

Report Publisher = Off

In this case, the Report Publisher is not installed on your system. Please contact Dionex if you are interested in purchasing the add-on product.

Reserved Relay, Remote Input, and Signal Names

The following names are reserved for special functions:

	Description
3DFIELD	The signal **3DFIELD** is composed of the absorption values recorded at the time t at different wavelengths using a photodiode array detector. Each absorption value is entered as a data point in a wavelength by time grid, producing a three-dimensional data field. The number of data points is determined by the optical resolution and the selected bandwidth (limits) of the 3D-field.
INJECT	refers to the signal that is recognized as the INJECT signal by the system and that defines the start of the chromatogram.

Resolution

The **Resolution** peak result variable is the distance between two adjacent peaks. This resolution is a measure for the separating capability of the column. It is calculated based on the following formulas (EU and US standards):

US standard:	R = 2 x (Tnext - Tret) / (BWnext + BWret)
EU standard:	R = 1.18 x (Tnext - Tret) / (W50%next + W50%ret)

With:

Tnext / Tret	Quotient of the retention times of the two peaks
BWnext / BWret	Quotient of the ➢*Peak Widths* of the two adjacent peaks
W50%next / W50%ret	Quotient of the width of the two adjacent peaks at 50% of the peak height

The distance between the peak maxima is divided by the arithmetic average of the peak widths.

Select the column in the report, choose the **Column Properties** command from the context menu, and select the variable in the selection box. Press the **Parameter** button to define whether the calculation is based on the EU (EP formula) or the US (USP formula) standard.

These abbreviations refer to:

EP = European Pharmacopeia

USP = United States Pharmacopeia.

Response

Response is the time the detector requires for reaching 98% of the full deflection. With a longer time interval, the ➢*Signal to Noise Ratio* improves, but the resolution is reduced.

Response Factor

The **Response Factor** peak table parameter is a peak-specific, multiplicative factor without dimension. Its default value is 1.000 and is changed for special applications. The response factor is entered in the corresponding column of the **Amount Table** in the ⇒*QNT Editor*.

Also, see ⇒*Response Factor*

Restore (File)

The **Restore** command allows restoring files previously stored via the ➢*Backup* function. The procedure is described under **How to ...: Actions in the Browser** **Restoring Backup Files**.

To execute the **Restore** command, select **Import/Restore** in the Browser **File** menu.

***Tip**:* The easiest way to open these archive files, which have the extension *.cmb, usually is to double click on them in the Windows Explorer.

Retention Index

The retention index serves for achieving uniform scaling of the ⇒*Retention Time*

Also, see ⇒*Response Factor*

For information how to enter the retention index, see **How to...: Actions in the QNT Editor** **Defining the Retention Index and the Kovats Index**.

Retention Time

The retention time is used for peak identification. The **Retention Time** peak variable refers to the time (in minutes) that passed since the injection (also, see ⇒*Dead Time*). The retention time of a peak is defined by the time of the data point with the highest absorbance value. (This does not have to be the data point with the largest distance to the baseline.)

In the Dionex Chromatography Management System, the retention time is especially important at two points:

- In the ⇒*QNT Editor* as part of the peak table
- In the Report / ➢*Printer Layout* on the **Integration**, **Peak Analysis**, and **Summary** sheets.

QNT Editor

On the page **Peak Table** in the **QNT Editor**, the retention time can be entered either manually by the user or automatically by the system.

Also, see ⇒*Response Factor*

Report

In contrast to the QNT editor, the actually measured retention times of the corresponding samples are stated in the report. This is the default setting for the **Retention Time** variable of the **Peak Results** category. With this variable, it is also possible to indicate the actual nominal retention time. Then, the settings of ⇒*Use Recently Detected Retention Times* are taken into account.

However, it is also possible to include the expected retention times (from the peak table of the QNT editor) using the category **Peak Table**. Choose the **Retention Time** variable from the report category **Peak Table**. It is not always the nominal retention time that is displayed.

Retention Time Correction

See ⇒*Use Recently Detected Retention Time*

Retention Time Deviation (Ret. Deviation)

The **Retention Time Deviation** peak result variable indicates the deviation of the actual retention time from the nominal ⇒*Retention Time* according to the peak table (in [minutes]).

Retention time deviation = T ret. (nominal) - T ret. (actual)

The retention time deviation can be set via two different methods. The setting can be either

- Absolute, i.e. in minutes, or
- Relative, i.e. relative to the retention time.

Select the column in the report, choose the **Column Properties** command from the context menu, and select the variable in the selection box. Press the **Parameter** button to determine whether the deviation is expressed as a relative or absolute value.

Retention Time Interpretation

This QNT file parameter determines the appearance of ⇒*Retention Times* in the peak table.

Select the **Absolute Times [min]** option to display the retention times as usual (time interval between injection and peak maximum).

Instead of this representation, relative time intervals to any peak can be displayed in the peak table (reference peak).

Select the **Time distance to Reference peak [min]** option to express the difference to the reference peak in minutes.

Select the **Time ratio to Reference peak [%]** option to express the difference to the reference peak in % values.

As the reference peak can be located in the center of the chromatogram, the difference expressed in minutes or percent can assume negative or positive values, or values below or above 100%.

⚠ ***Caution***: For difference and relative retention times also, relative (time) ⇒*Window* are interpreted as percentage values of the absolute retention time! Only the retention times of identified peaks are corrected! In the peak table, you can choose between the three options, as required. The retention time column is re-calculated automatically.

Retention Time Spectrum

The retention time of a peak is determined at the peak maximum. The spectrum the photodiode array detector records at this time is referred to as retention spectrum.

Retention Time Window

See ➢*Window*

Retention Window Width

The **Retention Window Width** peak variable provides the width of the ⇒*Retention Window* (in minutes) that was used to detect the peak. This variable is also available for not identified peaks.

RF Value (Amount/Area)

The ascending slope of the calibration curve, specified as amount/area value, is referred to as **RF Value**. This is the reciprocal value of the ➢*Slope* c1.

Note: The RF value is sometimes called Response Factor. Do not confuse this term with the ➢*Response Factor* used in the peak table.

Rider Peak

In a series of non-resolved peaks, all peaks - with the exception of the largest peak (reference peak) - are referred to as **rider peaks**. Alternatively, they are called **skimming peaks**.

Depending on the position of the rider peak (in the ascending or descending flank of the reference peak), a distinction is made between rider up and rider down.

The ⇒*Rider Threshold* and ⇒*Maximum Rider Ratio* detection parameters determine the peaks that are classified as rider peaks within a series of non-resolved peaks.

Peaks classified as riders are recognized in the chromatogram plot by the skimming tangent. In the result report, they are labeled **Ru** (**Rider up**) or **Rd** (**Rider down**).

Rider peaks can be skimmed in different ways (see ⇒*Rider Skimming*).

Rider Skimming

This parameter indicates how ➢*Rider Peaks* are skimmed.

Also, see ⇒*Rider Skimming*

For information on how to apply the detection parameters, see **How to ...: Actions in the QNT Editor Modifying Detection Parameters**.

Rider Threshold

The **Rider Threshold** detection parameter decides whether individual peaks in a series of non-resolved peaks are classified as ➢*Rider* or as main peak.

Also, see ⇒*Rider Threshold*

For information on how to apply the detection parameters, see **How to ...: Actions in the QNT Editor Modifying Detection Parameters**.

Right Mouse Button

The most common commands and functions are available in the context menu. The choice is context-sensitive, i.e. the commands most likely to be used in the current situation will be offered.

Pressing the right mouse button usually opens a context-sensitive menu (= context menu).

Right Limit

Normally, peak integration is performed automatically. It is possible to limit or extend integration on the left, right or on both sides with the appropriate peak table parameters.

Each (minute) limit is relative to retention time, i.e., the peak is integrated between the retention time - left integration limit .... and .... retention time + right integration limit. The value 0 deactivates the limit.

Example: For the right and the left integration limit, the value 0.5min is entered. The peak maximum is at the retention time of 8 minutes. The peak is integrated from 7 minutes 30 seconds to 8 minutes 30 seconds.

Example: For the left integration limit the value 0.5min and for the right integration limit the value 0 is entered. As before, the peak maximum is at the retention 8 minutes. The peak is integrated from 7 minutes 30 seconds. The end of the integration is then automatically determined.

Right Width

If a perpendicular line is dropped to the baseline from the peak maximum, the ➢*Peak Width* is divided in a left and right section. The two sections are referred to as **left width** and **right width** and can be expressed as separate peak result variables.

The Dionex Chromatography Management System also determines the left and right peak width at 5, 10, and 50% of the peak height. As described under Peak Width in the Glossary, the selected height is very important for the calculation of the peak width. This also applies to the calculation of the left and right peak widths. The abbreviations for the left and right peak widths are **LW** and **RW**.

Select the column in the report, choose the **Column Properties** command from the context menu, and select the variable in the selection box. Press the **Parameter** button to determine at which peak height to determine the peak width.

Rise Time

Rise Time is a measure of how quickly the detector responds to a change in signal. Rise time is defined as the time it takes the output signal to rise from 10% of its final value to 90% of its final value. Choosing an appropriate rise time value can optimize performance by keeping the ➢*Signal to Noise Ratio* at a minimum level. A longer rise time allows averaging of the noise frequencies, and subsequently, the baseline will contain much less short-term noise. However, longer rise times may have the following effects on peaks:

- Peak shape will become asymmetric.
- The peak maximum will be shifted.
- The peak height will be reduced.

 ***Note:*** The rise time should be approximately 25% of the peak width at half height of the narrowest peak of interest.

For example, for a peak width of 5 seconds, calculate the rise time as: 1/4 (5 sec) = 1.25 sec. Because 1.25 seconds is not one of the available settings for rise time, select the next fastest rise time, which is 1 second in this case.

 ***Tip***: In the AD25 and PDA-100 detectors, rise time applies to both digital and analog output.

RPC (Remote Procedure Calls)

The RPC technology introduced with Windows 95/NT allows running a program on a different computer.

Unlike true full-control programs as PC-DUO or PC-ANYWHERE, the amount of transferred data is considerably lower with this type of control. Processes started from a remote computer run almost without any time delay. For the user

it is not possible to determine whether the process is performed on the local or on a remote PC.

RPC requires a functioning network connection between the involved computers. It is irrelevant whether the computers are part of the same network or whether they are linked via a modem connection. Communication also functions between different networks (Novell, Windows), provided the networks communicate via a common protocol.

The Dionex Chromatography Management System generally communicates via the network protocols IPX/SPX, TCP/IP, or NetBEUI. Under Windows NT/2000, the protocol **Named Pipes** is also valid.

Sample Data

Data that contributes to characterize a single sample is stored in a database by the Dionex Chromatography Management System. This does not only include the entered data (name, volume etc.), but all results calculated from the ➢*Raw Data* and the chromatographic conditions under which the sample was analyzed (column, temperature, solvent, instruments etc.).

Sample Name

The **Name** ⇒*Sample Variable* serves to identify a sample and also to label graphics and result reports. The user generally enters the sample name.

When creating a sample list with the  **Sequence Wizard**, automatic sample name generation will be possible.

Also, see ⇒*Name* (sample name)

Sample Needle Height (AS50 Command)

The **Sample Needle Height** AS50 ➢*Autosampler* command positions the tip of the needle at the specified height (in mm) above the bottom of the vial. A value of 0 is closest to the bottom of the vial; a value of 46 is closest to the top. This height is used for all sample injections. It is also the default for sample preparation steps unless a separate ➢*Needle Height* command is specified.

Sample-Oriented Operation

Due to the object-oriented concept of the Dionex Chromatography Management System, emphasis is on samples and ➢*Sequences*, not on methods or activities.

The user selects the sample or sequence to process and automatically receives the corresponding view, i.e. calibration methods are displayed in the calibration window, integration samples in the integration window and sequences in the sample editor, etc. For each sample or sequence, only the selectable or expected views, methods, or functions are available to the user. This saves time and reduces the number of simultaneously active windows.

This context-sensitive procedure is also valid for options selectable in the context menu. The selection depends on the position and the time of the mouse click.

Sample Position

The **Pos**. ⇒*Sample Variable* determines the position of the sample in the ➢*Autosampler*.

If you use a controllable autosampler, the entered position is transmitted automatically to the sampler. The sampler approaches the corresponding sample for injection. If using a non-controlled autosampler or a hand-operated valve, this column only serves for documentation purposes. If the sample position parameter is not entered, the previous (current) value is used.

Also, see ⇒*Pos.* (sample position) and ⇒*Position* (autosampler command).

Sample Preparation Vial Positions

In AS50 autosampler sample preparation operations, a vial position can be specified either as an absolute position or as a relative position.

To specify an absolute position, enter the number of the vial's position in the tray. Valid numbers depend on the tray type in use: 1 to 100 for the 2 ml tray; 1 to 49 for the 10 ml plastic tray.

To specify a relative position, select **CurrentVial** for the current sample vial, **CurrentVial+1** for one vial past the current vial, **CurrentVial+2** for two vials past the current vial, and so on, up to **CurrentVial+9**.

Some operations let you specify **FlushPort** instead of a vial.

Sample Status

The **Status** ⇒*Sample Variable* determines the current sample processing status. A sample is either unprocessed (Single), or Finished, or due for multiple processing (Multiple).

The Dionex Chromatography Management System also maintains a log of the sample status, i.e. a Single sample is automatically assigned the status Finished as soon as processing is completed. A sample may also be excluded from processing by assigning the status Finished.

The sample status has a special significance for the built-in ➢*Power-Failure Protection*. Upon recovery from a power failure or starting the sample batch after a manual interruption, the Dionex Chromatography Management System begins processing the sample batch according to the selected power-failure handling option.

Also, see ⇒*Status* (sample status)

Sample Type

The ⇒*Sample Variable* **Type** specifies which type of sample is used.

Select the **Unknown** option if the sample is an unknown analysis sample. This sample type is indicated by the symbol:  .

Select the **Standard** option if the sample is a standard sample with known concentration. This sample type is indicated by the symbol:  .

Select the **Validate** option if the sample is a ➢*Validation Sample* ().

Select the **Blank** option if the sample is a ➢*Blank Run Sample* (). If a sample is corrected by the ➢*Raw Data* e.g. of a blank run sample, this is referred to as ➢*Blank Run Subtraction*.

Select the **Matrix** option for a ➢*Matrix Blank Sample*. This sample type is indicated by the symbol: 

Also, see ⇒*Type* (sample type)

Sample Weight

The **Weight** ⇒*Sample Variable* has two functions. It serves to enter the sample weight but it can also be used as a weight correction factor.

Sample Weight is implemented as a multiplication factor in the ➢*Formula for Amount Calculation* of not explicitly entered amount values (dilution series). It is without dimension.

Also, see ⇒*Weight* (sample weight)

Sampler.Ready

See ➢*Ready*

Sampling Rate

The number of stored signal values per second is referred to as sampling rate (or Data Collection Rate).

The maximum of stored values corresponds to the number of values generated per second and depends upon the device, for example, Dionex UVD 170S/340S Detectors = 100, ➢*A/D Converter* = 100, 3D-field = 10, Dionex AD25 and PDA-100 Detectors = 10.

The reciprocal value, i.e., the time interval between data points, is called ⇒*Step* (Dionex UV detectors = 0.01, A/D converter = 0.01, 3D-field = 0.1, Dionex AD25 and PDA-100 detectors = 0.1).

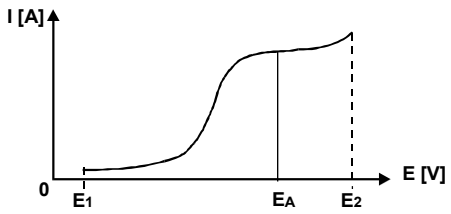
Tip: For Dionex detectors that are installed via the DX-LAN, a ➢*Data Collection Rate* command determines the data collection (sampling) rate and the step value is automatically set to the reciprocal of the selected data collection rate. For other Dionex devices, only the step value is set and a separate Data Collection Rate command is not used. See **How to...: Device Control** **Defining Step and Average** for details.

SCAN Mode

The SCAN Mode of an electrochemical detector serves to determine the analytical potential of a substance.

At a constant concentration in the flow cell, e.g. realized by strongly reducing or by stopping the pump flow, the potential between reference and working electrode is changed linearly.

The change is either a linear increase or decrease between two values (E1 and E2; **Half scan**), or an increase with a subsequent decrease (**Full scan**). If the increase and decrease are constantly repeated, this is referred to as **Continuous scan**.



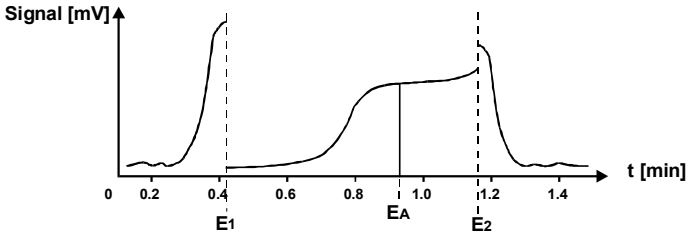
In all three cases, current/voltage curves (here represented by a **half scan**) are recorded. The working electrode potential (= E_A) here corresponds to the optimum analytical potential of a substance. Determining this potential is required for accurate analysis in the ➢*DC Mode* and the ➢*PULSE Mode*.

Practical Application with the Antec Detector DECADE

The analysis is performed in the DC mode or the PULSE mode. If the peak of a substance is detected for which the analytical potential is to be determined, stop the pump flow, switch to the SCAN mode, and slowly change the potential. When the final value is reached, return to the previous mode and reset the pump flow to its original value.

The entire process can be performed by a key click, if the required commands are placed on a Command Button.

In the signal plot of the ➢*Control Panel*, the following curve can be observed.



Unlike the pump, the chromatogram run time is not stopped. The retention times of the subsequent peaks will be shifted accordingly. However, the signal height of the peaks will be lower as part of the substance is "used up" during the **Scan** mode.

The optimum analytical potential cannot be directly read on the y-axis (time axis), but is determined with the printed chromatogram.

Self-Regenerating Suppressor (SRS)

See ➢*Suppressor*

Sensitivity (Detection Parameter)

The **Sensitivity** detection parameter determines the signal height from which the detected data points are interpreted as peak or as noise. It is always interpreted in the installed dimension (e.g. mAU).

☞ ***Tip***: Always consider this parameter in combination with the ⇒*Peak Slice* detection parameter!

Also, see ⇒*Sensitivity*

For information on how to apply the detection parameters, see **How to ...: Actions in the QNT Editor Modifying Detection Parameters**.

Sensitivity (Signal Parameter)

The **Sensitivity** parameter adjusts the data system to the sensitivity of the detector (i.e. to the ➢*Signal to Noise Ratio*). The fluorescence detector RF 1002 supplies the values LOW and HIGH, the model RF 2000 supports the values LOW, MED (Default) and HIGH.

Sequence, Sequence Table, Sample List

A sequence combines samples that belong together due to their origin or processing. The names of all samples that belong to one sequence from the user's point of view are entered in the sample list (also called sequence table). A sequence is thus a container for various samples.

To create a sequence, use the  **Sequence Wizard**.

Also, see ⇒*Sequence*

Sequence Data

Data that serves to characterize a ➢*Sequence* instead of a single sample (!) (see ➢*Sample Data*), is referred to as sequence data.

This includes, e.g. the date of the last change, the corresponding timebase or the name of the user who created the sequence. As the sample data, this information is stored in a database.

(Chromatography) Server

PCs connected to the components of an HPLC system via a serial interface can be used as chromatography servers.

A chromatography server is automatically installed on the PC during the installation of the Dionex Chromatography Management System. The chromatography server controls the data exchange between the system and the PC. Upon starting, each server is capable of serving up to six controlled or 16 non-controlled systems (timebases). The server receives the commands entered by a ➢*Client* PC in a ➢*Control Panel* and executes them at the specified time (e.g. by transmitting them to the corresponding device driver of the HPLC system). In the opposite direction, the server also assumes this buffer function. Thus, the raw data of each system is stored at the location specified by the client and the entire system-relevant data is forwarded to the client.

Starting (loading) the server can be performed manually or automatically. Select the required options in the ➢*Server Monitor Program*. For optimum functionality, the server must be configured. This is performed via the ➢*Server Configuration* of the Dionex Chromatography Management from any client PC.

If the server and the client software of the data system are located on the same PC, the installation is local, if not, it is a network installation (see **Network**).

☞ ***Tips***: In the case of manual data acquisition, the ➢*Raw Data* from the system is always stored in the PCNAME_LOCAL server directory. In the case of ➢*Batch Processing*, each user can choose where to store the data.

To minimize the risk of losing data, raw data should always be stored temporarily on the server. In the course of archiving, it can be transferred to a different computer.

Server Configuration

The Server Configuration includes information on the assignment of HPLC devices to ➢*Timebases*, the connection of servers to timebases, and the configuration of the individual devices. It is defined in the **Server Configuration** program.

The information is saved in an installation file (*.CFG file). The current configuration is always saved in the CMSERVER.CFG file on the chromatography server.

The user can create different installation files in the **Server Configuration**, transfer them to any server via the Import function, and use them accordingly.

Executing the **Save** command saves the current configuration as the new CSERVER.CFG file on the server.

For further information, see **How to ..: Actions in the Server Configuration** **Changing the Server Configuration**.

Server Monitor Program

The program required for starting and monitoring the chromatography server is called the Server Monitor. During installation, it can be included in the Autostart group of the operating system.

When starting the Server Monitor, an additional icon appears on the Windows status bar indicating the status of the server.

- Move the mouse cursor over the icon to view the server status via a quick info field.
- Open the corresponding context menu (right mouse button) to start or to stop the server (**Start/Stop Server**), or to exit the monitor program (**Quit Monitor**).
- Double-click the icon for further options, e.g. automatically starting the server when booting the computer.

The server status is also indicated by the icon's color:

Icon	Color	Message
	Crossed out red	*CHROMELEON (PeakNet) Server is not running.*
	Yellow	*CHROMELEON (PeakNet) Server is starting / is closing.*
	Green	*CHROMELEON (PeakNet) Server is active.*
	Turquoise	*CHROMELEON (PeakNet) Server is reconfiguring*.
	Gray	*CHROMELEON (PeakNet) Server is running idle.*
	Yellow/ red	*CHROMELEON (PeakNet) Server needs attention.* The server waits for the response to a message (⇒*Message* command). For example, after a power failure the user must decide how the program should continue the interrupted sample processing.

Sharable Devices

The Dionex Chromatography Management System records signals from several devices and controls different instruments. Via PC plug-in boards (such as the Dionex **A/D Converter** or the **Pump Control Board**) or via the ➢*UCI-100* Universal Chromatography Interface the signals are sent to the

➢*Server* PC. In order to avoid that an individual board or interface has to be available for each device from which signals are recorded and to which signals are sent, respectively, the boards / interface provides several channels.

The different devices need not necessarily be part of the same ➢*Timebase*. To enable e.g. signal recording by detectors from different timebases the PC plug-in boards or the interface should not be assigned to one specific timebase. Instead, the devices of different timebases address the same board / interface, i.e., the board / interface is shared between these timebases. Therefore, the PC plug-in boards / interfaces are called **Sharable Devices**.

Each slot of a PC plug-in board / interface corresponds to a channel. The used channels must then have a signal assigned in the ➢*Server Configuration*. Install the corresponding device driver and assign the signals on the **Signals** page. The ➢*Remote Inject* and the ➢*Integrator Driver* are available for non-controlled systems (usually GC, but also non-controlled HPLC systems). The Integrator Driver can also be used to record the pump pressure.

The advantage of this conception is that you do not have to rewrite all ➢*Programs* concerned if you plan to connect a device to a different channel. Instead, just change the A/D port assignment in the respective driver.

Shared Relays and Inputs

Relays and remote inputs of the PC-plug-in boards (e.g. **A/D Converter** or **Pump Control Board**) and the ➢*UCI-100* Universal Chromatography Interface that are installed under ➢*Sharable Device* in the **Server Configuration** are **timebase-independent** (**Sharable Device**), e.g. they can by used and addressed by different ➢*Timebases*.

To make these relays and remote inputs visible as controls on a ➢*Control Panel* and usable in the case of a relay, the corresponding relay or the used remote input must be installed below the corresponding timebase.

As for any other device, it is necessary to load a device driver (**Add Device** command). For relays and remote inputs, choose the **Shared Relays and Inputs** device driver.

After installing the device driver, double-click the driver name to enable configuration. A tab dialog box will appear for relays (**Relays**) and another one for remote inputs (**Inputs**).

Each of the two tab dialog boxes shows the current assignment of the currently used relays and/or remote inputs. If there is no entry in the list, either no **Sharable Device** component was previously installed or the relays and remote

inputs have not been assigned. Press **ADD** to install a new relay or remote input.

Signal

The data transferred directly from an instrument (ideally a detector), either in analog or digital form via ➢*A/D Converter* or RS232 interface to the data system, is referred to as *physical* signals. If an instrument delivers several signals, these are also called channels (e.g. two different wavelengths of a UV detector). Calculated data, such as the arithmetic average of several channels, can represent a signal. This type of signal is called ➢*Virtual Signal*.

Each signal has its own signal name that is assigned during instrument installation. The symbolic name of each signal must be clear. Some special signals have pre-defined signal names assigned to them.

The properties of a signal are determined via separate ➢*Signal Parameters*. They can be modified manually or program-controlled (➢*PGM File*) at any time.

The measuring data of the different physical and virtual signals is stored in uniform raw data files.

Signal Name

The symbolic signal name is freely selectable, however, it must be unique. Within one system, no other signal can have the same name. ➢*Virtual Signals* also receive a signal name. This name is defined by the data system.

⚠ ***Caution***: The signal name is also stored within a partial method or a file. To be able to read and use older data at any time, the chosen names should not be changed!

Signal Noise

See ➢*Noise*

Signal Parameters

Each signal delivered by a detector has detector-specific parameters. These **signal parameters** can be modified on the instrument, or in the case of controlled systems, via the data system. A manual or program-controlled (➢*PGM File*) alteration is thus possible during chromatogram run time.

The following parameters are available for Dionex instruments and third party instruments controlled by the Dionex Chromatography Management System via device drivers:

Signal type	Parameter	Signal type	Parameter
UV channel	⇒*Step*	**Fluorescence channel**	➢*Excitation*
	⇒*Average*		➢*Emission*
	➢*Data Collection Rate*		➢*Gain*
	⇒*Wavelength*		➢*Response*
	⇒*Bandwidth*		➢*Sensitivity*
	⇒*Reference Wavelength*		⇒*Step*
	⇒*Reference Bandwidth*		⇒*Average*
3D-field	➢*Min/Max Wavelength*	**Electrochemical channel**	⇒*Step*
	⇒*BunchWidth*		⇒*Average*
	⇒*Step*		➢*Data Collection Rate*
	⇒*Reference Wavelength*		
	⇒*Reference Bandwidth*	**ESA channel**	⇒*Step*
			⇒*Average*
MS Channel	Min/MaxMass		
	FilterIndex		

☞ ***Tip***: In controlled systems, user input on the instrument is disabled.

Signal to Noise Ratio

The signal to noise ratio serves to characterize electronic components such as the ➢*A/D Converter* or a UV or photodiode array detector. The lower the noise, the smaller the possible signal variations that can be recorded. As a general rule, the average of a signal should be at least twice, better three times the standard deviation of the signal value.

The signal to noise ratio of the Dionex Photodiode Array Detector UVD340S is 0.5/100000 AU. Measurement of this technical specification is within a clearly defined scope. This includes the wavelength information (254nm), the

bandwidth, and the ⇒*Step*. The values can only be realized with an empty flow cell and a new but burnt-in lamp (approx. 40 h). The maximum signal variation (in AU) is measured at maximum light radiation through the flow cell.

If establishing comparable specifications is not relevant, the signal to noise ratio can be improved by the following operations:

- Selecting a low ➢*Sampling Rate*
- Using photodiode bunching (➢*Bandwidth*)
- Selecting the ➢*Optimum Integration Path*

Signal Value at Peak End

This peak result variable gives the signal value at the time of the peak end. The peak end is determined via the right peak delimiter.

Signal Value at Peak Start

This peak result variable gives the signal value at the time of the peak start. The peak start is determined via the left peak delimiter.

Signature

See ➢*Electronic Signature*

SIM (Selected Ion Monitoring)

SIM is the ➢*Mass Spectrometer* method used for recording an MS chromatogram at a specific mass. As only single ions are recorded with specific masses, the SIM mode is more sensitive than the ➢*Full-Scan* mode. You can use up to 32 channels, which are called SIM_1 to SIM_32, for data acquisition. In the SIM mode, too, one TIC channel is recorded which is the sum of the results of the individual SIM channels.

With SIM chromatograms, the counts of specific masses (or more exactly: with a particular mass-to-charge ratio) are added up. Thus, contrary to ➢*TIC* chromatograms, SIM chromatograms contain data of a specific mass.

Contrary to ➢*Mass Traces* that are extracted later from ➢*Mass Spectra* (see **How to ...: Actions Related to the aQa-MS Extracting Mass Traces**

Afterwards), SIM chromatograms are always recorded during data acquisition. If an important SIM channel is not taken into account during data acquisition, it can be extracted later as mass trace.

Also, see: **How to ...: Actions Related to the aQa-MS**  **Defining the Number of MS Channels**.

Single-Point and Multiple-Point Calibration

If the position of the calibration curve is determined only by the ➢*Calibration Points* of one ➢*Calibration Level*, this is called single-point calibration. In this case, the ⇒*Calibration Type* **linear** must be chosen.

If calibration points on different levels determine the position of the calibration curve, this is referred to as multiple-point (e.g., two-point, three-point, etc.) calibration. The number of calibration levels determines possible calibration types.

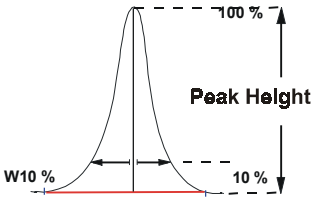
In both cases, the number of replicates is irrelevant for the number of calibration levels. Replicates only serve to statistically secure the measuring results.

Skewness

Similarly, to **Asymmetry**, the **Skewness** peak result variable is a measure for the column quality.

Its definition is also similar. This peak result variable is frequently mentioned in HPLC literature.

Skewness	Calculation
S	S = (RW10 + LW10) / (2 x LW10)
With:	
LW10	Left peak width in 10% of the peak height
RW10	Right peak width in 10% of the peak height



Also, see ➢*Asymmetry*.

Slope c1

The **Slope c1** calibration variable indicates the c1-value of the currently used ➢*Calibration Function*.

Smoothing

Data smoothing serves to reduce signal noise and help improve chromatogram appearance and reproducibility of peak baselines applying different digital filters without altering the raw data. The Dionex Chromatography Management System makes the following filter types available in the context menu of the Chromatogram window:

Moving Average (Boxcar)

The **Moving Average** (or **Boxcar**) filter equally weights each point. Thus, its ability to discriminate between noise and signal is limited (also, see ➢*Signal to Noise Ratio*).

Olympic

Compared to the **Moving Average** filter, the **Olympic** filter provides better rejection of impulse noise (spikes).

Savitzky-Golay

Savitzky-Golay smoothing is useful for reducing high-frequency noise of a data set that is continuous (such as a chromatogram) without significantly degrading the underlying signal.

For further details, see **How to ...: Actions in the Chromatogram**  **Performing Data Smoothing**

In addition, the Dionex Chromatography Management System allows smoothing MS chromatograms during acquisition or mass trace extraction using the Gaussian and Boxcar (= Moving Average, see above) filters which are both offered by ➢*Xcalibur*.

Gaussian

The Gaussian filter applies the Gaussian distribution for chromatogram smoothing.

For further information see **How to...: Actions Related to the aQa-MS** **Extracting a Mass Trace**.

For details on the different filter types and their respective parameters, see **Data Smoothing** in the Integration section.

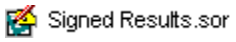
Snap to Grid

Use the **Snap to Grid** function to reduce, enlarge, or move the control frame in units of the mesh size.

Select **File/Preferences** to determine the mesh size of the grid.

SOR File (Signed Off Results)

SOR files (Signed Off Results) are electronically signed sequences (see: ➢*Electronic Signature*). They are indicated as follows:



SOR files merely contain the tabs with the corresponding data for the sequence that have been selected in the respective ➢*Report Definition File (RDF)*. The data cannot be changed unless the signature is undone. However, to do so, the user must have the **UndoSignResults** ➢*Privilege*. He/she has to re-enter his/her user-ID and the respective signature ➢*Password* if this has been defined accordingly in the ➢*CmUser* program (**File** menu > **Database Properties** > **Electronic Signature** tab).

Sound

The **Sound** command allows playing WAV files. The PC must be fitted with a sound card to support this command. WAV files are part of the Windows installation and contain various acoustic signals. Numerous example files are supplied e.g. in the WINNT/MEDIA directory (full Windows installation).

The command syntax of the Dionex Chromatography Management System for playing a WAV file is:

```
0.000  Sound    File= "Example.wav"
```

If the command cannot be performed due to a missing sound card, a default sound is generated at the PC speaker.

Also, see ⇒*Sound*

Spectra Calibration

Dionex UV Detectors UVD170S and UVD340S perform a spectra calibration after each **Lamp on** command. A ➢*Holmium-Oxide Filter* allows calibrating UV/VIS spectra recorded with the detector, due to the typical absorption spectrum of holmium oxide.

Dionex AD25 and PDA-100 detectors perform a spectra calibration at power up. New wavelengths are assigned to each pixel, based on the emission spectrum from the deuterium lamp.

With defined absorption maxima, spectra calibration ensures that the data delivered by the detector corresponds to the expected wavelength values.

Spectra Criteria

Apart from absorption values, each spectrum in a library contains various ID data fields that are freely editable by the user and that facilitate spectra searches. The following fields are available:

Column	Description
Name	This column shows the name under which the substance is included in the spectra library. Select a column entry to assign a new name to the corresponding substance.
ID	This column shows the short ID that is assigned to the spectrum. Use this column to save several spectra under the same substance name in a spectra library. The Ids (e.g. consecutive numbers). Then distinguish the spectra. ID
Column	**Description**
#Extrema	This column shows the number of extreme values in the spectrum determined by the system. Select a column entry to change the number.
Solvents:	This column shows the solvent in which the spectrum was recorded. Select a column entry to edit.
Comment:	Use this column to document details on the saved spectrum.
WL-Range:	This column indicates the wavelength range of the recorded spectrum.
WL-Resolution:	This column shows the ⇒*Bandwidth* with which the spectrum was recorded.
Ret.Time:	This column indicates the retention time at which the spectrum was

extracted from a peak.

Acq.Step: This column indicates the Step with which the underlying ➢*3D-Field* was recorded.

Detector: This column indicates the detector with which the spectrum was recorded. The name is taken from the **Server Configuration**.

Detector Serial No.: This column indicates the serial number of the detector from the **Server Configuration**.

Timebase: This column indicates the name of the timebase with which the spectrum was recorded.

Sequence: This column indicates the name and the patch of the sequence from which the extracted spectrum is taken.

Sample Name: This column shows the name of the sample from which the extracted spectrum is taken.

Acq. Date/Time: This column shows the date and time at which the spectrum or the underlying 3D-field was originally acquired.

Program: This column shows the name of the ➢*PGM File* which was used for generating the underlying chromatogram.

Extract Date/Time: This column shows the data and time at which the spectrum was extracted and saved.

Extract Operator: This column shows the name of the user who extracted the spectrum and saved it to the spectra library.

SQL (Structured Query Language)

SQL is a computer language that has been developed especially for queries in databases. The Dionex Chromatography Management System uses an adapted SQL for ➢*Queries* in the Browser (queries for specific samples/sequences) as well as for "Database Queries" in the report and in the ➢*Printer Layout*.

Standard

The **Standard** column input in the peak table defines the reference peak to be used for calibration. The term **Standard** can also be used for a calibration sample or a standard sample. Calibration can be performed with an external and/or internal standard.

Also, see ⇒*Standard*

Standard Deviation

Extracting the square root of the variance value produces the **Standard Deviation** calibration variable:

$$Std.Dev. = \sqrt{Variance}$$

Thus, the square standard deviation is the ➢*Variance*.

Status Bar

In the status bar on the lower window margin, messages regarding the current system status are shown on the left, the current timebase and the currently executed command are shown on the right.

The display of the status bar can be enabled and disabled via the **View** menu.

Step

The time interval between two successively recorded data points is referred to as step; the sum of all recorded data points is called raw data. The reciprocal value of the step value is the ➢*Sampling Rate*.

Also, see ⇒*Step*

Step Gradient

Immediate modifications to the solvent composition are referred to as step gradients. They ensure a rapid change of the elution conditions. The realization of the gradient on the column depends among others on the size of the dead volume between the pump and the column end.

Stop Flow

The **Stop Flow** command switches off the pump flow and interrupts data acquisition. A running batch is stopped, as in the hold mode.

Also, see ⇒*StopFlow*

Suck

See ➢*Draw*

Sucked

See ➢*Ready*

Suppressor

The Self-Regenerating Suppressor (SRS) and Atlas Electrolytic Suppressor (AES) are patented electrolytic eluent suppression devices from Dionex Corp. The suppressors reduce background signals and enhance analyte signals in ion chromatography using conductivity detection. Ion chromatography requires eluents that contain strong electrolytes. These electrolytes can interfere with detection of the ionic analytes of interest. The suppressors use ion exchange to neutralize (suppress) the electrolytes in the eluent, thus reducing the background conductivity. In addition, the ion exchange mechanism replaces a less conductive counter ion, with one that is highly conductive (hydronium ions in anion exchange and hydroxide ions in cation exchange). Because both the analyte and the counter ion produce the detector response, the analyte signals are increased. For details, see the Self-Regenerating Suppressor manual or the Atlas Electrolytic Suppressor manual.

Also, see: **How to ...: Device Control** **Controlling a Suppressor** and **Setting Atlas Suppressor Currents**.

Syringe Speed (AS50 Command)

The **Syringe Speed** AS50 ➢*Autosampler* command sets the speed of the sample syringe. Select the default value of 5 (the fastest) for water; select a slower setting for more viscous samples. The table below lists the sample syringe flow rates at each speed setting.

Syringe Setting	Flow Rate (ml/min)
1	0.06
2	0.12
3	0.24
4	0.6
5	2.4

Syringe Type

The volume that can be injected with an autosampler depends on the installed syringe type. Many autosamplers support several syringe types and thus allow

using a different type with a larger or smaller volume. In addition to the default types 25, 50, 100, 250, 500, 1000, and 4000 µl, using special syringes is possible. If the syringe type is changed, the new type must be specified in the **Server Configuration** of the Dionex Chromatography Data System. In addition, when installing a new autosampler, the currently used syringe type must be defined by configuring the corresponding device driver.

Caution: For the autosampler Dionex GINA 50, syringe types with the volumes 250 µl and 1000 µl are supported. If using different syringe types, the reproducibility stated in the instrument's specification cannot be guaranteed.

System Suitability Test (SST)

As defined in cooperation with EURACHEM, System Suitability Checking (SSC) or System Suitability Test (SST) is "a series of tests to check the performance of a measuring process " [P. Bedson and M. Sargent, Accred. Qual. Assur. (1996) 1, 265-274]. Aim and objective of System Suitability Testing is to ensure the performance of the operating system and the system.

SST or SSC can be applied to single measuring processes and thus may be part of the validation process. The System Suitability Test establishes for example that the operational conditions required for a specific measurement process are being achieved.

Tip: If you want to perform a System Suitability Test, ensure to enter the QNT file into the sample list before starting the analysis. Otherwise, the batch cannot be aborted in case of **Fail Action** - **Abort Batch** because the SST will not yet be performed during the batch run!

In addition to the System Suitability Test, ➢*Operational Qualification* and ➢*Performance Qualification* are also important for validating instruments and software (see **Validation**).

For details on how to perform a system suitability test in the Dionex Chromatography Management System, see **How to ...: Actions in the QNT Editor Defining the System Suitability Test**.

Tailing/Fronting Sensitivity Factor

This detection parameter is an implicit threshold for setting the peak end. The **Fronting sensitivity factor** refers to the peak start, respectively.

Also, see ⇒*Tailing/Fronting Sensitivity Factor*

For information on how to apply the detection parameters, see

How to ...: Actions in the QNT Editor Modifying Detection Parameters.

Temperature Compensation Factor

A temperature coefficient used in conductivity detection to stabilize conductivity readings. The temperature compensation factor corrects for changes in ambient temperatures that occur during a run and normalizes conductivity measurements to 25 °C.

If the cell is installed in a ➢*DS3 Detection Stabilizer* or a chromatography oven, the default factor of 1.7% is appropriate. When operating without a DS3 or oven, the compensation factor can be optimized to help minimize the baseline drift caused by fluctuations in ambient temperature. See the detector operator's manual for details.

Template

Templates facilitate entering data. The Dionex Chromatography Management System offers various pre-defined templates, e.g. report templates (DEFAULT.RDF and DEFLTDAD.RDF).

Theoretical Plates

The **Theoretical Plates** peak result variable is a measure for the separating capability of the column. Theoretical plates are calculated from the peak width and the corresponding retention time. As with asymmetry, there are different US and EU standards:

Name	Calculation	Comment
Theoretical Plates	$TB = 5.54 * (TRET / W50\%)^2$	EU standard
Theoretical Plates	$TP = 16.0 * (TRET / BW)^2$	US standard
Theoretical Plates	$TB = 5.55 * (TRET / W50\%)^2$	JP standard

With:

TB or TP:	Number of theoretical plates
TRET	Retention time
W50%	Peak width at 50% height (half-width)
BW	➢*Peak Width* on the base line.

TB or TP do not have a dimension. If they are placed in relation to the currently used column (L), the result is the theoretical plate height (H):

$$H = L / TB \quad \text{or} \quad H = L / TP$$

However, the reciprocal value says more about the quality of the currently used column. It gives the number of theoretical plates per column meter.

$$1 / H = TB / L \quad \text{or} \quad 1 / H = TP / L$$

Select the report column, choose the **Column Properties** command from the context menu, and select the variable in the selection box. Press the **Parameter** button to determine whether the calculation is based on the EU, US, or JP standard.

TIC (Total Ion Current)

TIC chromatograms add up all counts at the respective retention time. Contrary to ➢*SIM* chromatograms, TIC chromatograms include the data of the entire mass range.

Independent of the mode in the MS method (Full-Scan or SIM), a **TIC** channel is recorded. In ➢*Full-Scan* mode, up to four additional **TICF**_n channels can be recorded for which the data acquisition conditions may vary (e.g., the acceleration voltage in the ➢*Mass Spectrometer*). The channels are called TICF_1 to TICF_4. The **TIC** channel summarizes the results of these individual channels. A TIC channel can be recorded in SIM mode as well. In this case, it corresponds to the sum of the results of the single SIM channels.

From the ➢*Mass Spectrum*, separate ➢*Mass Traces* (this may be mass ranges as well) can be extracted and saved as new channels (see **How to ...: Actions Related to the aQa-MS**  **Extracting a Mass Trace**. In this way, you can limit the size of the mass range of TIC channels according to your requirements.

Also, see: **How to ...: Actions Related to the aQa-MS**  **Defining the Number of MS Channels**.

Time

The Dionex Chromatography Management System stores the time stamps as universal time (Greenwich time). However, the date notation is displayed according to the local settings chosen in the operating system (also, see ⇒*Inj. Date/Time* (Time of Injection)).

Timebase

All components combined in a chromatography system to enable the chromatographic separation and related in a time context with each other, are assigned to the same timebase.

A timebase can be a very complex system (e.g. two pumps, one autosampler, one column oven and two detectors switched in series). However, an isolated integrator or a gas chromatograph can be a timebase as well.

Only another system that is completely independent represents a new timebase. Administration of different timebases is on one or several ➢*(Chromatography) Servers*.

The name of a timebase and the assignment of the devices are specified in the ➢*Server Configuration*.

Toolbars

Frequently used commands and features are available as icons; related functions are combined on toolbars directly below the menu bar. When starting the Dionex Chromatography Management System, the standard toolbar is displayed. Select the **Toolbars** command from the **View** menu to enable or disable the display of individual toolbars. The following toolbars are available:

- Standard (standard functions)

- Online (commands for the ➢*Control Panels*)

- Layout (commands for the ➢*Layout Mode* are via the ➢*Layout Toolbar*)

- Method (for changing to other method sections, samples, or channels)

- Integration (commands for processing chromatograms)

- ➢*Status Bar* (enables/disables the Status Bar)

Move the mouse pointer over an icon to view its name in the **quick info** display.

Transmission

Transmission is 100%, when light passes through the UV detector flow cell without restraint. Transmission decreases with increasing absorption. For the UVD 340S detector, the maximum transmission value is determined via zero order at a reference wavelength of 630nm.

Caution: The substance mixture passing through the flow cell must not absorb in the reference wavelength range. If this is the case, either change the reference wavelength or select transmission without reference.

Tray Temperature (AS50 Command)

The **Tray Temperature** AS50 ➢*Autosampler* command sets the temperature of the sample tray to between 4°C and 60°C. This command is available only when the AS50 sample temperature control option is installed.

Trigger Commands

A trigger refers to the automatic execution of a command as soon as a condition becomes true.

The **Trigger** command can be included in a ➢*Program* or a programmable button, but not in the online control. The following syntax is valid:

```
Time    Trigger TRIGGERNAME    Condition,True,Delay,Limit,Hysteresis
        Reaction 1
        Reaction 2
        Reaction ...
Time    EndTrigger
```

Note: A pure basis license does not include the advanced feature **Trigger** (also, see **Options of the Dionex Chromatography Management System**).

Also, see ⇒*Trigger Commands*

TTL

TTL (Transistor-Transistor Logic) inputs and outputs are electronic switching devices for controlling instruments.

TTL Input Mode

The PDA-100 TTL inputs respond to four types of device output signals. The default TTL signal mode, normal edge, is compatible with the output signals provided by Dionex modules.

If the device connected to the PDA-100 outputs a different signal type, select a different signal mode

The four input signal modes are:

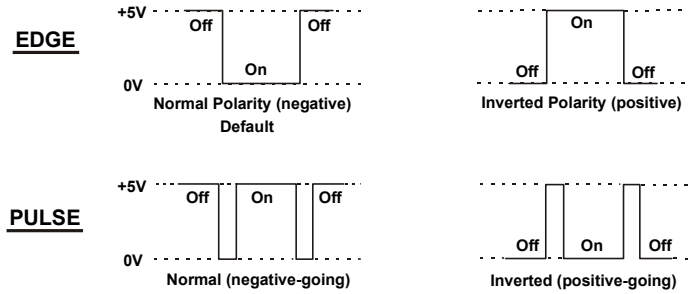
Normal Edge: In normal edge operation, the negative (falling) edge of a signal turns on the function and the positive (rising) edge turns off the function.

Inverted Edge: The inverted edge mode works identically to the normal edge mode, except that the positive and negative edges are reversed in function.

Normal Pulse: In normal pulse operation, the negative (falling) edge of the TTL signal is the active edge and the positive (rising) edge is ignored.

The minimum pulse width guaranteed to be detected is 50 ms. The maximum pulse width guaranteed to be ignored as noise or invalid is 4 ms. The action of the PDA-100 is undefined for pulses less than 50 ms or greater than 4 ms.

Inverted Pulse: The inverted pulse mode operates identically to the normal pulse mode, except that the positive and negative edges are reversed in function.



Type (Peak Type)

The **Type** peak result variable classifies a peak as main peak (M=Main) or ➢*Rider* (R=Rider). This variable also indicates the type of baseline contact (B=Baseline) and whether the peak data has been manually modified (*=modified).

Also, see ⇒*Type (Peak Type)*

UCI-100 Universal Chromatography Interface

The UCI-100 Universal Chromatography Interface serves as a data acquisition and device control module. It provides several different interfaces and makes them available to the chromatography server:

- Analog inputs
- Serial RS232 ports
- Digital inputs
- Digital outputs
- BCD inputs

For communication between the different devices and the server's chromatography data system, either a USB or an Ethernet connection can be used.

☞ ***Tip***: Use the RS232 interfaces (COM ports) via USB only (**no** TCP/IP)! NT4 computers do not support USB. Thus, if LAN connections are required, additional Equinox boards must be used for instrument control via RS232. We recommend using a peer-to-peer connection for analog data acquisition via LAN

(= installation of a second network interface card (= NIC; in the operating system = adapter) in the server PC - see **Connecting the UCI-100 via a Peer-to-Peer Connection under NT4**).

☞ ***Tip***: Always connect instruments requiring a GSIOC cable (such as **GILSON** devices and the **VARIAN/RAININ** (Pumps)) to the multi-serial 8-fold PCI interface board (Equinox 8-RS232 Multi-COM card, Dionex part no. 5906.2095). Otherwise, communication problems might occur with other RS232 ports (e.g. with the COM ports of the PC or the Dionex Universal Chromatography Interface (UCI-100)). The power supply of the GSIOC adapter (type 605) is directly via the RS232 interface. The RS232 ports of the UCI-100 Universal Chromatography Interface, however, are not designed for this.

Also, see **Dionex Universal Chromatography Interface (UCI-100)**

UI20 Universal Interface

The UI20 Universal Interface functions as a communications and control link between the PC and instruments that are not directly connected to the ➢*DX-LAN*. This enables the Dionex Chromatography Management System to collect data from any chromatographic detector with an analog output. The UI20 collects up to two analog detector voltage signals and converts them to digital data with 20-bit resolution.

Unzoom

The **Unzoom** command undoes the last zoom operation.

In the signal plot, the Unzoom command can be performed by double-clicking in the ➢*Overview Window*.

Use Recently Detected Retention Time

This ⇒*QNT Editor* parameter (**General** sheet) defines whether the retention time stored in the peak table (nominal time) is used by default to identify a peak or whether the actual retention time of a peak in the last sample is used.

The parameter serves to compensate many types of drift appearances (e.g. evaporation of volatile components in pre-mixed solvents or column aging).

Also, see ⇒*Use Recently Detected Retention Time*.

User Database

The user database defines the user rights (= ➢*Privileges*) and the membership of the individual users in ➢*Access Groups*. Creation of the user database is in the ➢*CmUser* program. Activation of the user database is in the CmSecure program so that the ➢*User-Mode* is enabled.

☞ ***Tip***: Due to the similarity of the term, do not confuse a user database with a ➢*Datasource* (database) of the Dionex Chromatography Management System. Although both may be e.g. ACCESS databases (= mdb container), they are two completely different databases.

User-defined Columns

The Dionex Chromatography Management System contains tables with different meanings at various positions within the program, for example:

- The different tables in the **Report** and in the ➢*Printer Layout*
- The sample list in the **Browser**
- The peak table in the ⇒*QNT Editor*... .

While the user defines the Report and the Printer Layout, anyway, the form of the sample list and peak table is mainly default. Nevertheless, you can define your own columns in all three tables.

In the Report and the Printer Layout, new columns can be created via the ➢*Report Publisher* to display special aspects of your data. For further information, see **How to ...: Actions in the Printer Layout Entering User-defined Formulas**.

User-defined columns in the sample list and the peak table can be used as further variables for generating a report. In the sample list, they can be used in addition as further search words for a ➢*Query*. Also, see **How to ...: Actions in the Browser Creating User-defined Columns**.

***Tip**:* Be careful when creating user-defined columns in the sample list of the Browser. Do not assign column names twice in different ➢*Datasources* or even on different computers that may communicate with each other. Otherwise, unless the column definitions are identical, problems may occur when copying sequences or during the **Restore** of backup files.

User Mode

The User Mode (= Access Control) can be enabled and disabled via the CmSecure program. When the User Mode is enabled, the Dionex Chromatography Management System offers numerous options to limit user access to ➢*Servers*, ➢*Timebases*, ➢*Clients*, and ➢*Datasources*.

System access is password-protected. Access is only granted to users who are identified by the system after password input.

Each user identified by the system is granted personal privileges. The system administrator assigns these privileges. Via the ➢*Access Group* and ➢*Privilege* group membership of a user, the administrator defines the operations the user can perform within the system.

If access control is disabled, each user receives all rights. Datasources or directories that have access groups assigned cannot be accessed when the User Mode is disabled. With enabled User Mode, the user can access an object if he/she is a member of a group granting access to the respective object. If no access group is assigned to an object, each user can access the object independently of his/her access group membership.

Enabled User Mode allows the user to access any object provided it is part of the respective access group. The sum of all privileges granted to the user (depending on his P-group membership) determines what the user is allowed to do with the object. Signing sequences electronically (see ➢*Electronic Signature*) is possible with enabled User Mode only.

For a detailed description, see **Access Control**.

UV Cutover

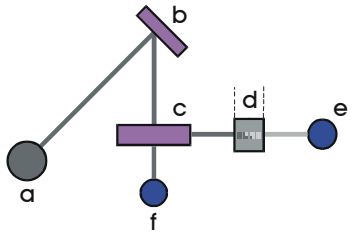
The **UV Cutover** command for the AD20 Absorbance Detector sets the wavelength above which the second order filter is inserted in the light path. Typically, the UV cutover wavelength is 380nm.

UV Detector

UV detectors (strictly speaking UV/VIS detectors) serve to quantify absorption of UV/VIS-active substances in the range from 190 to 380nm (UV range) and 380 to 900nm (VIS range). UV detectors provide high sensitivity and a large linearity range. UV detectors are relatively independent from temperature fluctuations; they can be used for gradient elution (%-gradient).

Functionality

A grating (b) disperses the light that is emitted from a light source (a) in a discontinued spectrum. Simultaneously, the grating serves as a filter and directs only the wavelengths required for detection to a beam splitter (c). A portion of the beam is directed through the flow cell (d) onto a photodiode (e), the other part is used as a reference (f).



Theory

Depending on the absorptivity (ε) of the substance, the light beam is more or less attenuated when traversing the flow cell. For the absorption (*E*), the following is true:

$$E = \varepsilon \, c \, d$$

As the length of the cell (*d*) is constant and the absorptivity (ε) depends only on the substance itself or the absorbed wavelength, there is a direct connection between the substance concentration (*c*) and the absorption (*E*). The absorption measured in AU ("absorbance unit") is thus proportional to the number of particles in the beam path ("Lambert-Beer absorption law").

Spectra Calibration

Spectra calibration is performed automatically after each ⇒*Lamp On/Off* or ⇒*Connect* command (**detector calibration**). The **CheckWavelength**

command allows you to include the largest wavelength deviation of this calibration in the **Audit Trail**.

A calibration is possible only when certain conditions are met:

1. During calibration, the baseline must be sufficiently stable. This may not be the case e.g. when the solvent composition was modified or when there were air bubbles in the solvent.
2. The solvent in the cell must not be fully absorbing in the wavelength range that shall be calibrated. This will be the case e.g. if the cell is filled with 96% hexane / 4 % ethyl acetate.
3. Ensure for the calibration that the deuterium lamp is already warm because its spectrum changes much during the first minutes after switching on the lamp.

If these conditions are not met, the process will be interrupted with the corresponding error message. When the problem is solved, repeat the calibration using the **Disconnect** command first followed by **Connect**.

Detector Calibration

To calibrate the detector, the transmission spectrum of the deuterium lamp is compared with that of the holmium oxide filter. With the resulting spectrum, the maxima are determined and are compared with the holmium oxide values stated in the literature. If, for a maximum, a difference is detected between the measured and the known value, an interpolation is performed between this maximum and the two adjacent maxima to correct the wavelength allocation of the affected photodiodes. The spectra calibration can take up to 2 minutes. During this time, data acquisition is not possible.

Also, confer ➢*Photodiode Array Detector*.

UV Lamp

This command switches the UV lamp on Dionex absorbance and PDA detectors on and off. For the AD20 Absorbance Detector (see ➢*UV Detector*), the command options are Low, High, and Off.

☞ ***Tip***: If you switch the AD20 lamp from Off to Low or High, there is a 22 second pause while the UV lamp warms up. During this time, the status of the lamp on the ➢*Control Panel* remains at Off. Once the warm-up period is complete, the status changes to the selected setting (Low or High). The Audit Trail window logs the

UV_Lamp command and the warm-up time.

☞ ***Tip***: Detector lamps require a considerable warm-up time for high-sensitivity and drift-free operation. Therefore, the ⇒*Inject* command should be placed 10 minutes (minimum) after the lamp is switched on. Note also that lamp(s) should never be switched off during a sample batch.

Validation Sample

Samples of known concentration that serve to verify a calibration are referred to as validation samples. In the sample list, they are labeled with the sample ⇒*Type* **Validate** and have the following symbol: .

Verification is by regular insertion of the validation samples in the normal analysis. The resulting (actual) area values are converted into amounts via the ➢*Calibration Function* and parameters and are then compared with the expected (nominal) values in the ⇒*Amount* table. The result of the nominal/actual comparison can be displayed as direct amount (Result Variable **Amount Deviation**) or as deviation in percent (**Rel. Amount Deviation**).

Checking can also be performed visually if you display the validation samples (marked by colors) in the calibration curve. They will not be considered for calibration, though.

Validation samples can also be injected from vials that are normally used for injection of standard (calibration) samples. Validation samples are not relevant for the calculation of the calibration function!

For further information on validation samples, see **How to ...: Actions in the QNT Editor**:

Entering the Concentration/Amount of the Validation Sample

Validating the Calibration Curve

Valley to Valley

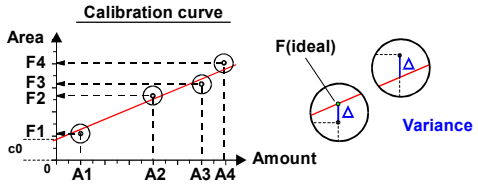
The activated **Valley to Valley** detection parameter draws the baseline from peak minimum to peak minimum below non-resolved peaks, i.e., from peak end to peak end.

Also, see ⇒*Valley to Valley*

For in formation on how to apply detection parameters, see **How to ...: Actions in the QNT Editor** **Modifying Detection Parameters**.

Variance

The **Variance** calibration variable is the average deviation of all area values F from the corresponding ideal area value in a calibration. The ideal area value is the value at the point of intersection between the calculated calibration curve and the corresponding amount value.



Variance is therefore a criterion for the measuring accuracy in the calibration. With an increasing value, calibration points are increasingly scattered.

The mathematical description of the variance is as follows:

$$Variance = \frac{1}{N-m}\sum_{i=1}^{N} W_i * (Y_i - F(X_i))^2$$

N: Number of standard samples involved in the calibration,

m: Number of coefficients to determine (depending on the ⇒*Calibration Type*: LIN: *m* = 1; LOFF: *m* = 2; QUAD: *m* = 2; QUOFF: *m* = 3 and EXP: *m* = 2),

i: Index for standard samples,

F(x): Model function of the calibration,

Xi: X-value of the standard sample no. i,

Yi: Y-value of the standard sample no. i,

Wi: Weight factor of the standard sample no. i, and

Δ i: *Yi - F(Xi)*

If the square root of the variance value is extracted, the result is the ➢*Standard Deviation* calibration variable, i.e., the square standard deviation is the variance.

Variance Coefficient

The **Variance Coefficient** calibration variable can be considered a type of **normalized** ➢*Variance* value. It is more meaningful when comparing variances

of different peaks with different concentrations. A variance coefficient near zero means that the calibration curve well approximates the calibration points.

Thus, the variance coefficient indicates how well the data points correspond to the theoretically assumed course of the curve. Similar to ➢*Coefficient of Determination* and in contrast to the ➢*Correlation Coefficient* it depends on the calibration type. The mathematical description of the variance coefficient is as follows:

$$VarCoeff = \sqrt{\frac{\sum_{i=1}^{N} W_i * (Y_i - F(X_i))^2}{\sum_{i=1}^{N} W_i * Y_i^2}}$$

N: Number of standard samples involved in the calibration,

i: Index for standard samples,

F(x): Model function of the calibration,

Xi: X-value of the standard sample no. i,

Yi: Y-value of the standard sample no. i,

Wi: Weight factor of the standard sample no. i.

Virtual Channel Driver (VCD)

The Virtual Channel Driver offers the possibility to record, display, save, and export the system status (e.g. relay status, gradients, pump pressure) or ➢*Virtual Signals* (e.g. UV_VIS_1/UV_VIS_2) as signals. The **Virtual Channel Driver** allows you to calculate any arithmetic expression during data acquisition, and then display the result as a signal channel and save it. Any combination of numeric characters can be used as terms in the expression.

For information on how to install the Virtual Channel Driver (VCD), see **Virtual Channel Driver: Installation**.

Virtual Signals

Signals that are composed of or calculated from several readings at the time t are referred to as virtual signals (e.g. the arithmetic average of several channels or the signal of a photodiode array detector). Virtual signals frequently have ➢*Reserved Signal Names* (e.g. 3DFIELD).). Virtual signals are generated with the ➢*Virtual Channel Drivers*.

As virtual signal cannot be generated manually, the corresponding program must be started. For information on how to enter commands, see **How to ...: Device Control Virtual Channel Commands**.

Visible Lamp

This command switches the visible lamp of Dionex absorbance (see: ➢*UV Detectors*) and ➢*Photodiode Array Detectors* on and off. For the AD20 Absorbance Detector, the command options are Low, High, and Off.

☞ ***Tip***: Detector lamps require a considerable warm-up time for high-sensitivity and drift-free operation. Therefore, the ⇒*Inject* command should be placed 10 minutes (minimum) after the lamp is switched on. Note also that lamp(s) should never be switched off during a sample batch.

Volume

See ➢*Injection Volume*

Wait

The **Wait** command interrupts program execution until the specified remote input signal arrives. During this time, program time and data acquisition are stopped. Controlled pumps are kept in the **Hold** mode.

For examples for using the **Wait** command, see the following topics: **How to ...: Device Control**:

Control - Autosampler

Special Commands, Relays, and Others

Also, see ⇒*Wait*

Wait for Stable Temperature (AS50 Command)

The **Wait for Stable Temperature** AS50 ➢*Autosampler* command delays the start of a timebase program until the temperature of the thermal compartment and/or sample tray has stabilized.

Wash

The **Wash** command causes the autosampler to lower the needle into the needle seat and to rinse the sample loop and needle with solvent in the **Inject** state. This corresponds to the normal solvent flow following an ⇒*Inject Command*.

☞ ***Tip***: Use the **Wash** and ⇒*NeedleUp* commands to wash the sample loop and thus prevent crystallization of substances in the sample loop.

Also, see ⇒*Wash*

Waveform

A series of steps, defined as points on a plot of potential vs. time. A waveform must be defined when using the Dionex electrochemical detector in ➢*Integrated Amperometry Mode*.

Wavelength

➢*UV Detectors* and ➢*Photodiode Array Detectors* are the most commonly used detector types in HPLC. Simple UV detectors record chromatograms at a defined wavelength (λ) while PDA detectors record them in a defined wavelength range. The wavelength and the wavelength range, respectively, depend on the detector and can vary between 190 to 900 nm.

This value indicates the wavelength at which a chromatogram is measured.

On Dionex photodiode array detectors, the wavelength is not set directly on the instrument, but via the PC. In Dionex Chromatography Management System installations with a controlling option, the wavelength can also be entered manually during the analysis or in the ➢*PGM File*.

In the case of the UV-VIS, 3DFIELD, and SPECTRA signals, wavelength means the central wavelength, i.e., the wavelength around which a field with a symmetrical ⇒*Bandwidth* is formed.

Also, see ⇒*Wavelength*

Wavelength Switching

The exact switching of the measuring wavelength on a UV detector is referred to as wavelength switching.

Wavelength switching allows simultaneously measuring substances with strongly differing absorption maxima and no or little absorption at the wavelength of the other maximum.

Generally, switching the wavelength is program-controlled, i.e., the switch times at which the wavelength of a specific channel is changed, is entered in a control ➢*Program*. This can also be performed by extracting the ➢*Optimum Integration Path* from an opened ➢*3D-Field* (**Extract: Opt.Int.Path to Clipboard**).

***Note**:* With fluorescence detectors, wavelength switching is also possible. In virtually all cases, the excitation wavelength must be changed at the exact time in addition to the detection wavelength.

Weights

The **Weights** calibration variable indicates the weighting (see **How to ...: Actions in the QNT Editor Weighting and Averaging Calibration Points** in the **Creating a Peak Table** chapter) assigned to the individual ➢*Calibration Points* when creating the calibration curve.

Define the weighting in the ⇒*Calibration Type* column of the ⇒*QNT Editor*. The following options are available:

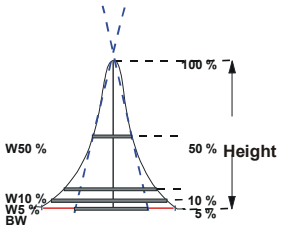
No weight	Default: higher weighting of higher amounts.
1/Amount (X)	Nearly cancels out the weighting of higher amounts/signal values.
1/Amount^2 (XX)	Causes over-proportional weighting of smaller amounts.

1/Response (Y) Nearly cancels out the weighting of higher signal values. In this case, the Y-values (dependent signal values) of the ➢*Calibration Points* are used as weight factors instead of the X-values (nominal amounts).

1/Response^2 (YY) Causes over-proportional weighting of smaller signal values. In this case, the Y-values (dependent signal values) of the calibration points are used as weight factors instead of the X-values (nominal amounts).

Width

This peak result variable refers to the peak width *extrapolated* on the baseline. Peak tangents are drawn from the turning points of the ascending and the descending flanks. Then the points of intersection with the baseline are calculated. The time distance between the two points of intersection is defined as the base width. If the base width is used for calculating other parameters, the abbreviation is **BW**.



The Dionex Chromatography Management System also determines the peak width at 5, 10, and 50% of the peak height (abbreviations: W5%, W10% and W50%).

⚠ ***Caution***: In contrast to the base width **BW**, the peak widths at 5, 10, and 50% of the peak height (W5%, W10%, and W50%) are not only measured up to the point of intersection with the two tangents, but up to the signal curve!

Determining the peak width is only possible if the peak is resolved at least to half the height.

If you wish to display the peak width in the report, please proceed as follows: Select the column in the report, choose the **Column Properties** command from the context menu and select the **Width** variable in the selection box. Press the **Parameter** button to determine at which peak height to determine the peak width.

Window

The **Window** peak table parameter defines the tolerance interval, within which the peak is expected. Adding and subtracting the window value to the retention time (retention time +/- window value), determines the window size, i.e., the window always has twice the width of your input. In addition, the value can be interpreted as absolute or relative value:

Also, see ⇒*Window*

Wizard

Various input procedures such as creating a ➢*Sequence*, or a ➢*Program* or defining ➢*Query* conditions are facilitated by using **Wizards**. The system prompts the user to define conditions and to enter the required information. The Wizard then adds default elements and thus completes a basic structure. If required, the user can extend or modify this structure according to individual requirements.

Use the Wizards to avoid unnecessary typing, syntax errors in command entries and overlooking important information and parameters.

Worklist

The format for reading data (sequences) of a ➢*LIMS* in the Dionex Chromatography Management System is referred to as Worklist (WLE file). The worklist describes the contents and the structure of a sequence (also, see ➢*Worklist Format*).

Choose the **New...** command from the **File** menu and then **Sequence (From LIMS Worklist)** to import an existing worklist.

If importing is possible, the imported sequence is listed in the Browser. The existing worklist is deleted to prevent importing it again.

If an error occurs when importing, the Dionex Chromatography Management System reports an error describing the error and the error location in the worklist. The error message is also saved in a log file. This log file carries the worklist name and the extension **log**. The incorrect worklist file is renamed to ***.err**.

Worklist Format

Worklists have the file extension **.wle** (Work List Export). The structure and the syntax of the ➢*Worklists* are similar to the Windows **INI** files.

There are various sections. Each section starts with a new line. The name of he section is written in brackets. There are one or several entries below the section name, with the syntax *name* = *value*. Comments start with a semicolon and finish at the end of the line.

Example of a valid worklist:

```
; Worklist generated by MegaLIMS 3.11.5622.00a
; Wed 05/27/98, 16:25:02

[options]
Application = CHROMELEON
Delete Worklist = No
Rename On Error = No

[file names]
; datasource, path, and name for the generated sequence
Sequence = \labor2_local\sys58\sequences\lims4711
; default for the program column
pgm = pgm0815
; default for the QNT method column.
qnt = qnt0815
; copy ➢PGM Files from here (datasource, and path)
pgm templates = \server1\templates\hplc

; copy ➢Quantification Methods (QNT Methods) as stated here (datasource, path, and name)
[qnt files]
qnt0815 = \server1\templates\hplc\pah\qnt0815
noint = \server1\templates\common\noint

[defaults]
; default for injection volume
Injection Volume = 10.0
```

[1]
Name=Wash
Type=Blank Run
Pos=1
; use the "Wash" program instead of the default ("pgm0815")
PGM=Wash
QNT=NOINT
; default for the user-defined column **Water Contents** - the marking asterisk * is omitted with ➢*User-defined Columns*
Water contents = 72.3

[2]
Name=Std
Type=Standard
Pos=99

[3]
Name=Sample1
Pos=2

[4]
Name=Sample2
Pos=3

[5]
Name=Sample3
Pos=4

[6]
Name=Sample4
Pos=5

[7]
Name=Stop
Type=Blank Run
Pos=1
PGM=Stop
QNT=NOINT

With this worklist, a sequence named **lims4711** is created in the datasource **labor2_local** in the **sys58\sequences** directory. The sequence contains a rinse sample, a standard, four unknown samples, and a stop program.

All control programs are copied from the subdirectory **\templates\hplc** of the datasource **Server1** (central file server). The source must contain the **pgm0815**, **wash**, and **stop** programs.

The evaluation method for the rinse and stop samples is copied from **\templates\common\noint.qnt**, the method for the analysis samples is copied from **\templates\hplc\pah\qnt0815.qnt** (both in the datasource **server1**).

Path Information

The entire path information of the worklist is related to the data structure of the Dionex Chromatography Management System. Therefore, the path name starts with the ➢*Datasource*, not the hard disk name. Relative paths are not accepted. Path names can be expressed either in the internal syntax of the Dionex Chromatography Management System (**Moniker**) (e.g. SEQ::\labor2_local\sys58\sequences\lims4711) or in a simplified syntax (as above), which omits the type abbreviation and the double colon. In this case, a slash or a colon can be used instead of the backslash.

```
Sequence = SEQ::\labor2_local\sys58\sequences\lims4711
Sequence = \labor2_local\sys58\sequences\lims4711
Sequence = Labor2_local:sys58/sequences/lims4711
```

All of the above paths refer to the sequence lims4711 in the directory sys58/sequences of the datasource Labor2_local.

Do not include type extensions (**.PGM**, **.QNT**, **.SEQ**) in the path information.

Handling of PGM Files and QNT Files

The program and the method columns of the sequence only include the file name without the path information, as the files are always located in the sequence. The same applies to the corresponding options (PGM= and QNT=) in the WLE file (see below).

The LIMS import module creates these files by copying them to the sequence. There are two possibilities to specify where to find these templates to copy:

- If all used files of a type are located in the same directory (the template directory), its path can be determined in the section [file names] via

  PGM Templates = *path to template directory* or. **QNT Templates=** for QNT files

The Dionex Chromatography Management System searches the corresponding template directory for a file with the specified name and copies this file to the sequence.

- If the copy templates are located in different directories, the path of each section has to be given in the section '[PGM file]' or '[QNT files]'. On the left side of the equal sign, the file name is located, and on its right side, the complete path of the template is indicated.

  Technically, it may be possible that the file name of the template differs from the name of the copied file. However, this will not be accepted.

Both methods can be mixed. In case of doubt, the second method has priority. If there is an entry in the section [PGM files], the PGM template file is not searched.

If all samples use the same PGM and QNT files, it makes no difference which method is used.

Section [OPTIONS]

The options listed in this section will influence the import function. Usually, no entries are required here. When testing a worklist, it may be useful to disable the **Delete Worklist** and **Rename On Error** commands. Thus, the worklist is retained instead of being deleted after importing.

Application = Chromeleon indicates that this worklist is intended for the Chromeleon. If there is a different entry here, the worklist will not be accepted by the Chromeleon. In this case, no log file is created, and the worklist is neither deleted nor renamed.

Computer Name = <Name of PC> indicates where to copy the worklist. If this entry does not correspond to the local computer, the worklist is not accepted. In this case, no log file is created, and the worklist is neither deleted nor renamed.

Log Error = Yes creates a log file containing the error message in the event of an error.

Log Success = Yes creates a log file documenting the successful import.

Delete Worklist = Yes deletes the worklist when importing was successful.

Rename On Error = Yes renames the worklist in ***.err** in the event of an error.

Character Set = Windows indicates the character set of the worklist. Any generated log file is also written with this character set. Change this option if some special characters, e.g. umlauts, are not transferred correctly. Valid values: Windows or ANSI (system character set, i.e. no conversion) DOS or OEM (PC character set, conversion by Windows function OEMToAnsi).

Section [FILE NAMES]

This section determines various file names. **Sequence =** indicates the path and the name of the sequence to generate. This parameter must always be specified. **PGM =** or **QNT =** determines the default value for the PGM column or the QNT column. (The default value can be overwritten for each sample).

PGM Templates = and **QNT Templates =** determine the corresponding template directory (see above).

Sections [PGM Files], [QNT Files]

The sections define from where to copy the PGM and the QNT files. Entries in this section take priority over a template directory. Entries have the following syntax:

name = path

On the left side of the equals sign, the file name is located, and on its right side the complete path of the template.

Section [DEFAULTS]

This section defines default values for various sample variables. **Name=**, **Comment=**, **Pos=**, **Type=Unknown**, **Status=Single**, **Sample Weight=1.0**, **Dilution Factor=1.0** and **Injection Volume=20.0** have the same meaning as in the Browser. The corresponding value range is also identical.

Note: The default values for the PGM and the QNT files are defined in the section [FILE NAMES].

Section [SEQUENCE]

This section defines the properties of the sequence.

Title = Created from worklist <Name of Worklist> determines the name (description) of the sequence.

Timebase = determines the timebase on which the sequence is executed.

Report = determines the default value for the report template (appears in the print dialog)

Channel = determines the default value for the channel when printing (appears in the print dialog)

Section [n] (Sample Data Records)

Each sample is described by one section. The section must have the name [*n*], where *n* is the sample number (without leading zero). The samples must be numbered consecutively. With a new sequence, sample numbering must start with 1. Samples can be appended to existing sequences. In this case, sample numbering must start with the next free sample number in the sequence (as number of samples in the sequence plus one). A sample section can have the entries **PGM=**, **QNT=**, **Name=**, **Comment=**, **Sample ID=**, **Replicate ID=**, **Pos=**, **Type=Unknown/Blank/Validation/Standard/Matrix**, **Status=Single/Multiple/Finished**, **Sample Weight=1.0**, **Dilution Factor=1.0** and **Injection Volume=20.0**. Missing entries are completed by the defaults in the sections [DEFAULTS] and [FILE NAMES].

☞ ***Tip***: In the worklist, omit the asterisk (*) which marks ➢*User-defined Columns* in the Browser.

Workspace

The area between the menu bar or ➢*Toolbar* and the ➢*Status Bar* is called **Workspace**. Within this area, the currently open windows of the various "window types" are displayed.

The Workspace allows you to open a specific set of windows. Normally, this is the most recently used workspace.

Choose **Autosave Workspace** in the **Workspace** menu to open the most recently used workspace whenever starting the Dionex Chromatography Management System (e.g. two ➢*Control Panels* showing the status of two different HPLC systems).

Of course, it is also possible to save or open any view with a separate name. The Dionex Chromatography Management System stores this information in WSP files. Use this option to save a view for data processing and a view for peak purity analysis etc.

If you want to save settings of an individual window without changing the Workspace, you can use a ➢*Report Definition File (RDF)*. The RDF is used whenever a sample or a window is opened individually, not in connection with a Workspace.

Combining RDFs and a Workspace allows each user to have a personal representation of the screen. For a detailed description, see **User Profiles**.

Xcalibur

Xcalibur (= XC) is the software data system of ThermoQuest Corporation. Controlling the Finnigan aQa ➢*Mass Spectrometer* via the Dionex Chromatography Management System requires the Xcalibur software. Two XC setup programs are available on the installation CD. For installation information see **How to ...: Actions Related to the aQa-MS Installing MS Components**.

Xcalibur allows you to define programs for the aQa mass spectrometers in a ➢*PGM File*. You can create the control file via the Dionex Chromatography Management System (see **How to ...: Actions Related to the aQa-MS Creating a Method for the aQa-MS)** using the corresponding XC Editor.

Year 2000 Conformity

According to the document PD2000-1:1998 which was published by the British Standards Institution (BSI) "year 2000 conformity shall mean that neither performance nor functionality is affected by dates prior to, during and after the year 2000."

In particular, this means that the following rules are adhered to:

1. *General Integrity:* No value for current date will cause any interruption in operation.

2. *Data Integrity*: Date-based functionality must behave consistently for dates before, during, and after year 2000.

3. *Explicit/Implicit Indication of the Century:* In all interfaces and data storage, the century in any date must be specified either explicitly or by unambiguous algorithms or inferencing rules.

4. *Leap Year:* Year 2000 must be recognized as a leap year. (According to the Gregorian Calendar the year 1900 was not a leap year.)

Versions 4.20 and higher of the Dionex Chromatography Management System fulfill the BSI rules mentioned above. As previous versions (4.12 and lower) do not completely fulfill the year 2000 conformity, upgrading to the current version is recommended.

The Dionex hardware fulfills the BSI rules in the same way. Two instruments of the previous generation that is no longer available (M480 pump and GINA160 ➢*Autosampler*) the year 2000 are displayed as 1900. This, however, does not affect the functionality.

Please do not hesitate to contact Dionex Service for the corresponding Year 2000 Certificate.

Zoom

Press the left mouse button and draw a frame around a section of a signal plot or a 3D-field that you wish to zoom. Select ➢*Unzoom* to undo the last zoom operation. Select **Full size** to return to the original display (100% representation).

☞ ***Notes***: In the online signal plot, an ➢*Overview Window* is displayed in the upper right corner in addition to the enlarged section.

While drawing a zoom frame, the operation can be canceled by pressing the ESC key or the right mouse button. Use this function to prevent redrawing the window (e.g. a 3D plot) when the wrong frame was selected.

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