DIONEX

PeakNet Software User's Guide

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Finding Information Fast

PeakNet Software User's Guide

The *PeakNet Software User's Guide*, for PeakNet Software Release 5.2, is a reference guide that provides a complete description of each feature of PeakNet software. Use this manual when you want details about a PeakNet program, its menus, dialog boxes, and functions.

On-line Help

PeakNet provides extensive on-line Help, which is available from the MainMenu and from each PeakNet program. Use the Help for quick access to information about the program or dialog box you are using, and for step-by-step instructions on tasks you wish to perform.

There are several ways to access the on-line Help:

- Click on the Help button in the MainMenu
- Select Index from the Help menu of any PeakNet program
- Press the <F1> function key

For more information about using Help, see Chapter 3.

Release Notes

Any important information that was unavailable when this manual was printed is contained in the Release Notes of the PeakNet on-line Help. You can view the Release Notes automatically at the conclusion of the PeakNet setup procedure, or any time after installation from the PeakNet Help.

To view the Release Notes:

1. Access the PeakNet Help.
2. Click on the Help Topics button in the PeakNet Help window.
3. Select the Contents tab and then select Release Notes.

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8 • The Run Program

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1 • About PeakNet

1.1 Overview of PeakNet Workstations

PeakNet workstations are used to control instruments, collect data from the controlled instruments, process the data, and generate reports.

A PeakNet workstation consists of an IBM-compatible personal computer, an interface to the controlled instruments, a printer, and PeakNet software.

Two different types of instrument interfaces are supported:

- ***Via the DX-LAN instrument network***, PeakNet software controls and monitors up to eight instrument systems. Each DX-LAN system can consist of one DX-120 Ion Chromatograph or a set of up to eight DX-LAN modules, of which two can be UI20 Universal Interfaces. Each system, in turn, controls up to eight modules and collects and stores data from up to four detectors per system.
- ***Via ACIs (Advanced Computer Interface)***, PeakNet software controls and monitors up to four instrument systems (2 per ACI), and collects and stores data from up to two detectors per system. The ACI has two functions: a) to control the chromatograph and any accessories (such as autosamplers and sampling pumps) and b) to collect and store detector data until the computer is ready to process the data.

NOTE For detailed system requirements, refer to *Installing the Dionex PeakNet System* (Document No. 034941).

1.2 Overview of PeakNet Software

Family of Programs

PeakNet is a family of programs, each with specific functions. The PeakNet MainMenu organizes the programs into groups based on their functions and lets you start the programs from one convenient location.

Starting PeakNet Programs

NOTE Before turning on the power to the PeakNet workstation, first turn on the power to the module(s) to be controlled. This allows the DX-LAN network card to establish communication with the module(s).

To start the PeakNet MainMenu program, select the Start button on the Windows taskbar and select Dionex PeakNet MainMenu from the Programs list.

To start any other program, click on the MainMenu button that represents that program.

NOTE To have the MainMenu start automatically when Windows starts, select the corresponding option during PeakNet Setup.

Windows Environment

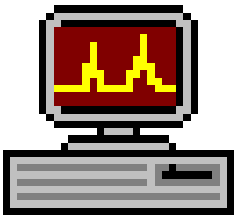
PeakNet runs under Microsoft® Windows® 95 or Windows NT® and follows the Windows conventions for menus, dialog boxes, toolbars, and other user interface features. The PeakNet on-line Help also follows the Windows conventions.

PeakNet supports the Windows Clipboard for cutting and pasting information to and from PeakNet and other programs.

If you are unfamiliar with Windows, refer to the Windows documentation before running PeakNet.

2 • Getting Started

2.1 The MainMenu



The **MainMenu** (MENUDX.EXE) is organized as a series of “tab pages” on which each PeakNet program is represented by a button. Resting the mouse on a button displays a brief description of the program’s function; clicking on a button starts the program.

There are five types of tab pages:

- A **DX-LAN** tab page (appears only if there are configured DX-LAN systems)
- An **ACI** tab page (appears only if there are configured Advanced Computer Interface (ACI) systems)
- An **Accessories** tab page for PeakNet accessory programs
- An **Options** page for modifications to default paths, the MainMenu, and the PEAKNET.LOG file
- An **About** page that indicates the PeakNet software release level

NOTE If no DX-LAN or ACI systems are configured, a Programs tab page appears instead of the DX-LAN or ACI tab page.

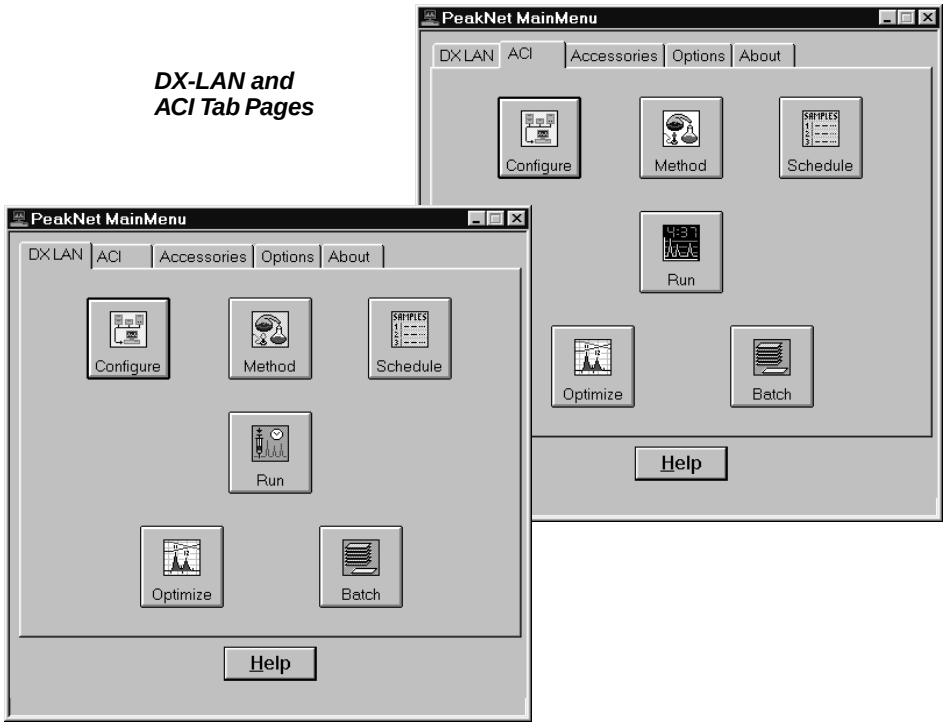
2.1.1 DX-LAN and ACI Pages

Each button on a DX-LAN or ACI page lets you access one of the PeakNet main programs.

The sequence of program buttons on a page corresponds to the typical sequence of events for automated operation: system configuration, creation of Methods and Schedules, data collection, and review and reprocessing of the data once data collection is complete.

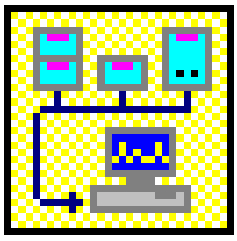
The number and sequence of program buttons included on the DX-LAN and ACI pages are the same. However, the Method Editor and Run buttons launch different versions of those programs, depending on the system type.

DX-LAN and ACI Tab Pages



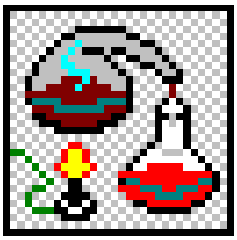
2.2 Main Programs

Connections

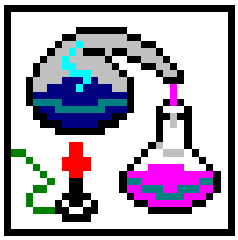


The **Configuration Editor** (CONFIGDX.EXE) configures the instruments, the Advanced Computer Interface, and the DX-LAN network to the analytical system(s) being used. Run the Configuration Editor during the initial installation of PeakNet software, as well as each time the instrument configuration is changed.

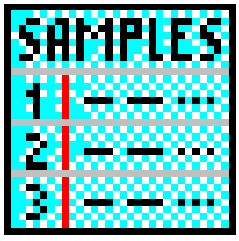
Preparation for Analysis



The **Method Editor** (METHODDX.EXE) creates and edits Methods for analyses or experiments conducted by liquid chromatography, ion chromatography, gas chromatography, and/or capillary electrophoresis. Each Method contains complete instrument control and data handling instructions for a single analysis. The Method Editor is used only with DX-LAN systems.

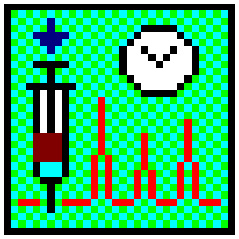


The **ACI Method Editor** (METACI.EXE) performs the same functions as the Method Editor, but is used only with Advanced Computer Interface systems.

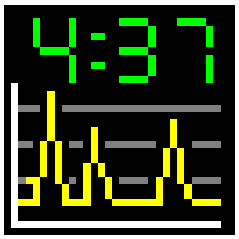


The **Schedule Editor** (SCHEDDX.EXE) creates, stores, and edits Schedules of analyses. Each line of a Schedule specifies a sample name, a Method to be used for the analysis, and any optional correction factors. Automatic calibrations can be incorporated into the Schedule, if desired.

Analysis

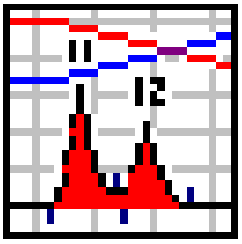


The **Run program** (RUNDX.EXE) loads a selected DX-LAN system with a Method or Schedule. Each system's status and real-time plot are displayed separately. When an analysis is complete, Run directs the computer to save the raw data. Run then detects and integrates peaks and calculates component concentrations, based on response factors calculated from calibration standards. Run will store and/or print the results of these calculations, depending on the instructions in the Method(s).



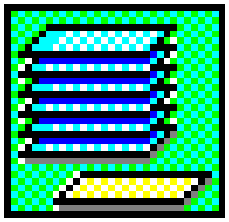
The **ACI Run program** (RUNACI.EXE) performs the same functions as the Run program, but is used only with Advanced Computer Interface systems.

Post-Analysis Data Processing



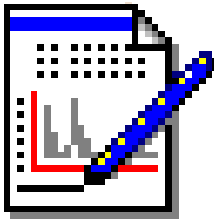
The **Optimize program** (OPTIMDX.EXE) retrieves raw data from the disk drive for additional processing. The data file is first shown exactly as it was processed at the time it was saved. Optimize commands enable you to test various treatments of the raw data; modify the data; and then update the Methods, data files, and report files.

Optimize lets you visually compare up to 12 stored chromatograms. These may be plotted on separate axes or overlaid on a single set of axes. Optimize also calculates and plots the mathematical sum, difference, or ratio of any two raw data files collected and stored by the Run or ACI Run program. Optimize can plot the first and second derivatives of a data file, store the calculation results as a new data file, and process the file just as it would any other data file.

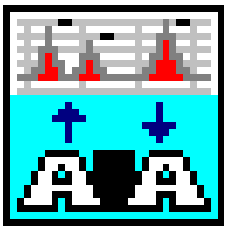


The **Batch program** (BATCHDX.EXE) reprocesses previously stored data files in a group, rather than individually. Using information from Schedules, Batch retrieves the names of the data files to be reprocessed and the Methods to be used. Batch then stores the reprocessed data as new files and generates new reports.

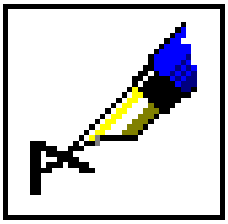
2.3 Accessory Programs



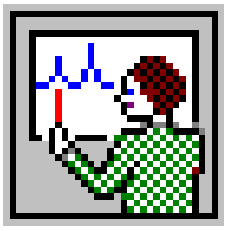
The **Report Designer** (REPORTDX.EXE) lets you create and edit custom formats for three types of single-injection reports: Sample Analysis, Calibration Update, and Check Standard. The Report Designer also lets you create formats for summary reports, generated by the Batch program from multiple data files.



The **AIA program** converts a PeakNet raw data file into the AIA data file format (Andi/Chromatography) for import into a different chromatography data system. The program also converts a raw data file in the AIA format into a PeakNet raw data file. In either case, the conversion process creates a new file; it does not change the existing file. Refer to the on-line Help for details.

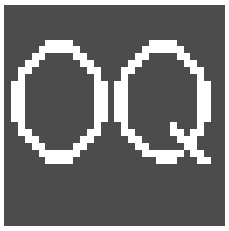


The **PeakNet event logger** automatically records significant events in the PEAKNET.LOG file, which is stored in the same directory as the PeakNet programs. You may review or print the event log, for informational or troubleshooting purposes, using Windows Notepad or other text editor.

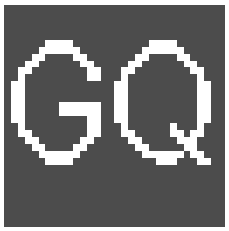


The **PeakNet Tutorial** takes you through an example PeakNet session.

The **Installation Qualification program** uses an error detecting technique called Cyclic Redundancy Check (CRC) to verify that all files are installed correctly during PeakNet setup. The Installation Qualification program runs automatically after PeakNet setup. It can also be run at any time from the MainMenu.



The **Operational Qualification program** checks PeakNet operation by generating reports and exported values from reference data files. The exported values are then compared with reference exported values.

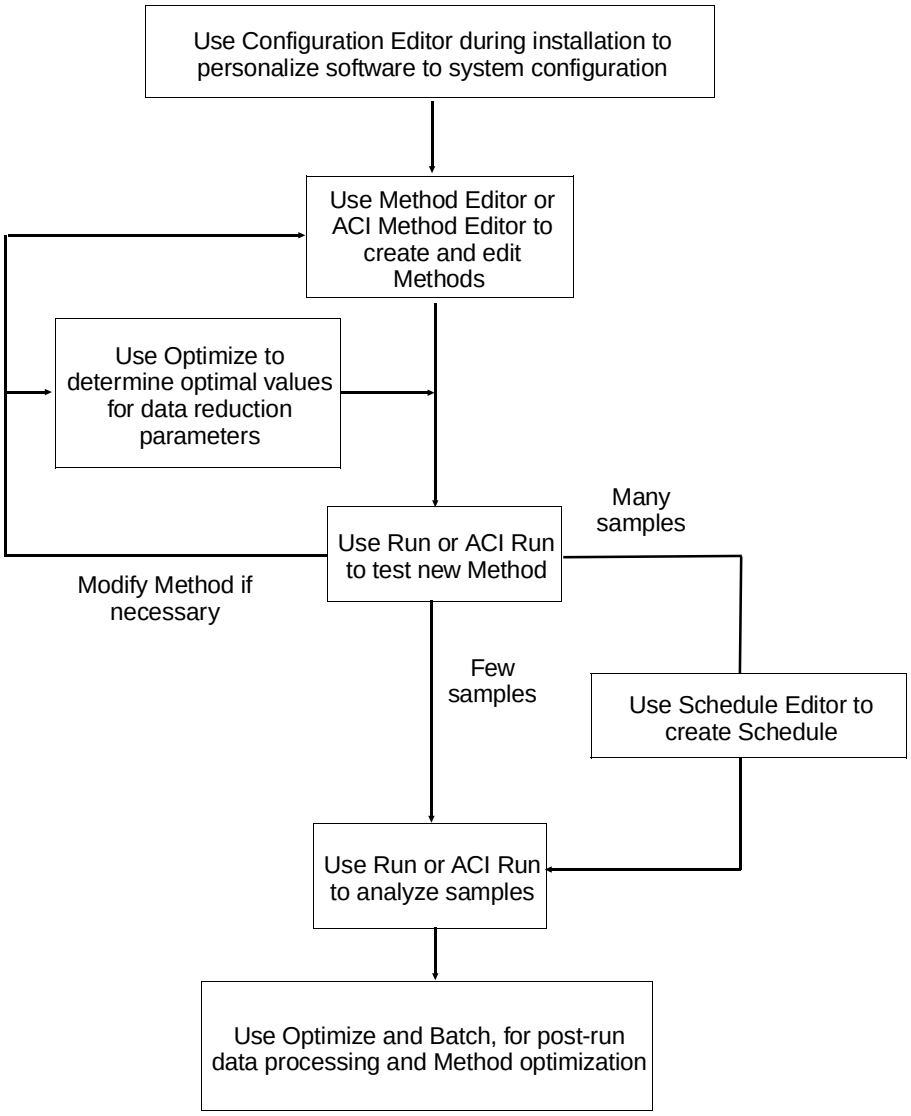


The **Gradient Pump Qualification program** tests for the correct operation of Dionex gradient pumps by analyzing gradient profile raw data files, created using example Methods supplied by Dionex. The program performs a series of tests to determine whether the pump is operating within specified performance limits.

2.4 Typical PeakNet Operation Sequence

After PeakNet has been installed and you are familiar with Windows, you are ready to begin using PeakNet. Below is a summary of the typical sequence of events.

1. Configure PeakNet to your instrument, using the Configuration Editor. Unless the system configuration changes later, you will not need to reconfigure PeakNet.
2. Develop one or more Methods for analyzing samples, using the Method Editor or ACI Method Editor.
3. Test the Methods by analyzing calibration standards, using the Run or ACI Run program.
4. If necessary, use the Method Editor or ACI Method Editor, or Optimize program to modify the Methods.
5. Use the Schedule Editor to create a Schedule of analyses that uses these Methods in a logical sequence. A typical Schedule includes Methods to equilibrate the system, calibrate it, analyze samples, and shut down the system.
6. Carry out the sample analysis via the Run or ACI Run program, using one Method or a Schedule of Methods.
7. Examine the analytical results, manipulate the data, and compare the results with those obtained from other analyses. For instance, you might first reprocess with the Optimize and Batch programs and then use Optimize to calculate ratios or differences, or compare plots.


Use Configuration Editor during installation to personalize software to system configuration
Use Method Editor or ACI Method Editor to create and edit Methods
Use Optimize to determine optimal values for data reduction parameters
Use Run or ACI Run to test new Method
Many samples
Modify Method if necessary
Few samples
Use Schedule Editor to create Schedule
Use Run or ACI Run to analyze samples
Use Optimize and Batch, for post-run data processing and Method optimization

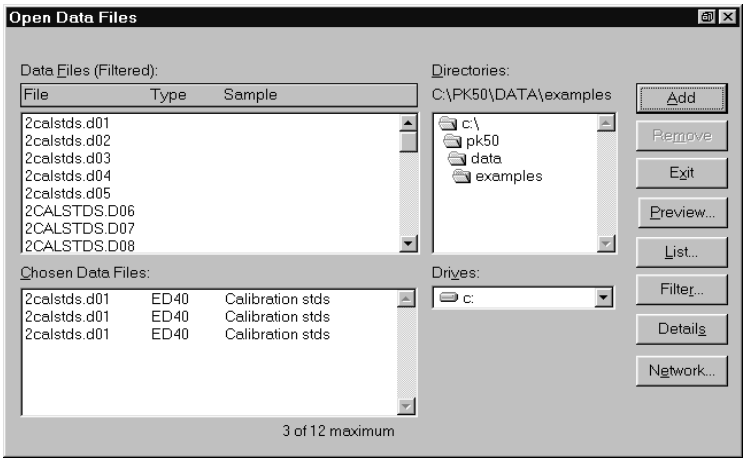
3 • General Functions

3.1 Data File Open Dialog Box

PeakNet uses two styles of Open dialog boxes. The first is the standard Open dialog box, common to most Windows programs; it is described in the Windows documentation.

The second style is the specialized PeakNet Open dialog box for data files that appears when you select Open... from a post-run program (Optimize and Batch). The dialog box controls let you display, sort, filter, and preview each file in a selected directory.

For instance, the following dialog box appears when you select Open... from within Optimize:



NOTE The PeakNet Open dialog box contains Add and Remove command buttons only if the program *and* the selected operation can use multiple files. For instance, the buttons are present when opening a Comparison Window in Optimize, but are absent when opening an Edit Window.

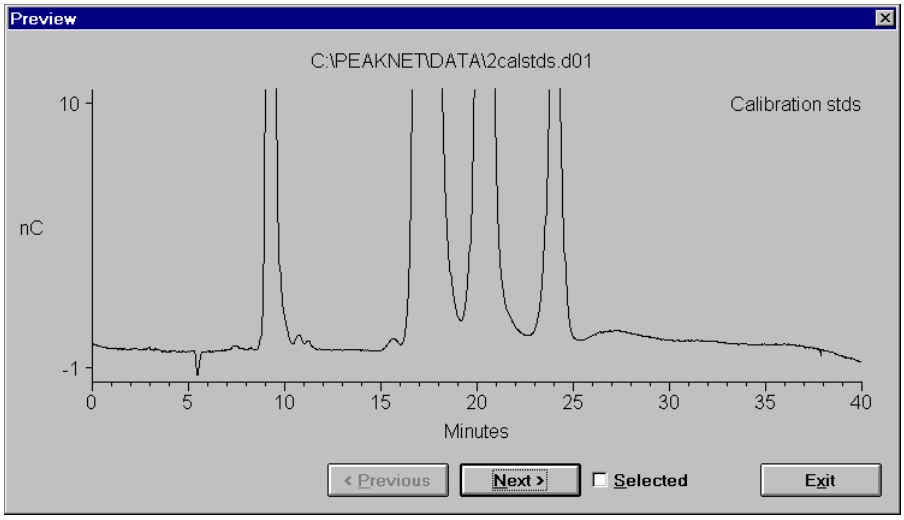
The File list box lists all files in the currently selected directory. The Chosen Data Files list box lists only the files you selected for an operation.

- To select a file for an operation, click first on the desired filename in the File list box and then on the **Add** command button. The file is added to the Chosen Data Files box.
- To remove a file from the Chosen Data Files box, click first on the filename and then on the **Remove** command button.

Exit closes the PeakNet Open dialog box.

Preview... lets you preview the data plot of a file. First, select a data file from the File list box and then click on the Preview... command button. This opens a dialog box displaying the trace and axes of the selected plot.

NOTE If you click on Preview... when more than one filename in the File list box is highlighted, the file with a faint dotted border (input focus) will be displayed.



The way in which the Preview dialog box controls operate varies slightly, depending on whether the current operation allows multiple-file selection, or only single-file selection.

- **Multiple-Selection Open Dialog Box**

  The **Previous** and **Next** command buttons let you change the displayed plot without exiting the Preview dialog box. However, displaying a plot does not select it.

  As each data plot is displayed, select or deselect the file by clicking on the **Selected** check box. A check in this box indicates that the displayed file is selected; no check means the file is not selected.

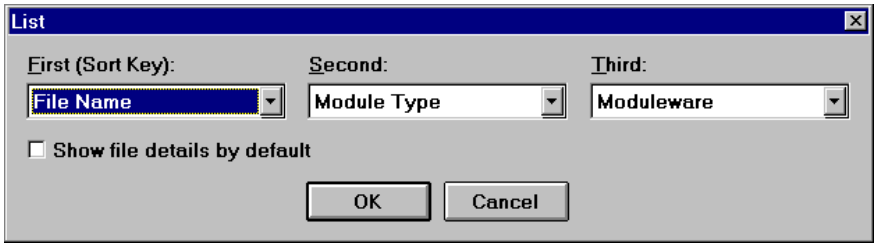
  After previewing files, click on **Exit** to return to the PeakNet Open dialog box. There, all of the selected files will be highlighted in the File list box.

- **Single-Selection Open Dialog Box**

  The **Previous** and **Next** command buttons let you change both the selected plot and the displayed plot. Click on **Previous** to display a data plot of the file listed just above the file currently selected in the File list box. Click on **Next** to select the file listed just below the current selection.

  The **Selected** check box is disabled during single-file selection.

Click on the **List...** command button to display the List dialog box:



Use the dialog box controls to display more information about each file in the File list box. The File list will be sorted according to the first listed item. Click first on the down-arrow beside the **First** edit box and then on one of these options (or sort keys):

None	System Name
File Name	Analyst ID
Sample Name	Column ID
Module Type	Inject ID
Module Name	Date/Time Collected
Moduleware	Date/Time Changed

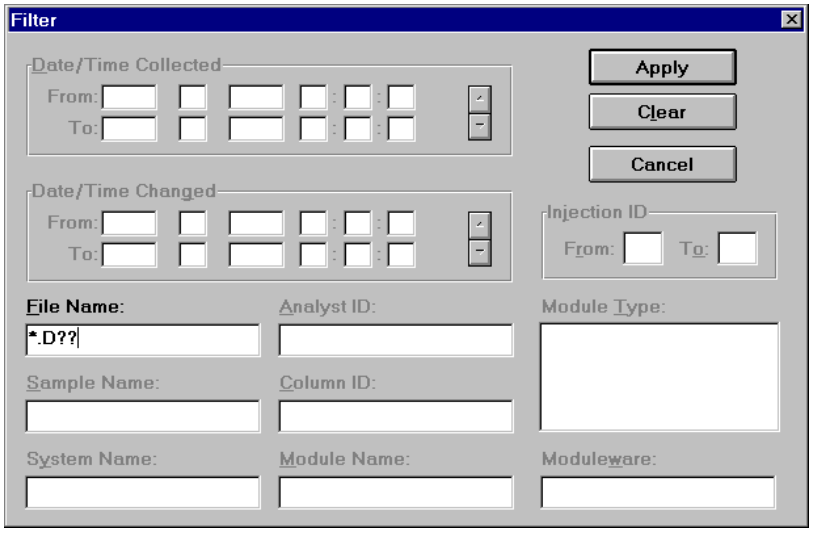
The selected information now appears after each file in the File list box. You may also select options from the **Second** and/or **Third** drop-down list box, if desired; those options are identical to the ones in the First list box.

The **Process with Method from Disk** check box determines which Method version is applied when you open a data file in Optimize. When the check box is not selected, the Method embedded in the data file is applied. When the check box is selected, the current version of that same Method file from the disk (if available) is applied.

Clicking on **OK** saves the selections in the List dialog box and returns you to the PeakNet Open dialog box.

Selecting the **Filter...** command button opens the Filter dialog box. Use its controls to limit the files listed in the File list box to those that match the criteria entered here.

NOTE The controls in the Filter dialog box are disabled when File Name is the only sort key selected from the List dialog box.



Date/Time Collected specifies limits for the date and time at which the data file was originally written. **Date/Time Changed** specifies limits for the date and time at which the data file was most recently written. Type in new values for the time period and clock time, or click on the double-arrows until the desired values are displayed.

Injection ID specifies a range of injections; type the first and last numbers of the range in the spaces provided.

File Name can be used to filter using standard DOS wildcards.

Sample Name, **System Name**, **Analyst ID**, **Column ID**, **Module Name** and/or **Moduleware** work in the same way. Each one sorts out only those files in which the characters specified in the edit box occur at the beginning of the specified item.

Module Type lets you specify a module (AD20 Absorbance Detector, CD20 Conductivity Detector, etc.). The default selection is all modules whose names appear in the Module Type list box. To deselect a module, click on its name in the list box. If a module

name is not highlighted, the module has been deselected. To select a module again, click on its name in the list box.

Click on **Apply** to save these selections and return to the Open dialog box.

Click on the **Clear** button to remove all filter criteria and restore the default selections.

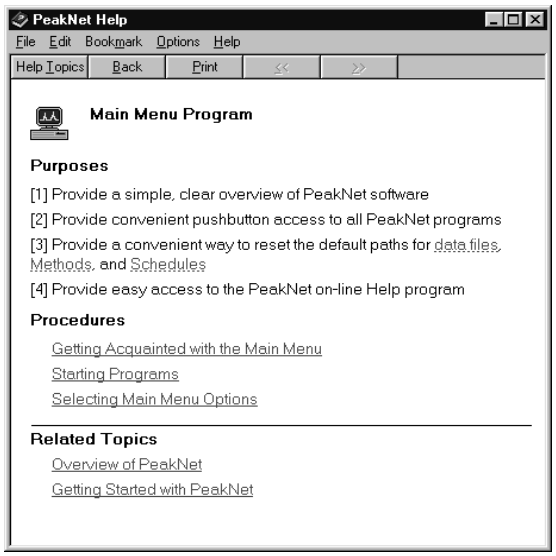
3.2 The Help Program

The on-line **Help program** is a convenient way to look up information about PeakNet menu commands, dialog boxes, terminology, and operating procedures. The Help program is typically used to answer questions that arise while you are running another PeakNet program.

To access Help from the PeakNet MainMenu, click on the Help command button. To access Help from other PeakNet programs use one of the following methods:

- To display an overview screen for the active program, click on the Help toolbar button (the question mark), or select Index from the Help menu..
- To display the PeakNet Help table of contents, click the Help Topics button at the top of the Help screen.
- To display context-sensitive information about an open dialog box, press <F1>.

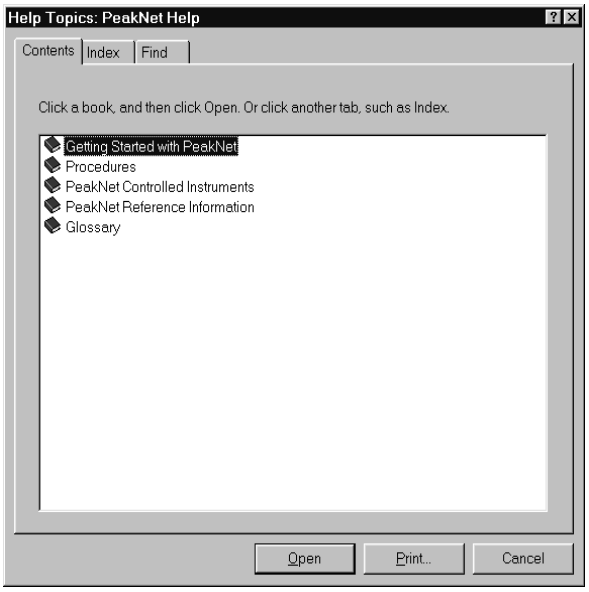
Besides a summary of the program's purposes, the overview screen includes an index of commands, procedures, and related topics (see below). Clicking on text which has a solid underline jumps you to a related topic; clicking on text which has a dotted underline displays a pop-up definition.



Clicking on the Help Topics button in a Help window opens the Help Topics dialog box. This dialog box provide three ways to look up Help topic information.

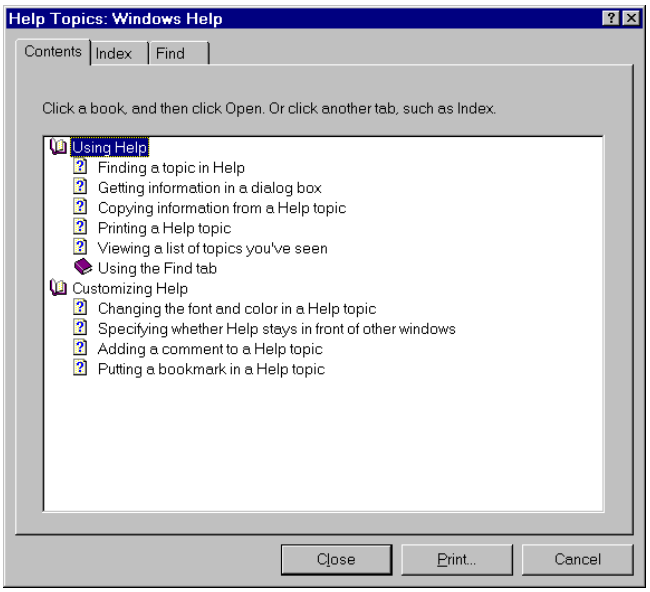
- To select topics by category or subject, use the Contents tab page.
- To select topics from a list of index entries, use the Index tab page; either type the word you're looking for or scroll through the list.
- To search for a word or phrase in the Help topics and display the topics containing the word or phrase, use the Find tab page .

PeakNet Help Contents Tab Page



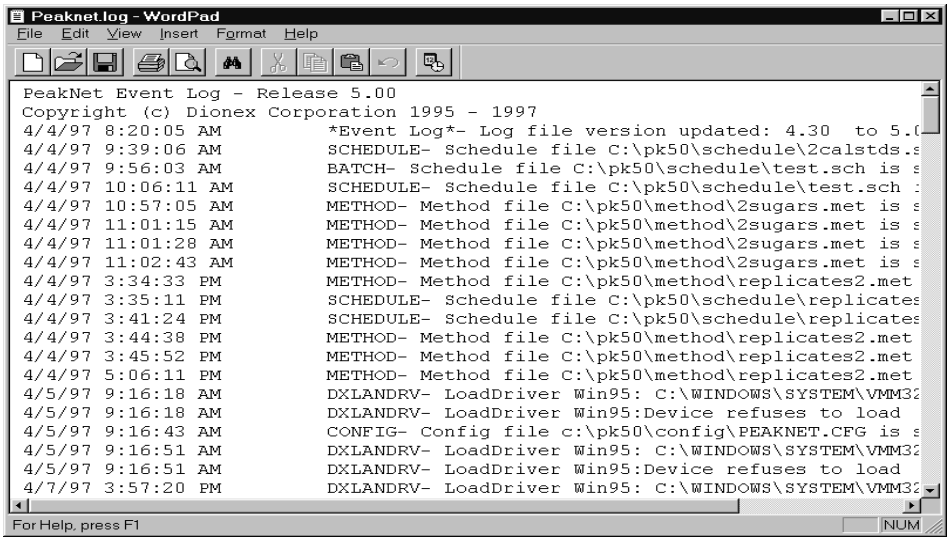
For additional information about how to use Windows Help, press the <F1> function key to display the Windows Help screen (see below). The Windows Help describes how to use the Contents, Index, and Find functions, and how to customize the Help display.

Windows Help Contents Tab Page



3.3 Event Log

The PeakNet event logger automatically records significant events in the PEAKNET.LOG file, which is stored in the same directory as the PeakNet programs. To review or print the event log, for informational or troubleshooting purposes, click on the Log button on the MainMenu Accessories tab page. The file opens in Windows WordPad.



Three types of events are logged:

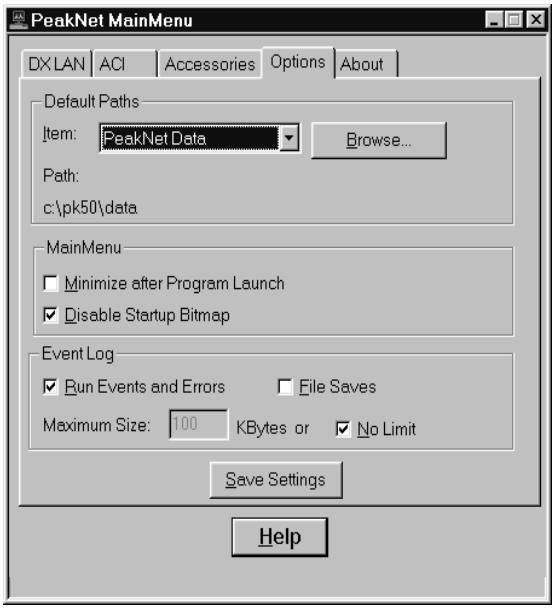
- File saving events are logged each time a Configuration Editor, Method Editor, Schedule Editor, Form Editor, Batch export, Batch setting, or data file is saved.
- Run and ACI Run status update events are logged each time the Run Program or ACI Run Program loads, starts, ends, or aborts a Method/Schedule, or when the program detects an error.
- Run-time errors are logged when an error occurs during a run.

  This is an example of a typical event description in the PEAKNET.LOG file:

12/01/97 09:46:27 AM RUN- Start Schedule MYSCHED.SCH

To modify the information saved in PEAKNET.LOG:

Select the Options tab page in the MainMenu.



- To record all Run or ACI Run status update events and errors, select the Run Events and Errors check box. (The default is on.)
- To turn file logging on or off, select the File Saves check box. (The default is on.)
- To specify the size limit of the PEAKNET.LOG file, enter a value (in 1 kilobyte increments) in the Maximum Size edit box. (The default is 100.)

NOTE When the maximum file size is reached, the earliest 25% of the events listed in PEAKNET.LOG are automatically deleted, except for the header, which is always retained. The file then grows until it again reaches the limit.

- To allow the PEAKNET.LOG file to grow indefinitely, select the No Limit check box (the default is off).

When you finish making changes on the Options tab page, click the Save Settings button to update the PEAKNET.INI file with the new settings.

To add a comment to the PEAKNET.LOG file:

Comments can be added from the Run program.

1. Select the Edit Log command from the Run program's File menu.

   The PeakNet Log dialog box will appear.

2. Type your comment (up to 128 characters) into the edit box.

3. To write the comment into the PEAKNET.LOG file, select Add to Log.

   The comment will be preceded by the date and time of the entry, along with the label "User Comment," as in this example:

```
12/01/00  09:46:27 AM  User Comment - Restarted system
with new buffers.
```

4. When you finish editing, select Close.

To erase the contents of the PEAKNET.LOG file:

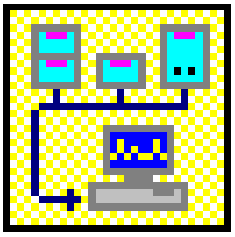
1. Select the Edit Log command from the Run program's File menu.

   The PeakNet Log dialog box will appear.

2. Select Clear Log.

This deletes all information in the log file except for the header, which is always retained.

4 • The Configuration Editor



The Configuration Editor lets you specify the connections of the modules and accessories in your DX-LAN or Advanced Computer Interface (ACI) instrument system, as well as the connections between the system and the computer. This information is stored in one or more configuration files that other PeakNet programs, including Run and ACI Run, must routinely access in order to communicate with each module.

You must run the Configuration Editor during the initial installation of the PeakNet workstation, as well as each time a module is added to or removed from the system.

In addition, you may use the Configuration Editor to quickly update DX-LAN modules with the latest version of Moduleware, the computer code in each module that controls its functionality.

4.1 DX-LAN Support

The PeakNet workstation includes a personal computer that communicates with DX-LAN modules and the UI20 Universal Interface via the Dionex DX-LAN network. In order for the PC to identify the modules on the network, the Configuration Editor assigns each module a unique identification and address.

The ***unique identification***, known as the DX-LAN ID, is a six-digit number assigned at the factory to each module. If any Moduleware is corrupted or lost, the module's address might be lost but its DX-LAN ID is always retained. Thus, the DX-LAN ID is the most important form of module identification available to the Configuration Editor.

The ***unique address*** consists of both a system number (from one to eight) and a module number (from one to eight). The number of systems that can be configured depends on which PeakNet model you have. You can configure as many as eight DX-LAN modules per system.

The Configuration Editor records the following information in the DX-LAN system configuration file, named PEAKNET.CFG:

- System numbers and names
- Number of modules in each system
- Name, type, unique address, and DX-LAN ID of every DX-500 module or UI20 in each system
- COM port assignments for the optional AS3500 Autosampler

The PEAKNET.CFG file is read by the MainMenu each time that program is started. The contents of the file determine the number, and type, of System tab pages built for the MainMenu.

The Configuration Editor records the I/O address and interrupt number of the DX-LAN computer interface card in your PC in the PEAKNET.INI file. PEAKNET.INI is stored in the Windows directory.

4.2 ACI Support

Each ACI (Advanced Computer Interface) system has multiple configuration files:

- The ACI communication configuration is stored under the filename CONFIG0.ACI.
- The module configuration for each ACI is stored in a file named CONFIGx.ACI, where x is a number from 1 to 2 which corresponds to the ACI being configured.
- The configuration notes you enter for each ACI are stored in a file named NOTEx.ACI,where x is a number from 1 to 2 which corresponds to the ACI being configured.

The ACI configuration files are read by the MainMenu each time that program is started. The contents of these files determines the number, and type, of System tab pages built for the MainMenu.

4.3 Starting the Configuration Editor

To open the main window, click on the Configure button in the PeakNet MainMenu or double-click on CONFIGDX.EXE in the directory that contains the PeakNet program files.

If you have a DX-LAN system, the Configuration Editor compares the module addresses, types, and DX-LAN IDs of all on-line modules with those listed in the PEAKNET.CFG file.

- When a module exists both in the PEAKNET.CFG file and on the DX-LAN, the system list box displays the DX-LAN ID and the module name in black.
- When a module exists in the PEAKNET.CFG file but not on the DX-LAN, the system list box displays the DX-LAN ID and the module name in red and labels the system ***Off line***.
- When a module exists on the DX-LAN but not in the PEAKNET.CFG file, you may assign the module to a system.

When an ACI is supported, it is represented by an icon in a special ACI child window; if no ACI child window is displayed, it is because ACI support was not installed. The number of ACIs that can be supported depends on which ACI model you specified when installing PeakNet software. Note that you cannot add or delete ACIs from the child window, as you can with DX-500 modules.

4.3.1 The Toolbar

Click on a toolbar button to quickly implement frequently used Configuration Editor menu commands and controls. Click on the icons for the PeakNet MainMenu and Help to display those programs.

From left to right, the toolbar button functions are:

1. Save
2. Print
3. COM Ports
4. Moduleware
5. Module Inventory
6. Help
7. Switch to MainMenu

4.4 File Menu

4.4.1 Save

Click on the Save toolbar button (or select the menu command) to save complete system configuration information. Other PeakNet programs routinely access the configuration file(s) in order to communicate with system modules.

NOTE Each system must have at least one module assigned to it. If the Configuration Editor detects a system with no modules, it will delete the "empty" system when the configuration is saved.

4.4.2 Database Export Options...

Opens the Database Export Options dialog box, which allows you to select the type of data to export to a database. This command is available only if you have already completed the following:

- Installed a database program that supports ODBC (for example, Microsoft Access) on the computer
- Set up PeakNet as a data source for the database program

Once the above have been completed, data is exported automatically after each run.

NOTE The options selected in the Database Export Options dialog box determine the type of information exported to the PeakNet database. If the Peak Table option is set to None, no data will be exported.

Setting Up PeakNet as a Data Source

NOTE The following instructions describe the setup procedure necessary to use the PeakNet database with Microsoft Access. To set up other database programs, use these steps as a guideline and also refer to the Microsoft ODBC Help.

1. Open the Windows Control Panel.

   Click the Start button on the taskbar, select Settings, and click Control Panel.

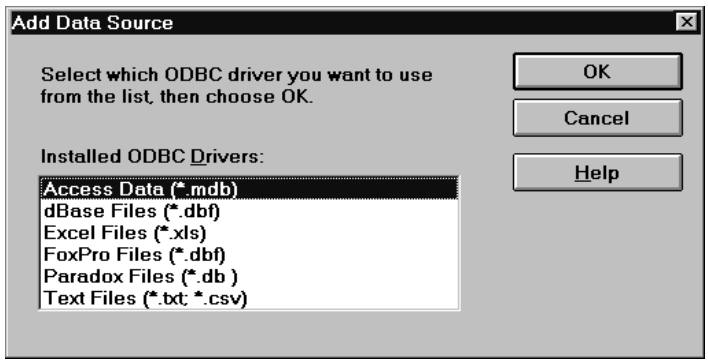
2. In the Control Panel, double-click the ODBC icon.

   NOTE If the ODBC icon does not appear, rerun the Microsoft Access setup to install the ODBC driver. You may also need to rerun the PeakNet setup to install the PeakNet database file if, after installing the Access ODBC driver, the Add button in the Data Sources dialog box is disabled, or if PeakNet.mdb is not listed in the Select Database dialog box (see Step 7).

   The Data Sources dialog box appears.

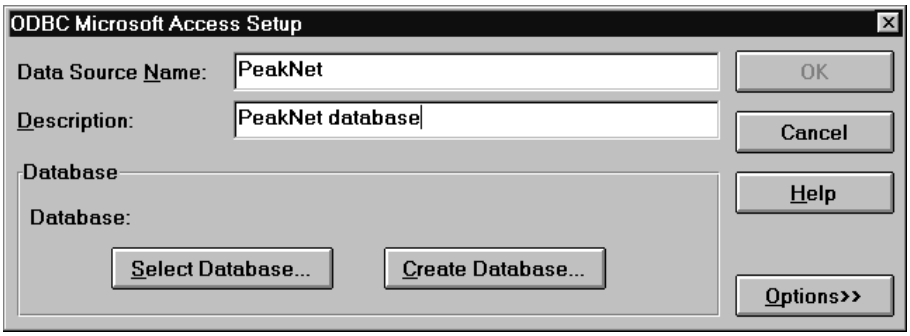
3. Click the Add button.

   The Add Data Source dialog box appears. (If you are running under Windows NT, the appearance of the next three dialog boxes will vary slightly from the illustrations here, although the functionality is similar.)



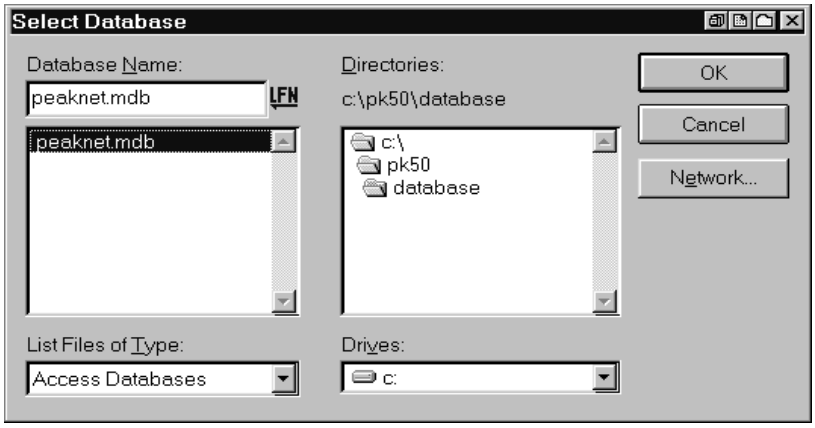
4. Select the Access Driver (*.mdb) and select OK.

   The ODBC Microsoft Access Setup dialog box appears.



5. In the Data Source Name box, enter **PeakNet**.
6. In the Description box, enter **PeakNet database**, or any other desired description.
7. Click the Select Database button.

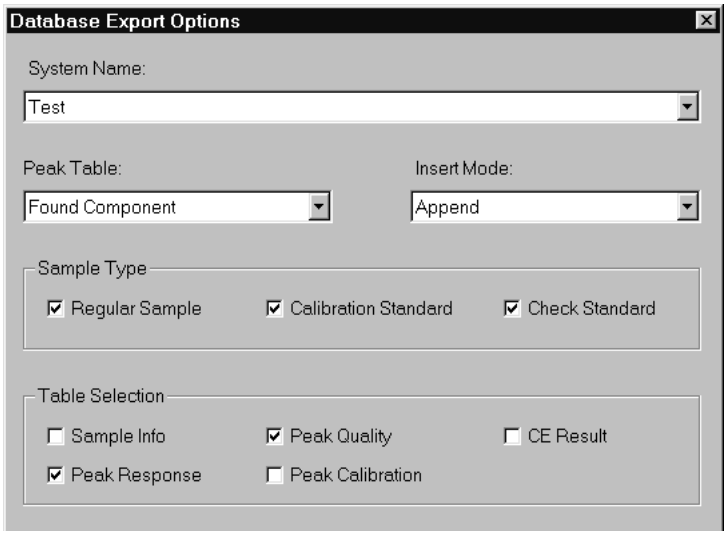
   The Select Database dialog box appears.



8. Navigate to the location of the PeakNet database. The default location is c:\PeakNet\Database.
9. Select **peaknet.mdb**.
10. Select OK through two dialog boxes, and click Close to exit the Data Sources dialog box.

Setting Database Export Options

Selecting the Database Export Options... command opens the following dialog box:



System Name lists all of the available PeakNet systems (eight) and the available ACI systems (four). Names assigned to systems configured in the Configuration Editor are shown. Default names are shown for unconfigured systems. All other options in the dialog box will apply to the selected system. You can select different options for each system.

Peak Table lists the types of Peak Tables that can be exported.

None specifies that no data will be exported to the database. When selected, all other options in the dialog box are disabled.

All Peaks exports data for all peaks.

All Components exports data for all the components expected to be in the injection

Found Components exports data for components that were matched to peaks detected in the chromatogram.

Insert Mode specifies how the data will be added to the database.

Append adds the data to the end of the database.

Overwrite searches the Injection Table for the most recent record with the same Method start time and replaces the old record with the new.

Sample Type selects the types of injection data to export: Sample, Calibration Standard, and Check Standard.

Table Selection selects to which tables data will be exported.

To save the options, select OK. The options selected for all systems are saved.

4.4.3 Print...

Click on the Print toolbar button (or select the menu command) to print a report containing the following information for the current DX-LAN or ACI system:

- The number of installed systems
- The name of each system
- The name and type of the modules which comprise each system
- The DX-LAN ID of all DX-500 modules
- The COM port assignment for each Advanced Computer Interface (ACI) and AS3500 Autosampler

4.4.4 Print Setup...

Displays the Windows common Print Setup dialog box for the current printer. Use the dialog box controls to select the report options (printer, print quality, paper size, etc.) or to select a different printer.

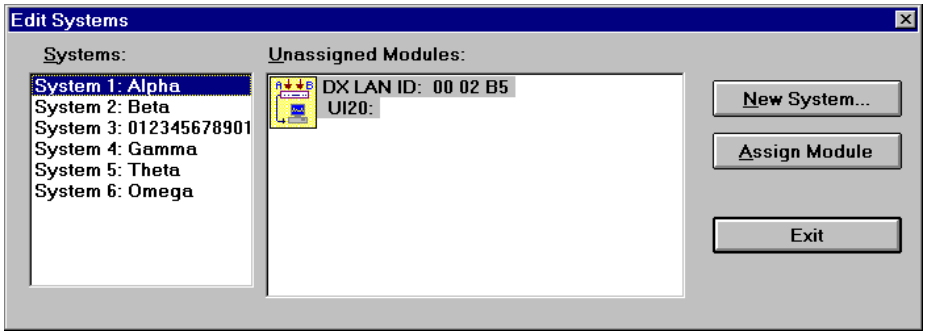
4.4.5 Exit

Closes the Configuration Editor.

4.5 Configure Menu

4.5.1 Systems...

The Systems... command is enabled only when the Configuration Editor detects an unassigned DX-LAN module. Select Systems... to open the Edit Systems dialog box and create new DX-LAN systems, or add modules to existing systems. Up to eight DX-LAN or UI20-based systems can be configured.

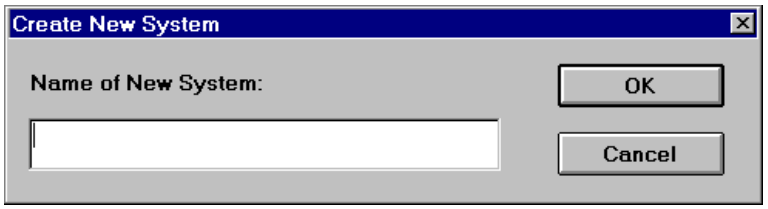


The dialog box contains two list boxes:

The **Systems** list box indicates the names of existing systems on the network.

The **Unassigned Modules** list box indicates the types and DX-LAN IDs of any on-line modules not currently assigned to a system.

To create a new DX-LAN system, click on the **New System...** command button to open this dialog box:



Enter a new system name (of up to 31 characters) in the space provided, then click on OK to save the name and return to the Edit Systems dialog box.

The new system name is now displayed in the Systems list box and a window for the new system is now displayed in the Configuration Editor main window.

To assign a module to a system:

1. Highlight the system name in the Systems list box.
2. Highlight the module in the Unassigned Modules list box.
3. Click on the **Assign Module** command button. You may assign up to eight modules to each system.

Exit closes the Edit Systems dialog box.

4.5.2 Delete Module

To delete a DX-LAN module from its assigned system:

1. Highlight the module in the appropriate system window by clicking once on the module icon. (Do not double-click; this will open the Names dialog box.)
2. Select the Delete Module command. This removes the module from the system and, if it is on-line, leaves it free for reassignment to another system.

4.5.3 Delete System

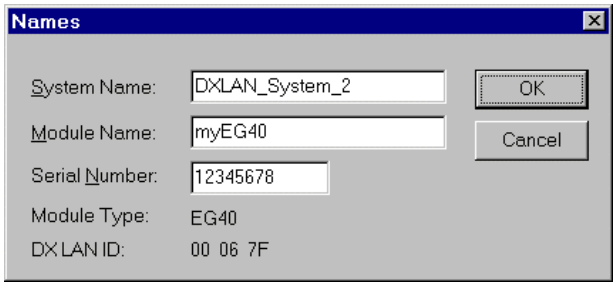
To delete a DX-LAN system and all modules assigned to it from the PEAKNET.CFG file:

1. Highlight the appropriate system window.
2. Select the Delete System command from the Configure menu.
3. When the confirmation message box appears, click on Yes. All modules formerly assigned to the system are now available for reassignment to other DX-LAN systems.

4.5.4 Names...

This command opens the Names dialog box, where you can enter a name for a DX-LAN system or a module assigned to a system, or the serial number for a module.

NOTE You cannot edit the Module Type or the DX-LAN ID.



1. To select a system for modification, highlight the system window.
2. Open the Names dialog box by selecting the Names... command or by double-clicking on a module name in the system window.
3. Type the new name (consisting of up to 31 characters) in the **System Name** and/or **Module Name** edit box.
4. Enter the module serial number (if any). The serial number is on the label on the rear panel of the module.

NOTE The next time this dialog box is opened, you will not be able to edit the serial number. To edit (or remove) the number, delete the module from the system and then re-assign it to a system.

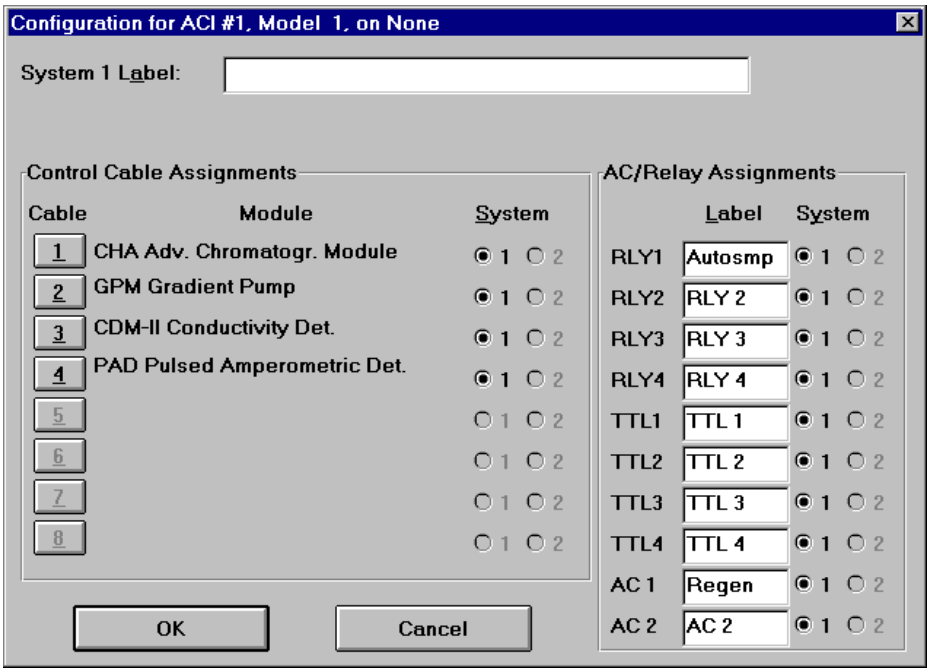
5. Click on **OK** to save the information.

4.5.5 Setup ACI...

If you have an ACI system, double-click on the icon in the ACI child window that represents the ACI you wish to configure. A dialog box showing this ACI's current configuration will appear. The dialog box controls will vary slightly, depending on which ACI model is selected. (If no configuration file has been stored for this ACI, a default configuration will be displayed for reference.)

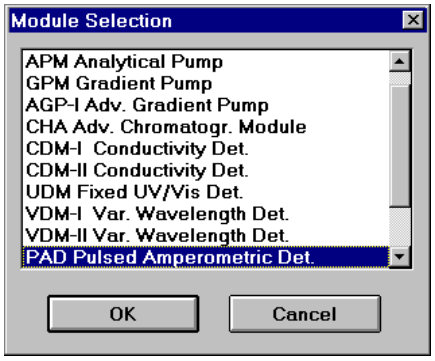
System 1 Label and System 2 Label (optionally) create a label (no more than 31 characters) for each ACI instrument system. The label will be stored in the \CONFIG subdirectory under the filename NOTEx.ACI, where x is the number of the ACI.

Control Cable Assignments displays the cable assignment for each ACI System. Each ACI provides parallel remote control of up to two complete instrument systems. (A system typically consists of a pump, one-half of a chromatography module, and one or two detectors.)



Each module is connected to the ACI rear panel by a 50-pin ribbon cable. These parallel remote cables are numbered 1 through 8 and correspond to the eight Cable buttons in this dialog box. The name of the module connected to each cable appears to the right of the Cable button. Make sure the cable assignments shown in the dialog box match the connections made to the ACI during installation.

If a cable assignment is incorrect, click on the button corresponding to that cable to display the Module Selection list box. To select the correct module, click on the module name and then on **OK**.



AC/Relay Assignment Each ACI includes four contact-closure relays, four TTL control lines, and two controlled AC outlets for control of additional accessories (for example, a Dionex Automated Sampler). However, Data System Model 1R has no AC outlet control.

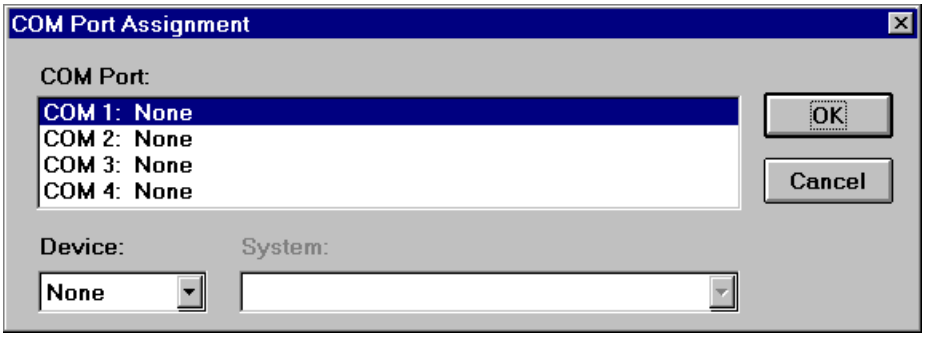
For a dual-channel interface, these can be allocated as desired between the two systems. A label of up to 9 characters can be entered for each control.

4.5.6 COM Ports...

If the PeakNet workstation includes an AS3500 Autosampler or an Advanced Computer Interface (ACI), you must specify to which computer COM port each device is connected.

Each ACI system and each DX-LAN system can support one AS3500; therefore, a PeakNet workstation can support up to two autosamplers.

Click on the COM Ports toolbar button (or select the menu command) to open the following dialog box.



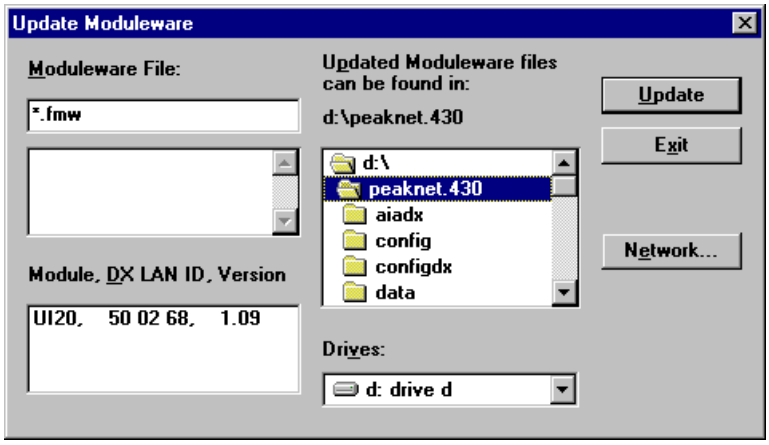
1. Highlight the COM port name in the list box.
2. From the drop-down list box, select the **Device** to which the COM port will be connected. The Device name will be added to the COM Port list box.
3. If the device is an AS3500, select the **System** to which the device will be assigned. The System name will be added to the COM Port list box.
4. When you finish assigning COM ports, click on **OK** or press <Enter>.

4.5.7 Moduleware...

Moduleware is the computer code in each DX-500 module that controls the functionality of the module. Use the Moduleware... command to check the revision levels of all installed Moduleware, or to download the latest Moduleware file to an out-of-date module.

CAUTION Downloading a new version of Moduleware overwrites the previously-installed version.

Click on the Moduleware toolbar button (or select the menu command) to open the Update Moduleware dialog box:



Moduleware File lists the names of the files that contain the current Moduleware versions. The name indicates the module type and Moduleware version; for example, GP40_114.FMW contains Revision 1.14 of the GP40 Gradient Pump Moduleware.

Module, DX-LAN ID, Version lists the DX-LAN ID for each on-line module, as well as the Moduleware version currently installed in the module.

To update Moduleware:

1. Insert the diskette with the updated Moduleware version into the computer's diskette drive.
2. Select the path for the diskette drive.
3. Select the file to be updated (from the Moduleware File list box).

4. Select the module to be updated (from the Module, DX-LAN ID, Version list box).
5. Click on **Update** or press <Enter>. A message box asking for confirmation always appears before the Configuration Editor begins the update; other message boxes may appear, also. In a few seconds, a message box will inform you that the download is complete and to warn you to wait until the module MAIN screen is displayed before downloading again to the same module. The updated version number is now listed in the list box titled **Module, DX-LAN ID, Version**.
6. Download Moduleware to another module, or click on **Exit** to close the dialog box.

4.5.8 Module Inventory

Whenever the Configuration Editor is opened, one or more modules may be off-line. If you subsequently turn on one of these modules, click on the Module Inventory toolbar button (or select the menu command) to instruct the program to poll the DX-LAN for on-line modules.

If you add a new module to the DX-LAN network, remember to use the Systems... command on the Configure menu to assign it to a system.

4.5.9 Computer Interface Card...

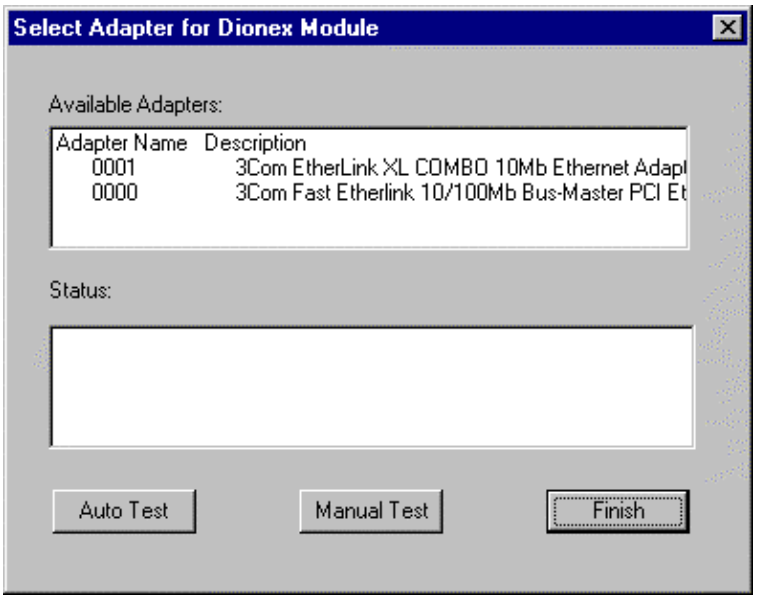
NOTE For instructions on how to install and configure DX-LAN cards, see *Installing the Dionex PeakNet System* **(Document No. 034941).**

Selecting Computer Interface Card... opens one of two dialog boxes, depending on which DX-LAN card is installed for PeakNet.

Select Adapter for Dionex Module Dialog Box

When a DX-LAN PCI card (P/N 052350) is installed, selecting Computer Interface Card... opens the Select Adapter for Dionex Module dialog box. The dialog box controls allow you to test one, or all, of the installed cards. Testing can only take place when at least one module on the DX-LAN network is connected and turned on.

NOTE This dialog box also appears if PeakNet does not detect a DX-LAN card when the Configuration Editor is opened initially.



Click **Auto Test** to initiate testing of the DX-LAN cards. PeakNet tests the cards one at a time, beginning with the first name in the Available Adapters list box, until it detects a card which is

connected to the network. At that point, the test is ended and the name of the detected card is saved in memory.

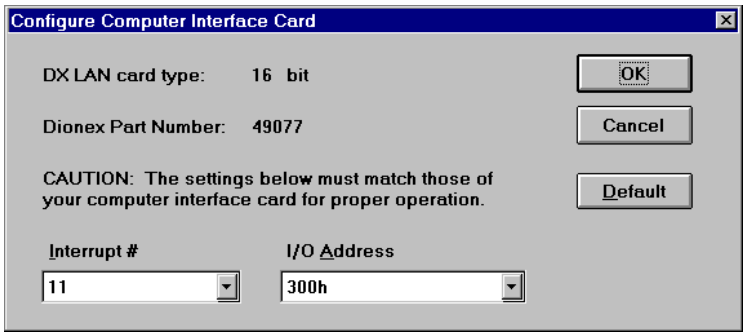
The **Manual Test** button lets you test one particular card. Highlight a card name in the Available Adapters list box and then click on Manual Test to initiate testing of the selected card. Select Manual Test if you suspect a problem with a card.

All test results are displayed in the **Status** list box. If at least one module in the network is connected and turned on, a test failure usually means that the selected card is not connected to the DX-LAN.

Click **Finish** to exit the dialog box.

Configure Computer Interface Card Dialog Box

When a 16-bit DX-LAN card (P/N 049077) is installed, selecting Computer Interface Card... opens the Configure Computer Interface Card dialog box.



DX-LAN Card Type indicates that a 16-bit computer interface card is installed. The 16-bit DX-LAN card is configured via software, so it cannot be configured until after both the card and PeakNet have been installed. (Releases prior to PeakNet 4.11 do not support the 16-bit card.)

Dionex Part Number is the part number of the 16-bit card.

Interrupt Number and **I/O Address** indicate the selected DX-LAN card interrupt request line (IRQ) and memory location, respectively.

NOTE If you change the IRQ or I/O address for the 16-bit DX-LAN card, write down the new setting. You must provide this information when reconfiguring the card.

Click on **Default** to restore the factory default settings, or click on **OK** to accept your selections and store them in the PEAKNET.INI file.

Clicking on OK also loads the CardAssistant (SETUP17.EXE) program, so that you can now reconfigure the card with the new settings. For instructions, see *Installing the Dionex PeakNet System* (Document No. 034941).

4.5.10 EG40 Service Command

EG40 Service Command is enabled only when an EG40 module is online. Selecting the command opens a pop-up menu with three commands.

The **Start EG40 I+E Diagnostic...** and **Start EG40 I/R Diagnostic...** commands are reserved for Dionex Service personnel use. Select these commands only when instructed to do so by a Dionex representative.

The **EG40 Leak Calibration** command initiates a calibration procedure for the EG40 leak sensor. After the leak sensor detects a liquid leak in the module, the sensor must be recalibrated. A message box will report the results of the calibration; click OK to close the box. If the leak sensor was not successfully calibrated, contact Dionex for help.

4.6 View Menu

4.6.1 Installed Options...

Displays a dialog box showing the optional equipment installed in the currently selected module. This command is disabled if no options are installed.

4.6.2 Toolbar

Shows or hides the toolbar.

4.6.3 Status Bar

Shows or hides the status bar.

4.6.4 MainMenu

Click on the MainMenu toolbar button (or select the menu command) to display the PeakNet MainMenu.

4.7 Window Menu

4.7.1 Cascade

Arranges child windows in an overlapping fashion so that each title bar is visible.

4.7.2 Tile

Resizes and positions all open child windows so that each is fully visible.

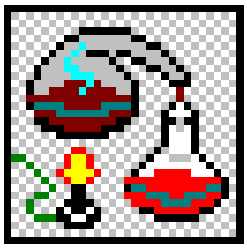
4.7.3 Arrange Icons

Automatically arranges icons neatly at the bottom of the window.

4.7.4 Open Windows List

Choosing the name of an open system window from this list makes the window active.

5 • The Method Editor



NOTE **The Method Editor is used exclusively with DX-LAN systems. ACI-based systems use the ACI Method Editor described in Chapter 6.**

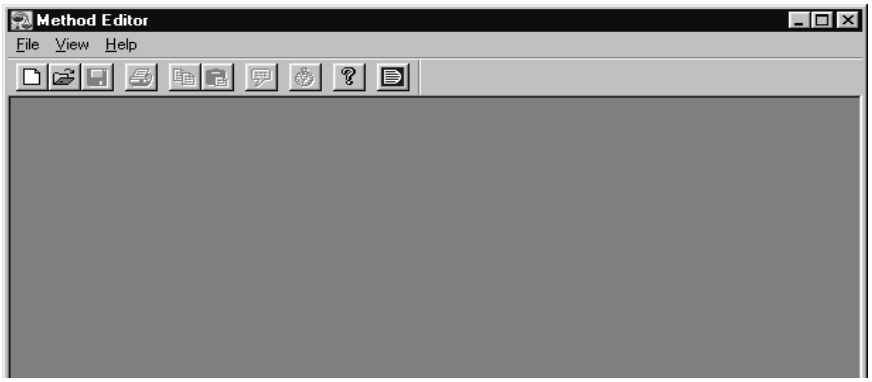
The Method Editor is used to create, edit, and store Method files. Methods contain instructions that tell PeakNet how to control the analytical system, collect and process data, and generate a report after an analysis is complete. Methods include a list of the names, amounts, and retention times of the components in the standard(s) that will be used for calibration.

Each Method is stored on disk under a unique file name. A new Method can be created by recalling an existing Method, modifying it, and then saving the new Method under a different name. PeakNet supplies default values for most Method parameters. These are a useful starting point when developing a new Method.

5.1 Starting the Method Editor

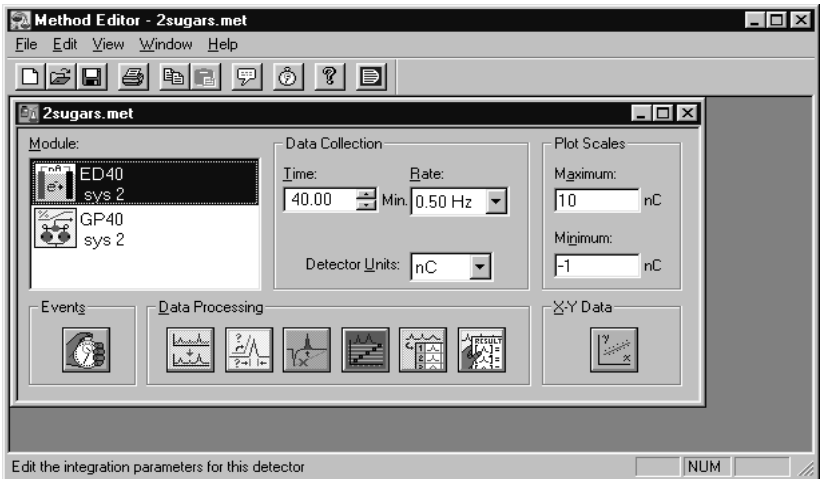
To open the Method Editor main window, click on the Method button in the PeakNet MainMenu or double-click on METHODDX.EXE in the directory that contains the PeakNet program files.

When the Method Editor is initially opened, only an abbreviated version of the File menu, plus the standard Help menu, are displayed.



After a Method is loaded, all menus, including the complete File menu, are available. The Method Editor lets you open multiple Methods at a time. Each Method appears in its own child window (see below).

Use the controls in the child window to set data acquisition, timed events, and data processing parameters for the Method. A few key parameters can be set directly from the window; icon buttons access a set of dialog boxes from which you can select many more parameters.



5.1.1 The Toolbar

Click on a toolbar button to quickly implement frequently used Method Editor menu commands and controls. Click on the buttons for the PeakNet MainMenu and Help to display those programs.

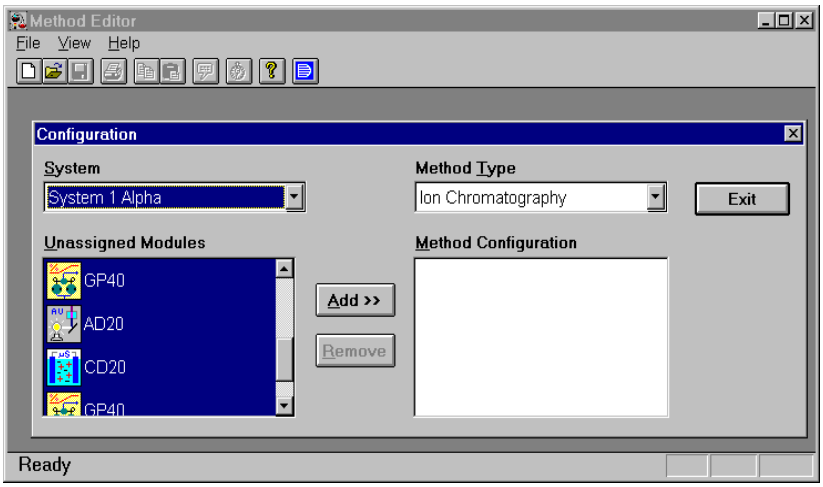
Pointing to a button displays a brief description of its function.

1. New
2. Open
3. Save
4. Print
5. Copy
6. Paste
7. Comments
8. Timed Events
9. Help
10. Switch to MainMenu

5.2 File Menu

5.2.1 New...

Click on the New toolbar button (or select the menu command) to open the Configuration dialog box and specify which modules a new Method will use.



Because Methods contain module-specific instructions, every Method must be created for a particular system. Any (or all) of the modules in a system configuration can be used in a Method configuration.

When the Configuration dialog box is initially opened, it highlights all modules in the first configured system by default. To use these modules for the new Method, click on **Add>>** and then **Exit**. If you want to modify the system configuration for the Method, use the dialog box controls (see Section 6.3.4).

5.2.2 Open...

Click on the Open toolbar button (or select the menu command) to display a Windows common Open dialog box. Select an existing Method file from the directory to open the Method in a new child window.

5.2.3 Close

Closes the active Method.

5.2.4 Save

Click on the Save toolbar button (or select the menu command) to rewrite a previously saved Method to disk under the same name.

If the Method was not previously saved, Save functions in the same way as the Save As... command.

5.2.5 Save As...

Save As... opens the Windows common Save As dialog box. Type in a file name to identify the Method. If you do not enter an extension, the Method Editor automatically adds the extension ".MET" to the file name. Unless you specify otherwise, the file name is added to the ...\METHOD subdirectory.

5.2.6 Print...

Click on the Print toolbar button (or select the menu command) to print the Method currently being edited.

5.2.7 Print Preview

Displays the current Method as it will look when printed.

Selecting Print Preview first opens the Method Table dialog box, which lets you select the modules and Method data to be previewed. See Section 12.10 for details.

After selecting the desired modules and Method data click on OK to close the Method Table dialog box and display the Print Preview window. If the number of columns for each row of the printout is wider than a single page on the printer, the Method will be displayed as a series of pages numbered from left to right, top to bottom. A header containing the Method file name and a footer with the page number will be printed on each page. The system number, default Method path, default data path, and any comments included in the Method will be printed after the last row of Method data.

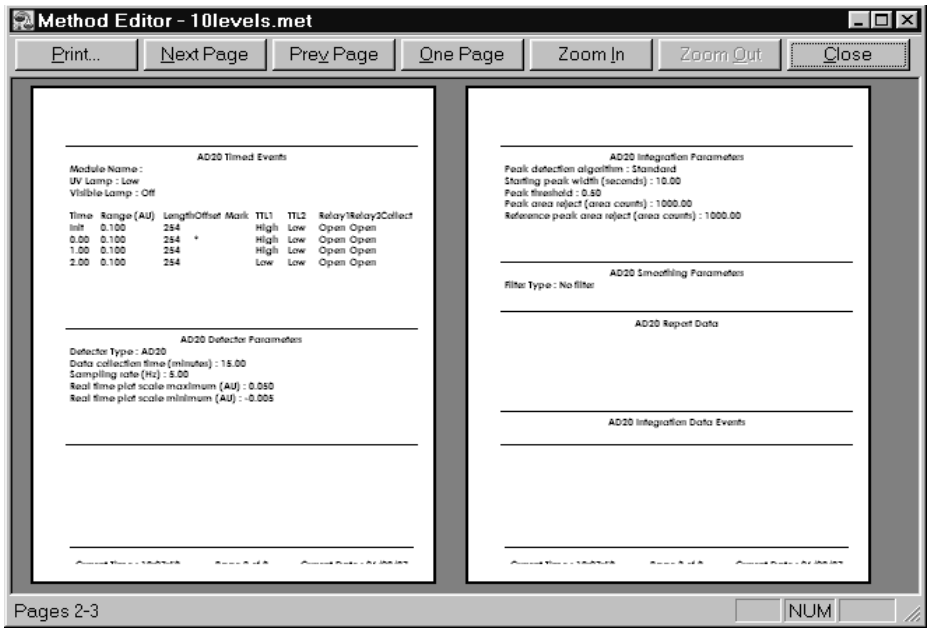
Click on the command buttons below the title bar to modify the display in the Print Preview window:

Next Page displays the next page of the Method.

Prev Page displays the previous page of the Method.

One Page switches from a two-page display (the default) to a one-page display of the last left-hand page displayed.

Two Pages reverts to the default view.



Zoom In switches from a full-page view to a magnified view. (This does not affect the printing size.)

Zoom Out switches from a magnified view to a full-page view. (This does not affect the printing size.)

To exit the Print Preview window without printing, click on the **Close** command button.

To print from the Print Preview window, click on the **Print** command button.

5.2.8 Print Setup...

Displays the Windows common Print Setup dialog box for the current printer. Use the dialog box controls to select the printer settings (print quality, paper size, etc.) or to change the printer.

5.2.9 Most Recently Used

Open one of the last four Methods used by clicking on its name here.

5.2.10 Exit

Closes the Method Editor.

5.3 Edit Menu

Commands in the Edit menu let you copy settings from one module to another, either in the same Method or in two different Methods. Only settings that are compatible between the two modules will be copied.

NOTE The procedure below summarizes the use of the Edit menu's Copy, Copy Special, Paste, and Paste Special... commands.

1. Select the source — the Method child window and the module you want to copy.
2. Click on the Copy button on the toolbar (or select the menu command) to copy all information for the selected module to the Windows Clipboard. Select Copy Special... to copy only the parameters selected in the Copy Special dialog box.
3. Select the destination — the Method child window and the module to which you want to transfer the contents of the Clipboard.
4. Click on the Paste button on the toolbar (or select the menu command) to paste all information from the Clipboard to the selected module. Select Paste Special... to paste only the sections selected in the Paste Special dialog box for that module.

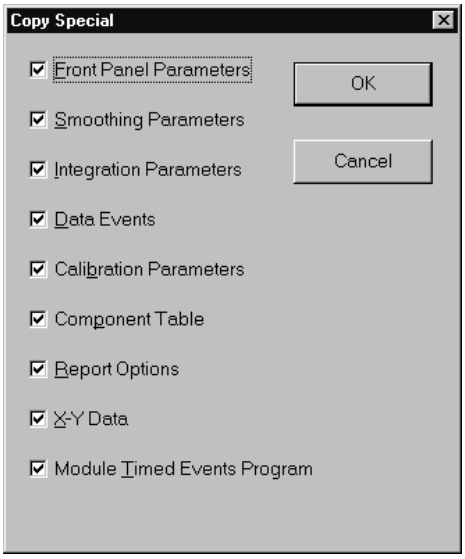
5.3.1 Copy

Click on the Copy toolbar button (or select the menu command) to copy the Method for the currently selected module to the Windows Clipboard in the form of text. From there, it can be pasted into other Methods or a text editor.

5.3.2 Copy Special...

Copy selected Method parameters for the module to the Windows Clipboard in the form of text for transfer to another Method or to a text editor.

Select the parameters in the Copy Special dialog box and click on OK.



Front Panel Parameters include the data collection rate and time, the plot scales, and the Method comments.

The remaining parameters correspond to the icons in the bottom of the Method child window.

5.3.3 Paste

Click on the Paste toolbar button (or select the menu command) to paste all information from the Windows Clipboard into the currently selected module, overwriting any existing Method for that module.

Information about the sampling rate, detector type, plot scales, and timed events cannot be copied from one detector to another.

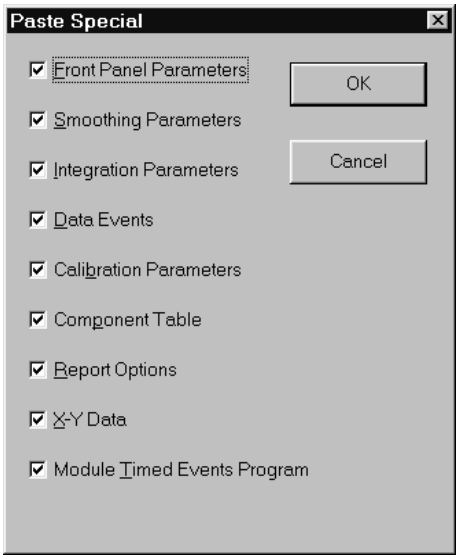
5.3.4 Paste Special...

Pastes selected Method parameters from the Windows Clipboard into the currently selected module. This overwrites those sections in the existing Method for that module.

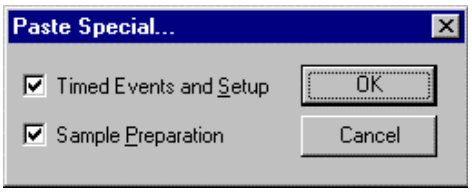
To select information to be pasted, click first on the corresponding check box(es) in the Paste Special dialog box and then on OK.

The Paste Special dialog box for detectors is shown below. Front Panel Parameters include the data collection rate and time, the plot scales, and the Method comments. The remaining items in the Paste Special dialog box correspond to the icons in the bottom of the Method child window.

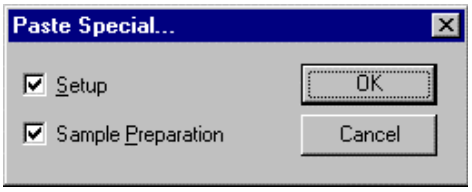
For pumps, Module Timed Events Program is the only available option.



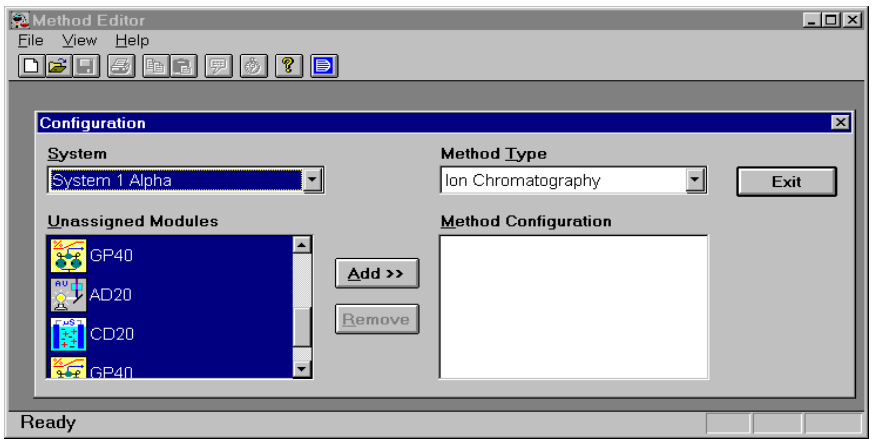
The Paste Special dialog boxes for the AS50 autosampler are shown below. The dialog box varies, depending on the types of AS50 Methods involved in the copy and paste. If the paste is occurring from a regular AS50 Method (*.MET file) to another regular AS50 Method, the following Paste Special dialog box appears:



If the paste is occurring from and/or to an AS50 sample preparation Method (*.SPR), the following dialog box appears:



5.3.5 Configuration...



System selects the name of a system whose modules can be used in the Method.

Method Type specifies whether the Method is for ion chromatography, liquid chromatography, gas chromatography, sample preparation, or capillary electrophoresis (CE). For the first three types, this simply sets the defaults appropriately. For Sample Preparation Methods and CE Methods, it also enables controls specific to these Method types.

Unassigned Modules lists modules in the currently selected system that are not included in the Method configuration. If you assign a custom name to a module (in the Configuration Editor), the custom name is shown here. (When the Method uses a UI20 Universal Interface for which two signals are defined, these are listed as UI20 Signal A and UI20 Signal B. Assign UI20 Signal A, UI20 Signal B, or both to the new Method.)

Method Configuration lists the names of all modules in the Method configuration. If a module is configured to the current Method but is not present in the current system configuration, it is labeled NOT PRESENT.

- To ***add a module*** to a Method configuration, highlight its name in the Unassigned Modules window and click on **Add**>>.

- To ***remove a module*** from a Method configuration, highlight its name in the Method Configuration window and click on **Remove**. (A Method must have at least one module.)

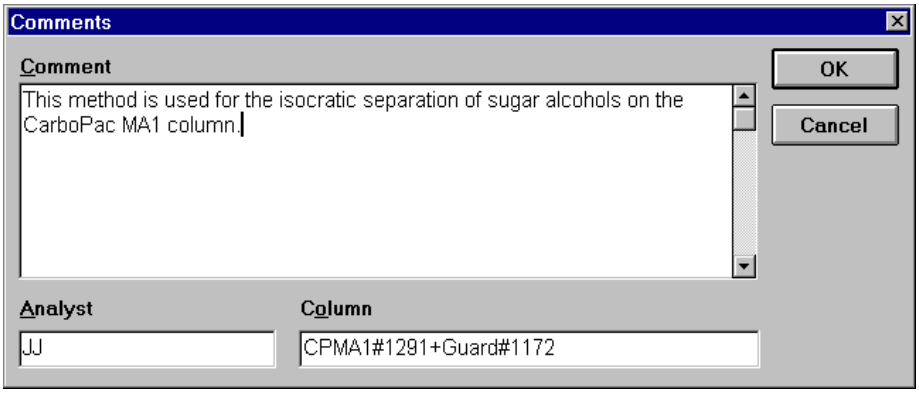
If a module in the Method configuration is missing from the system configuration, Run cannot load the Method and it can be used for reprocessing only. There are three ways to correct the situation:

- Assign the Method to a system that includes the required modules.
- Remove the missing module from the Method configuration.
- Run the Configuration Editor again and update the configuration to include the missing module(s).

Click on **Exit** to save your selections and close the Configuration dialog box. This automatically displays the Method child window, the starting point for setting data acquisition and data processing parameters (see Section 6.6).

5.3.6 Comments...

Click on the Comments toolbar button (or select the menu command) to record comments about the Method.



The **Comments** edit box can contain up to 4,095 characters of text describing the Method. To start a new paragraph, press <Enter>.

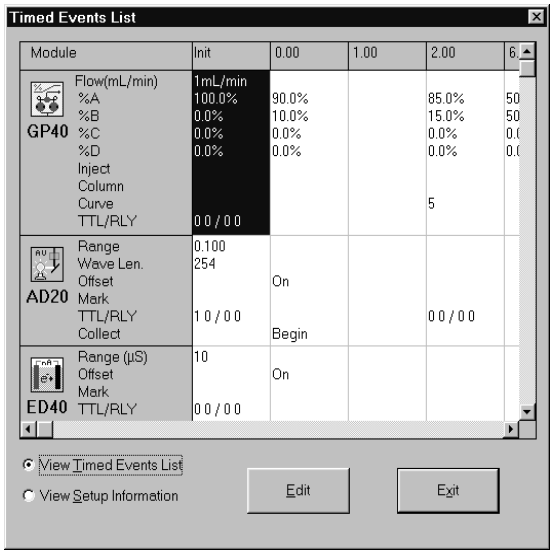
The **Analyst** and **Column** edit boxes can contain descriptions of 19 and 35 characters, respectively.

5.3.7 Timed Events List...

NOTE Sample Preparation Methods contain no timed events.

Click on the Timed Events List toolbar button (or select the menu command) to view all of the module timed events or initial setup conditions for a Method in a single list.

Use the controls in the Timed Events List dialog box to open other dialog boxes and edit the timed events or initial conditions. Saving these editing changes immediately updates the master list.



To View and/or Edit Timed Events:

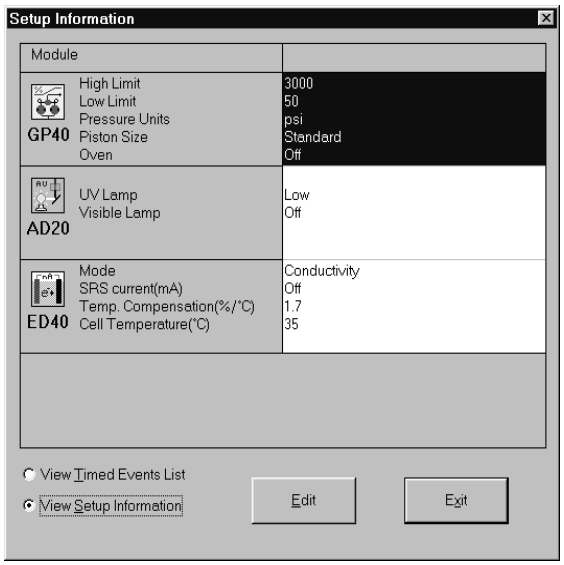
1. Click on the **View Timed Events List** option button (the default setting) if it is not currently selected.
2. Use the vertical scroll bar on the right side of the dialog box (if present) to view all of the modules in the Method. Use the horizontal scroll bar (if present) to view timed events that are not currently visible.

3. Timed events for modules must be edited from their Editor dialog boxes (see Section 6.7). There are two ways to open an Editor dialog box from the master timed events list:
   - Double-click on the module of interest.
   - Click first on any of the timed events for the module of interest, and then on the Edit command button.
4. Edit the timed events program as desired. Saving the changes returns you to the Timed Events List dialog box, where the updated timed events program is now displayed.

NOTE If you also want to change the setup conditions, that dialog box (GP40 Setup, AD20 Lamps, etc.) can be opened from the Editor dialog box.

5. When you finish editing, click on the Exit command button.

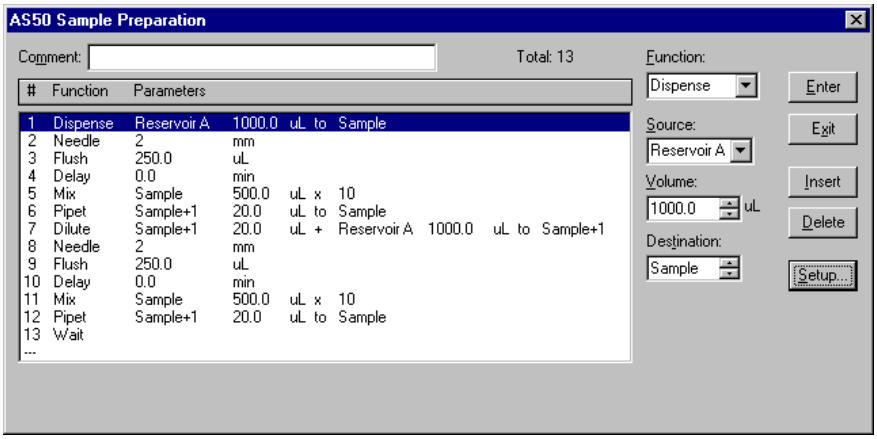
To View and/or Edit Setup Conditions:



1. Click on the **View Setup Information** option button.

2. Use the vertical scroll bar on the right side of the dialog box to view all of the modules in the Method. Use the horizontal scroll bar to view all of the setup conditions.
3. Setup conditions must be edited from the setup dialog boxes (see Section 6.7). There are two ways to open a setup dialog box from the master list of conditions:
   - Double-click on the module of interest.
   - Click first on any of the cells for the module of interest, and then on the Edit command button.
4. Edit the setup conditions as desired. Saving the changes returns you to the Timed Events List dialog box, where the updated conditions are now displayed.
5. When you finish editing, click on the Exit command button.

To View and/or Edit Sample Preparation Conditions:



1. Click on the **View Sample Preparation** option button.

NOTE **This button is present only when the AS50 Autosampler is equipped with the Sample Preparation option.**

2. Use the horizontal scroll bar to view all of the sample preparation conditions.
3. These conditions must be edited from the AS50 Sample Preparation dialog box. There are two ways to open the dialog box from the master list of conditions:
   - Double-click on the AS50 cell.
   - Click first on any of the cells for the AS50, and then on the Edit command button.
4. Edit the sample preparation conditions as desired. Saving the changes returns you to the Timed Events List dialog box, where the updated conditions are now displayed.
5. When you finish editing, click on the Exit command button.

5.4 View Menu

5.4.1 Toolbar

Shows or hides the toolbar.

5.4.2 Status Bar

Shows or hides the status bar.

5.4.3 MainMenu

Click on the MainMenu toolbar (or select the menu command) to display the PeakNet MainMenu.

5.5 Window Menu

5.5.1 Cascade

Arranges child windows in an overlapping fashion so that each title bar is visible.

5.5.2 Arrange Icons

Automatically arranges icons neatly at the bottom of the screen.

5.5.3 Open Windows List

To make an open Method window active, choose its name from this list.

5.6 Data Acquisition and Control

5.6.1 Module

The Module list displays the names and icons of all modules used in the Method. To select a module, click ***once*** on its icon in the list; to open a timed events Editor dialog box for that module, ***double-click*** on a module (or click on the Timed Events icon). See Section 6.7 for a description of the Editor dialog boxes.

All parameters selected from the Method child window (including selections from any dialog boxes opened via the child window) apply to the module selected in the Module list. To edit parameters for a different module, select it from the list. The Method stores all of the parameters for all modules in the system.

5.6.2 Data Collection

NOTE The Collection controls are enable only when the highlighted module in the Module list is a detector.

Time determines for how long (from 0.1 to 999.9 minutes) data is collected for the selected detector or UI20.

Rate sets the data collection rate for the selected detector. This determines how many data points per second are collected and stored in memory. A rate of 5 Hz (points per second) is adequate for most IC and HPLC applications. The data collection rate options depend on the module, as can be seen here:

AD20 Absorbance Detector: 0.1, 0.2, 0.5, 1, 2, 5, 10 Hz

AD25 Absorbance Detector: 0.1, 0.2, 0.5, 1, 2, 5, 10 Hz

CD20 Conductivity Detector: 0.1, 0.2, 0.5, 1, 5, 10, 20 Hz

DX-120 Ion Chromatograph: 0.1, 0.2, 0.5, 1, 2, 5, 10 Hz

ED40 Electrochemical Detector, Conductivity and DC Amperometry Modes: 0.1, 0.2, 0.5, 1, 5, 10, 20 Hz

ED40 Electrochemical Detector, Integrated Amperometry Mode: 1 to 5 times the waveform period

IC20 Ion Chromatograph: 0.1, 0.2, 0.5, 1, 5, 10, 20 Hz

UI20 Universal Interface: 0.1, 0.2, 0.5, 1, 2, 5, 10, 20, 50 Hz

In general, each peak should be defined by 20-30 data points. 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. Using a faster data collection rate than necessary does not improve accuracy, but it *does* slow down data processing and waste memory and disk space. See Appendix B for more information about data collection.

To select the desired units for a DX-500 detector or an IC20, select the **Units** that are most convenient for the analysis from the drop-down list box; for example, AU, mAU, or µAU for an AD20. This affects plot labeling and reporting only; it does not affect detector sensitivity.

To enter a proportion for converting input voltage received by the UI20 into detector units, use the **Number** and **Units** edit boxes.

1. Verify that the full-scale voltage shown is appropriate.
2. Enter the number of detector units which corresponds to this full-scale voltage.
3. Enter the abbreviation for the detector units.

5.6.3 Plot Scales

NOTE The Plot Scales controls are enabled only when the selected module is a detector or UI20 Universal Interface.

The **Maximum** and **Minimum** values are the defaults for the Y axis of the real-time data plot displayed during a run. An inappropriate plot setting can make peaks too small to see, or so large that the top of the peak goes off scale on the display. This setting also affects the printed output, unless you select the Autoscale option from the Plot dialog box. The range and units displayed depend on which detector is selected.

NOTE The plot scale setting affects only the display of the data, not the collection of raw data from the detector.

5.7 Timed Events

Timed Events are timed operations performed by a module during execution of a Method. All timed events programs must contain at least two steps: one at initial conditions (INIT) and another at time 0.0. The maximum number of steps in a timed events program depends on the module.

Module	Maximum Program Steps
All pumps	50
IC20 Ion Chromatograph	50
EG40 Eluent Generator	50
Other modules	32

- The INIT step typically contains standby conditions for each module in the system. This lets you include system equilibration conditions in each Method. The conditions in the INIT step are in effect from the time the Method is downloaded to the module until the Method is started.
- The conditions at time 0.0 take effect as soon as the module receives a START command. The conditions in the time 0.0 and INIT steps do not have to match.

Each module has a unique Editor dialog box from which you create and edit timed events. Follow the steps below to create a timed events program for a module.

1. To open an Editor dialog box, double-click on the module name in the Module list, or click on the Timed Events Edit... command button.
2. Enter a step time in the Time (Min) edit box of the Editor dialog box. Click on the Enter command button to add the new step time to the timed events window.
3. Select the conditions for this step, then click on Enter to accept the selections and display them in the timed events window.
4. Repeat Steps 2 and 3 until the timed events program is complete.

NOTE **If the time entered for a new step duplicates the time for an existing step, the parameters for the new step will overwrite the existing parameters.**

5.7.1 Common Timed Event Features

The following features are common to all of the Editor dialog boxes. Descriptions of the unique features of each of the module Editors follow this section.

Time (Min) specifies the time (from 0.00 to 999.99 minutes) at which the selected operating conditions will go into effect. Each time entry is a separate step in the timed events table. In the gradient pump Editors, each time entry determines the time at which each gradient step in the program occurs.

- To ***create*** a new step, type a new time in the edit box. After using the controls in the dialog box to select the conditions for the step, click on Enter to accept the new information.
- To ***copy*** an existing step, click on the down-arrow, select the step to be copied, type the new time, and click on Enter.
- To ***edit*** an existing step, click on the down-arrow, select the step to be edited, make the desired changes, and click on Enter.

Outputs

For all Editors:

TTL outputs control the TTL outputs of the module. These outputs provide control of accessories that need only a digital signal to trigger their operation.

RLY outputs control the relays of the module. The relays provide contact-closure control of accessories (e.g., stream-select valves).

For pump Editors only:

Inject switches the injection valve to the inject position.

Column switches the position of the column switching valve.

For detector Editors only:

Offset offsets the current detector value to zero.

Mark controls the transmission of a positive pulse to the analog recorder output as an event marker. The pulse is equivalent to 10% of the full-scale setting.

Enter adds the conditions selected for the module at a specified time to the timed events table. If this step time is the same as an existing time, the existing parameters will be overwritten.

Exit closes the Editor dialog box.

Delete removes steps from the timed events table. Click first on the step to be removed (to highlight it) and then on the Delete command button. The Delete command button is disabled when the INIT and time 0.0 steps are highlighted because these steps cannot be deleted.

5.7.2 GP40 Gradient Pump Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.

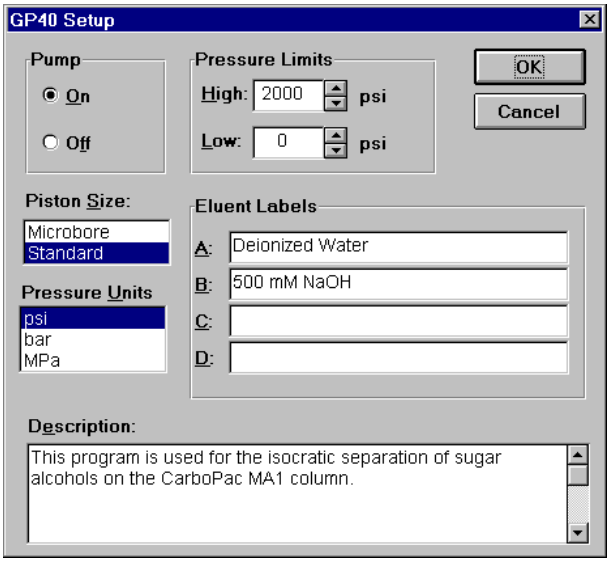
1. If you have not previously created a gradient program, open the GP40 Setup dialog box by double-clicking on the GP40 icon in the Method child window.
2. Use the controls in the GP40 Setup dialog box to set the initial pump conditions (pressure limits, piston size, etc.) and click on OK. Clicking on OK accepts these selections and opens the GP40 Editor dialog box.
3. Use the controls in the GP40 Editor dialog box to set the conditions for each step of the gradient program. A program can contain up to 50 steps.

NOTE Each gradient file must include a step at initial conditions (INIT) and a step at time 0.0.

GP40 Setup

The GP40 Setup dialog box appears when you invoke the GP40 Editor before a gradient exists, or when you click on the Setup... command button in the GP40 Editor dialog box.

When an EG40 Eluent Generator is present, the dialog box contains additional controls (see Section 5.7.6).



Pump turns the pump On or Off. When it is Off, no gradient can be entered. Use Off to shut down the pump at the end of a Schedule.

Pressure Limits are set using the arrow buttons, or by typing the desired values in the edit boxes. The following table indicates the pressure ranges and High limit default settings. (When an EG40 is present, the maximum allowable pressure is 3000 psi.)

	psi	bar	MPa
Low Pressure Default	0.00	0.00	0.00
Minimum Pressure	0.00	0.00	0.00
Maximum Pressure	5000	344.7	34.4
High Pressure Default	3000	206.8	20.7

Piston Size specifies the diameter of the pistons installed. The default is Standard.

Eluent Labels are displayed on the gradient graph and on Method printouts. The default labels are A, B, C, and D; up to 39 characters can be entered.

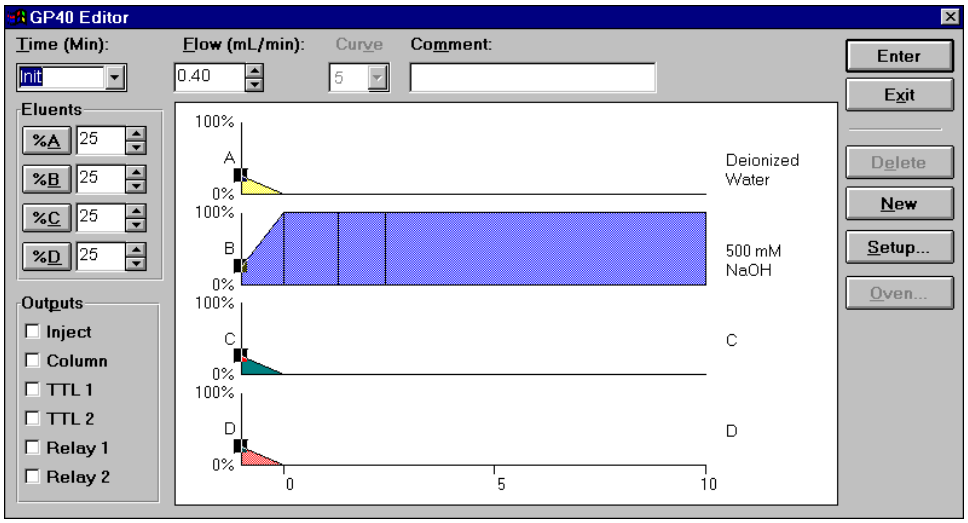
Description can be up to 319 characters. To begin a new line, press the <Ctrl> and <Enter> keys simultaneously.

When you finish editing, click on OK to save your selections and open the GP40 Editor dialog box.

GP40 Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.

NOTE When an EG40 Eluent Generator is present, the GP40 Editor contains additional controls (see Section 5.7.6).



NOTE When using a concentration gradient, be sure to inject sample at exactly the same point in the gradient each time. This is easily done by including several minutes of the eluent with the highest concentration at the beginning of the gradient program and following this with a re-equilibration step. Inject the sample at some set time after the equilibration is complete. For more information, see the *GP40 Gradient Pump Operator's Manual* **(Document No. 034856).**

Eluents

Each eluent has a **totalizer button** labeled %A, %B, %C, or %D; an **edit box** which displays the eluent percentage for the step being edited; and two **arrow buttons**. Type an eluent percentage in the edit box or use the arrow buttons to make a selection. The percentages of all selected eluents must total 100%. The gradient graph is updated dynamically so that you can see the effect of the eluent proportions as you select them.

NOTE A quick way to ensure that the eluent percentages total 100% is to click on the totalizer button for the final eluent selection. The value required to make the eluent totals equal 100% will automatically appear in this edit box, if possible (i.e., if the total of the previous selections is less than 100%). If the eluent totals already equal or exceed 100%, clicking on the totalizer button has no effect.

Flow (mL/min) displays the flow rate for the currently selected gradient step. The flow rate ranges are 0.0 to 10.0 mL/min for the standard bore GP40 and 0.0 to 2.50 mL/min for the microbore GP40. Type a value in the edit box or use the arrow buttons to display the desired flow rate.

Curve applies a curvilinear gradient to the preceding gradient segment. For an increasing eluent, gradient curves 1 through 4 are convex, curve 5 (the default) is linear, and curves 6 through 9 are concave.

C**omment** can be up to 29 characters, including spaces and punctuation, for each gradient step.

Gradient Graph

The gradient graph is updated dynamically, allowing you to see the profile of the eluent proportions as you select them.

To select a gradient step, click the mouse cursor on the perpendicular step line on the graph. A handle (a small darkened square) will appear at the top of the selected step line. Press the up or down arrow keys to select other steps, or select the step time from the Time drop-down list.

To change an eluent percentage, position the cursor over the step line handle. The cursor arrow will change to a double-headed vertical arrow. Press the mouse left button and move the step line handle up or down to adjust the eluent percentage. Click on the Eluents totalizer buttons as required to bring the percentage for eluents to 100%, or double-click on the makeup eluent graph.

To change the time of a gradient step, first click the cursor on the step line to select it. Next, position the cursor anywhere on the step line except on the handle (the cursor arrow will change to a right-left arrow). Now, change the step time by depressing the mouse left button and dragging the step line left or right along the time axis.

To duplicate a step at a different time, follow the procedure for changing the time of a gradient step, but depress the <Shift> key while dragging the time line. The position to which you drag the time line becomes a duplicate step. (The original step is retained.)

Or, select a step, type the time of the new step, and press <Enter>.

To clear all entries and create a new gradient, click New.

Setup... opens the GP40 Setup dialog box described previously.

Oven... opens the Oven Settings dialog box, which is used only if the GP40 is connected to an LC30 Chromatography Oven:

Temperature can be set between zero and 80 °C or Off, using the edit box or arrow buttons. The default setting is Off.

5.7.3 GP50 Gradient Pump Editor

Controls in the GP50 Editor and Setup dialog boxes are identical to those in the GP40 dialog boxes; refer to the preceding section for a description.

For more information about the GP50, refer to the *GP50 Gradient Pump Operator's Manual* (Document No. 031377).

5.7.4 IP20 Isocratic Pump Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.

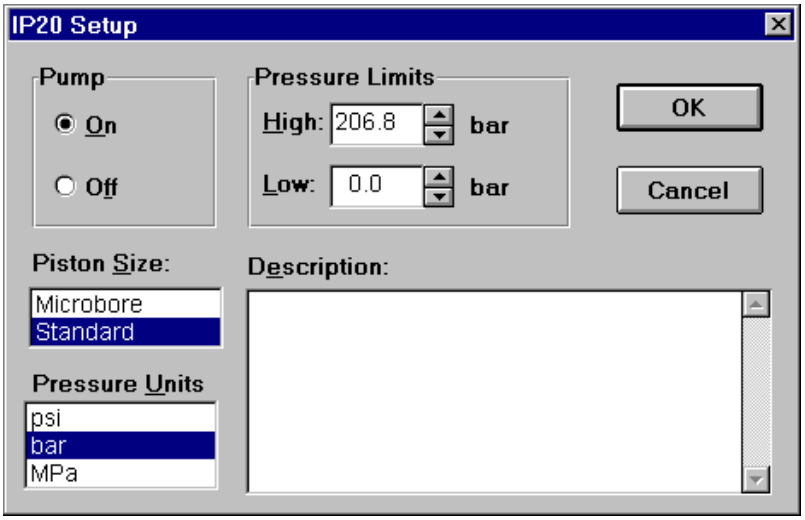
1. If you have not previously created an isocratic program, open the IP20 Setup dialog box by double-clicking on the IP20 icon in the Method child window.
2. Use the controls in the IP20 Setup dialog box to set the initial pump conditions (pressure limits, piston size, etc.) and click on OK. Clicking on OK accepts these selections and opens the IP20 Editor dialog box.
3. Use the controls in the IP20 Editor dialog box to set the conditions for each program step. A pump program can contain up to 50 steps.

NOTE Each file must include a step for the initial conditions (INIT) and a time 0.0 step.

IP20 Setup

The IP20 Setup dialog box appears when you invoke the IP20 Editor before an isocratic program exists, or if you click on the Setup... command button in the IP20 Editor dialog box.

When an EG40 Eluent Generator is present, the IP20 Editor contains additional controls (see Section 5.7.6).



Pump turns the pump On or Off. When the pump is Off, no program can be entered. Use Off to shut down the IP20 at the end of a Schedule.

Pressure Limits are set using the arrow buttons, or by typing the desired values in the edit boxes. The following table indicates the pressure ranges and High limit default settings. (When an EG40 is present, 3000 psi is the maximum allowable pressure.)

	psi	bar	MPa
Low Pressure Default	0.00	0.00	0.00
Minimum Pressure	0.00	0.00	0.00
Maximum Pressure	5000	344.7	34.4
High Limit Default	3000	206.8	20.7

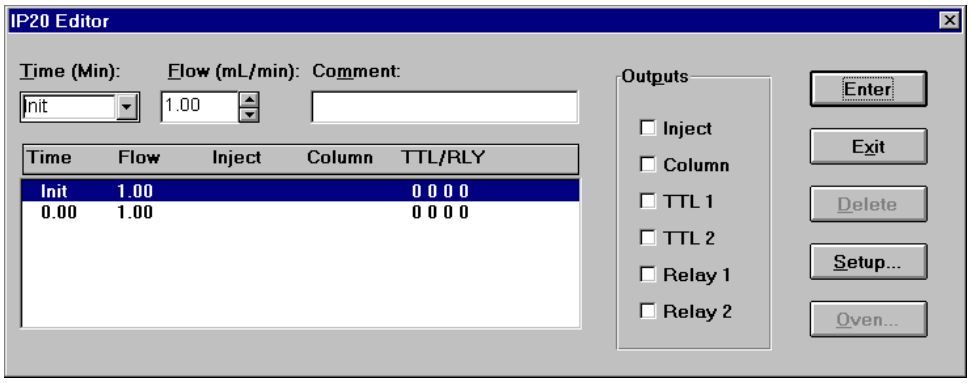
Piston Size specifies the diameter of the pistons installed. The default is Standard.

Description can be up to 319 characters. To begin a new line, press the <Ctrl> and <Enter> keys simultaneously.

When you finish editing, click on OK to save your selections and open the IP20 Editor dialog box.

IP20 Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.



Flow (mL/min) displays the flow rate for the currently selected step. The flow rate ranges are 0.0 to 9.99 mL/min for the standard bore IP20 and 0.0 to 2.50 mL/min for the microbore IP20. Type a value in the edit box or use the arrow buttons to display the desired flow rate.

Comment can be up to 29 characters, including spaces and punctuation, for each gradient step.

Setup... opens the IP20 Setup dialog box described previously.

Oven... opens the Oven Settings dialog box, which is used only if the pump is connected to an LC30 Chromatography Oven:

Temperature can be set between zero and 80 °C or Off, using the edit box or arrow buttons. The default setting is Off.

5.7.5 IP25 Isocratic Pump Editor

Controls in the IP25 Editor and Setup dialog boxes are identical to those in the IP20 dialog boxes; refer to the preceding section for a description.

For more information about the pump, refer to the *IP25 Isocratic Pump Operator's Manual* (Document No. 031379).

5.7.6 EG40 Eluent Generator Editor

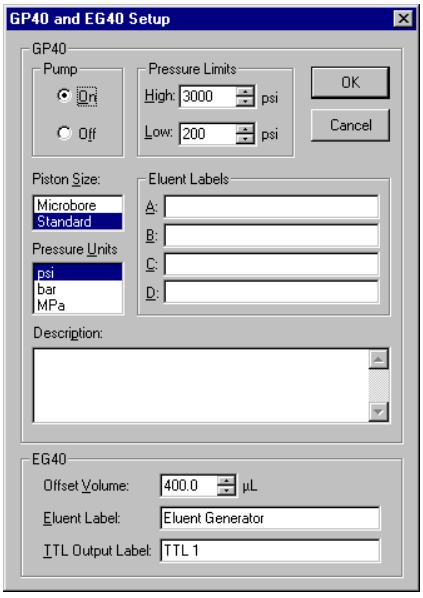
NOTE See Section 5.7.1 for a description of features common to all module Editors.

1. If you have not previously created a Method for the EG40, open the Setup dialog box. To do so, double-click in the Method child window on either the EG40 icon or the icon for the pump that is in the system with the EG40.
2. Use the controls in the Setup dialog box to set the initial conditions for the EG40 and pump (pressure limits, piston size, etc.) and click on OK. Clicking on OK accepts these selections and opens the Editor dialog box.
3. Use the controls in the Editor dialog box to set the conditions for each program step (up to 50 steps).

NOTE Each file must include a step at initial conditions (INIT) and a step at time 0.0.

EG40 Setup

A combination pump/EG40 Setup dialog box appears when you invoke the EG40 Editor before a program exists, or when you click on the Setup... command button in the pump Editor dialog box. The EG40 controls in each dialog box are the same, regardless of which pump is configured for the system. The GP40 and EG40 Setup dialog box shown below is an example.



Offset Volume specifies the loop volume (from 0 to 2000 µL) between the pump outlet and the injection valve. The Run program uses the offset volume to calculate the time delay in starting the EG40; this delay synchronizes the operation of the EG40 and the pump.

Eluent Label can be any desired text (up to 39 characters).

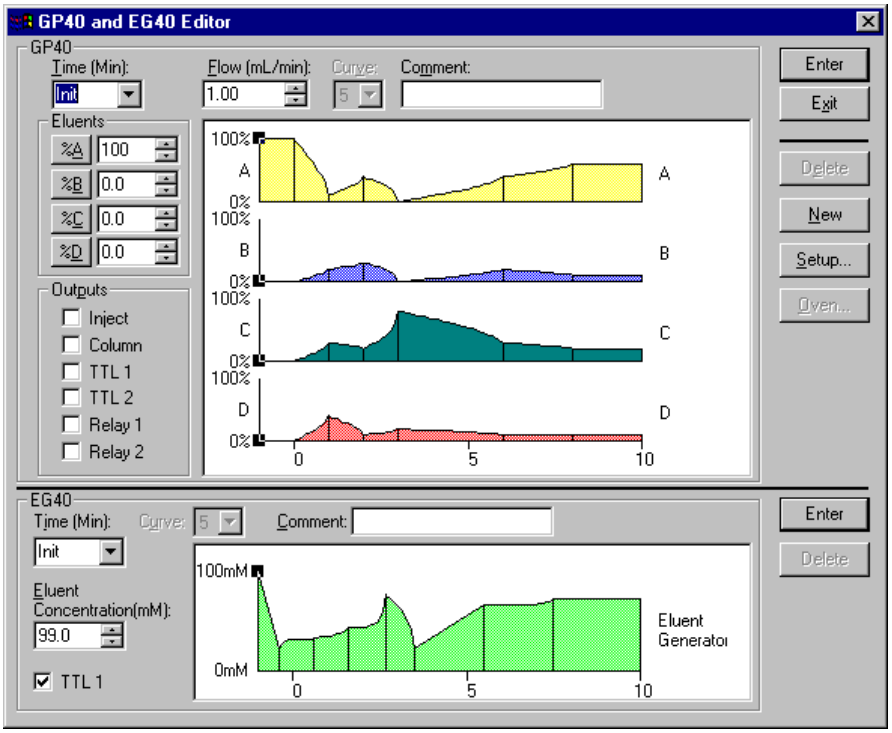
TTL Output Label can be can be any desired text (up to 15 characters).

When you finish editing, click on OK to save your selections and the combination pump/EG40 Editor dialog box will appear.

EG40 Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.

The EG40 controls are in the lower section of the pump Editor dialog box. The EG40 controls are the same, regardless of which pump is configured for the system. The GP40 and EG40 Editor is shown here as an example.



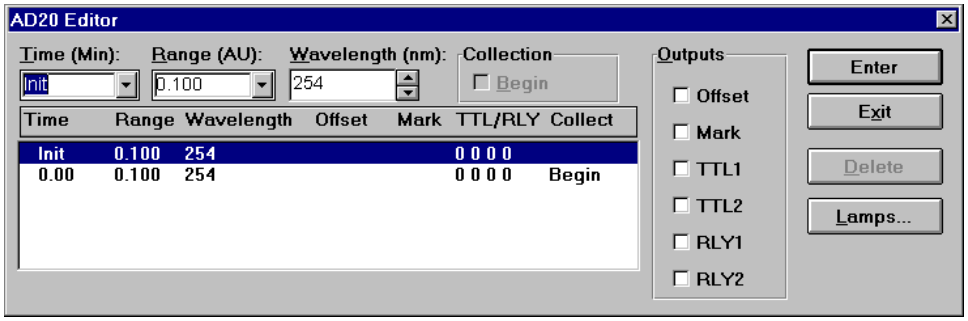
Eluent Concentration (mM) specifies the concentration in increments of 0.1 mM. The concentration range depends on the flow rate for the step.

Curve applies a curvilinear gradient to the preceding gradient segment. For an increasing eluent, gradient curves 1 through 4 are convex, curve 5 (the default) is linear, and curves 6 through 9 are concave.

Comment can be up to 29 characters, including spaces and punctuation, for each step.

5.7.7 AD20 Absorbance Detector Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.

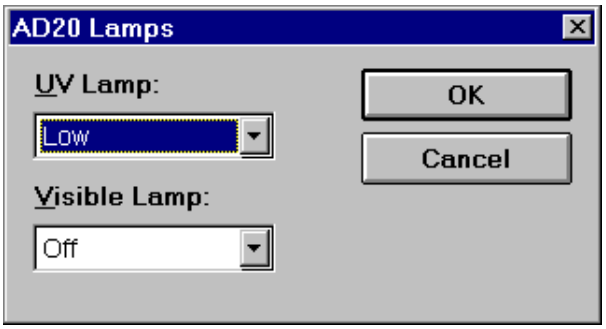


Range (AU) sets the full-scale recorder output range to between 0.001 and 2.0 AU. The default is 0.1 AU.

Wavelength (nm) sets a wavelength of 190 to 350 nm for the UV lamp, or 351 to 800 nm for the visible lamp. The default is 254 nm.

Begin Collection specifies when collection of detector data starts. This can only occur once in the timed events sequence. The default is the step at time 0.0.

Lamps... opens the AD20 Lamps dialog box:



Set the **UV Lamp** or **Visible Lamp** to Off, Low, or High. Turning both lamps Off disables the AD20 timed events. Use Off to shut down the AD20 at the end of a Schedule.

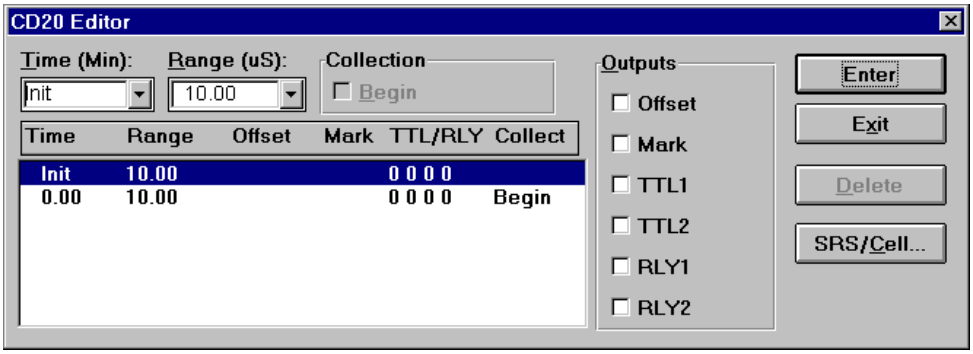
5.7.8 AD25 Absorbance Detector

Controls in the AD25 Editor and Lamps dialog boxes are identical to those in the AD20 dialog boxes, except that the lamp settings are Off and On only. Refer to the preceding section for a description.

For more information about the detector, refer to the ***AD25 Absorbance Detector Operator's Manual*** (Document No. 031647).

5.7.9 CD20 Conductivity Detector Editor

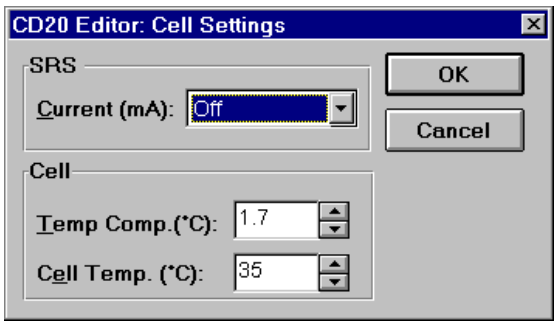
NOTE Also see Section 5.7.1 for a description of features common to all module Editors.



Range (µS) sets the full-scale recorder output range to between 0.01 and 3000 µS. The default is 10 µS.

Begin Collection specifies when collection of detector data starts. This can only occur once in the timed events sequence. The default is step at time 0.0.

SRS/Cell... opens the CD20 Editor: Cell Settings dialog box:



SRS

Current (mA) sets the SRS current to 50, 100, 300, or 500 mA or Off. The default setting is Off. Select from the drop-down list.

Cell

Temp. Comp. (^{o}C) sets the temperature compensation to a value from 0.0 to 3.0 %/°C. Use the arrow buttons to display the desired value, or type a value into the edit box.

Cell Temp. (^{o}C) sets the cell temperature to a value from 25 to 45 °C. Use the arrow buttons to display the desired value, or type a value into the edit box. A selection of 0.0 or Off turns off cell heating.

5.7.10 ED40 Electrochemical Detector Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.

ED40 Setup

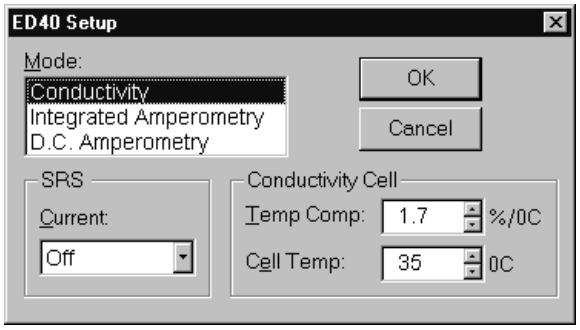
The ED40 Setup dialog box appears if you click the Setup... command button in the ED40 Editor. Use the Setup dialog box to select the ED40 operating mode and to select operating conditions for the cell and its heating source (if installed).

Mode selects the ED40 operating mode: Conductivity (the default), Integrated Amperometry, or D.C. Amperometry.

NOTE If you change to a different operating mode, a warning message informs you that the module program will be reset. If you continue, any timed events set for the previous mode will be deleted; the ED40 module control program will be reset to the new mode, and the ED40 Editor will display the default settings for the new mode.

The remaining controls in the Setup dialog box depend on the selected mode and the type of cell heating source (if any).

Conductivity Mode with DS3 installed



SRS (Self-Regenerating Suppressor)

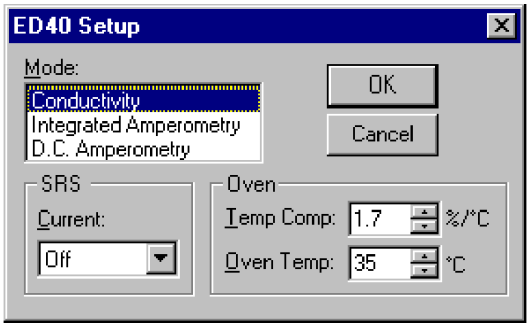
Current (mA) sets the SRS current to 50, 100, 300, or 500 mA or Off. The default setting is Off. Select from the drop-down list.

Conductivity Cell

Temp. Comp. (%/°C) sets the temperature compensation to a value from 0.0 to 3.0 %/°C. Use the arrow buttons to display the desired value, or type a value into the edit box.

Cell Temp. (°C) Set the cell temperature to a value from 25 to 45 °C. Use the arrow buttons to display the desired value, or type a value into the edit box. A selection of 0.0 or Off turns off cell heating.

Conductivity Mode with LC25 installed



SRS

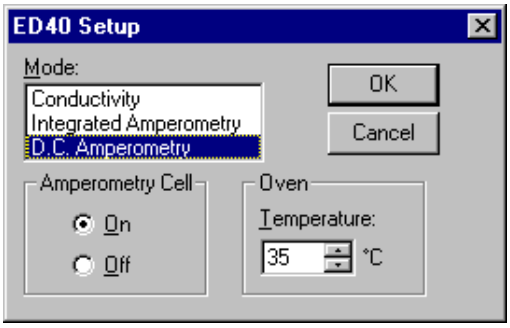
Current (mA) sets the SRS current to 50, 100, 300, or 500 mA or Off. The default setting is Off. Select from the drop-down list.

Oven

Temp. Comp. (%/°C) sets the temperature compensation to a value from 0.0 to 3.0 %/°C. Use the arrow buttons to display the desired value, or type a value into the edit box.

Oven Temp. (°C) sets the cell temperature to a value from 30 to 45 °C. Use the arrow buttons to display the desired value, or type a value into the edit box. A selection of 0.0 or Off turns off cell heating. This box is disabled if an LC25 oven is not installed.

Amperometry Modes with LC25 installed



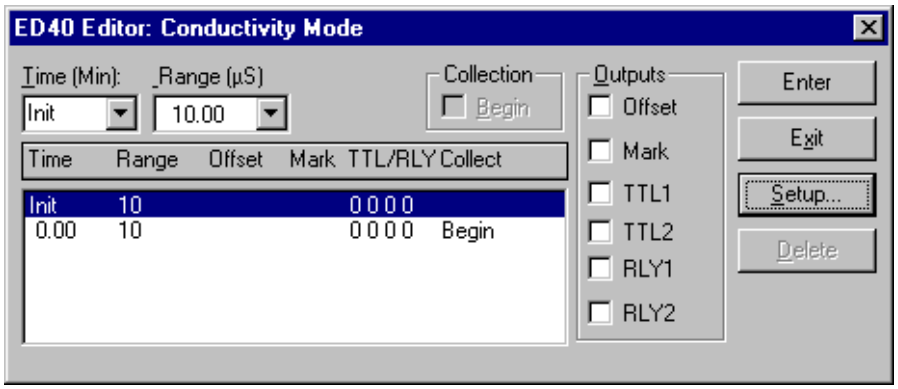
Amperometry Cell turns the cell on or off. Selecting Off, disables the Method timed events.

Oven Temperature (°C) sets the cell temperature to a value from 30 to 45 °C. Use the arrow buttons to display the desired value, or

type a value into the edit box. A selection of 0.0 or Off turns off cell heating. This box is disabled if an LC25 oven is not installed.

ED40 Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.

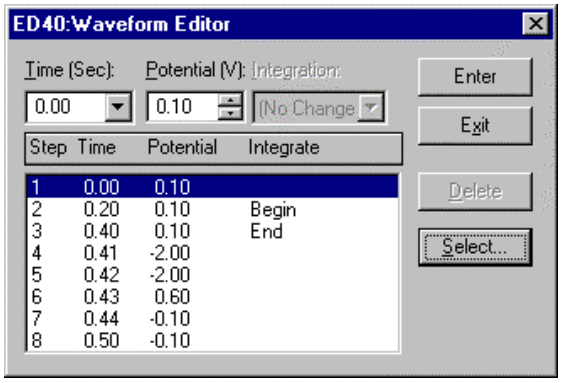


Range (µS) Set the full-scale recorder output range to between 0.01 and 3000 µS. The default is 10 µS.

Begin Collection specifies when collection of detector data starts. This can only occur once in the timed events sequence. The default is the step at time 0.0.

Setup... opens the ED40 Setup dialog box described previously.

Waveform... (Integrated Amperometry mode only) opens the ED40: Waveform Editor dialog box:



Time (Sec) Set the time to between zero and 2.0 seconds. The default is zero.

Potential (V) Set the potential to between -2.04 and +2.04 volts. The default is zero.

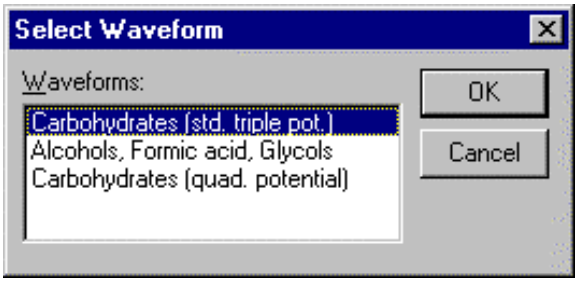
Integration options are **No Change**, **Begin**, and **End**. You must click on **OK** after each selection to accept it. The default is No Change.

Enter adds the selected step to the table.

Exit closes this dialog box and returns you to the ED40 Editor: Integrated Amp. Mode dialog box.

Delete removes the selected step from the table.

Clicking on **Select...** opens the Select Waveform dialog box. Select a standard waveform from the ones listed. The new selection replaces any waveform already in the Waveform Editor.



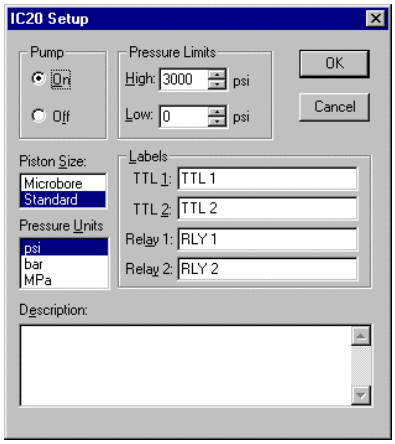
5.7.11 IC20 Editor

1. If you have not previously created an IC20 timed events program, open the IC20 Setup dialog box by double-clicking on the IC20 icon in the Method child window.
2. Use the controls in the IC20 Setup dialog box to set the initial conditions (pump on or off, pressure limits, etc.) and click on OK. Clicking on OK accepts these selections and opens the IC20 Editor dialog box.
3. Use the controls in the IC20 Editor dialog box to set the conditions for each program step (up to 50 steps).

NOTE Each file must include a step for the initial conditions (INIT) and a time 0.0 step.

IC20 Setup

The IC20 Setup dialog box appears when you click on the Setup... command button in the IC20 Editor dialog box or when you double-click on the IC20 icon in the Method child window.



Pump turns the pump On or Off. Use Off to shut down the IC20 at the end of a Schedule.

Pressure Limits are set using the arrow buttons, or by typing the desired values in the edit boxes. The following table indicates the

pressure ranges and High limit default settings. (When an EG40 is present, 3000 psi is the recommended maximum pressure.)

	psi	bar	MPa
Low Pressure Default	0.00	0.00	0.00
Minimum Pressure	0.00	0.00	0.00
Maximum Pressure	5000	344.7	34.4
High Limit Default	3000	206.8	20.7

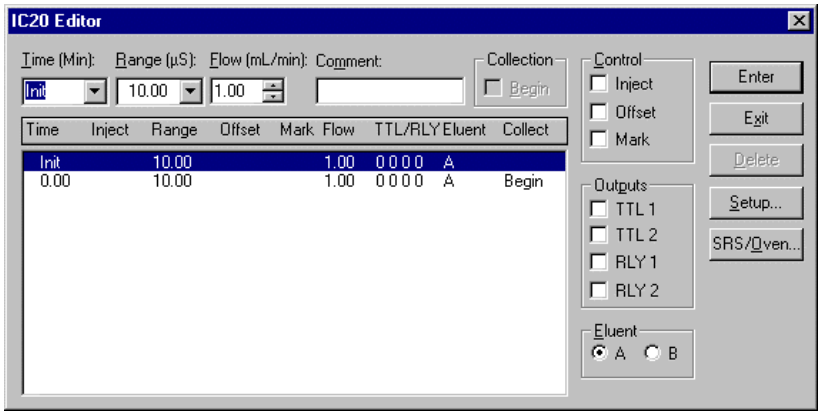
Piston Size specifies the diameter of the pistons installed. The default is Standard.

Description can be up to 319 characters. To begin a new line, press the <Ctrl> and <Enter> keys simultaneously.

When you finish editing, click on OK to save your selections and open the IC20 Editor dialog box.

IC20 Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.



Flow (mL/min) displays the flow rate for the currently selected step. The flow rate ranges are 0.0 to 9.99 mL/min for the standard bore IC20 and 0.0 to 2.50 mL/min for the microbore IC20. Type a value in the edit box or use the arrow buttons to display the desired flow rate.

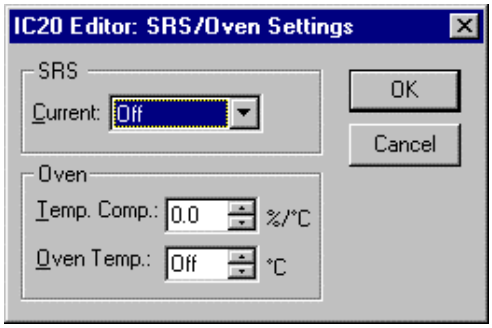
Comment can be up to 29 characters, including spaces and punctuation, for each gradient step.

Begin Collection specifies when collection of detector data starts. This can only occur once in the timed events sequence. The default is the step at time 0.0.

Eluent selects eluent A or B.

Setup... opens the IC20 Setup dialog box described previously.

SRS/Oven... opens the SRS/Oven Settings dialog box:



SRS

Current (mA) sets the SRS current to 50, 100, 300, or 500 mA or Off. The default is Off. Select from the drop-down list.

Oven

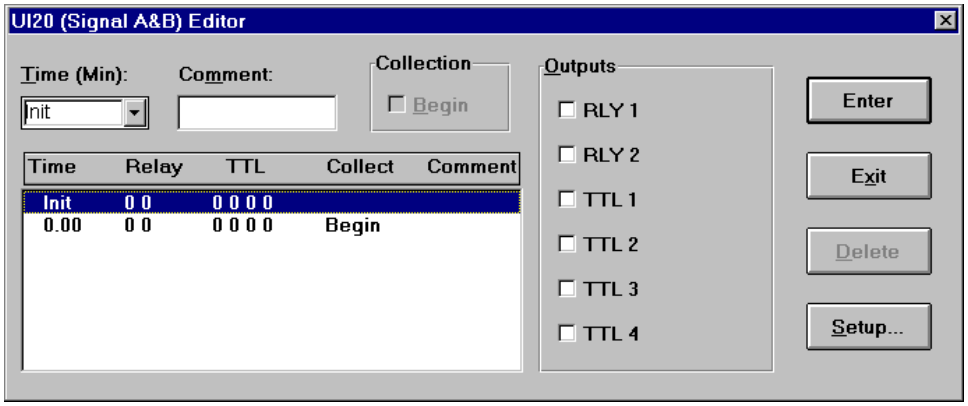
NOTE These controls are enabled only when the IC20 is connected to an LC25 Chromatography Oven.

Temp. Comp. sets the temperature compensation to a value from 0.0 to 3.0 %/°C. Use the arrow buttons to display the desired value, or type a value into the edit box.

Oven Temp. sets the oven temperature to a value from 30 to 45 °C. Use the arrow buttons to display the desired value, or type a value into the edit box.

5.7.12 UI20 Universal Interface Editor

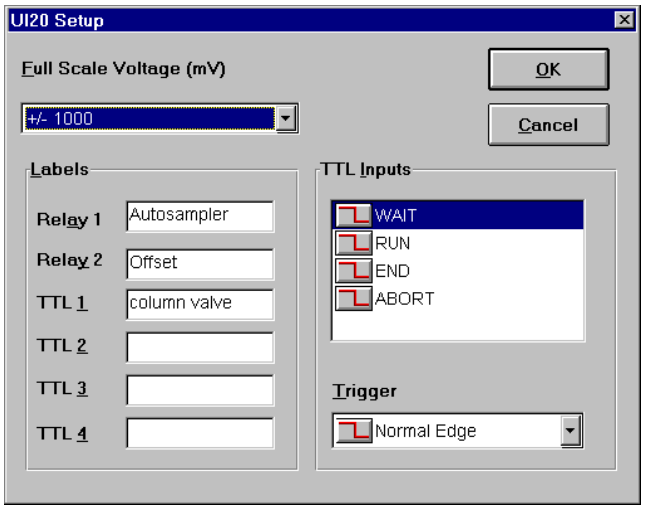
NOTE See Section 5.7.1 for a description of features common to all module Editors.



Comment (optional) can be up to 29 characters (including spaces and punctuation). Comments can be entered for each step.

Begin Collection specifies when collection of detector data starts, This can only occur once in the timed events sequence. The default is the step at time 0.0.

Setup... opens the UI20 Setup dialog box:



Full-Scale Voltage (mV) can be set to +/- 10, 100, 1000, or 10,000 mV to match the maximum output of your detector.

Labels can be up to 15 characters for any TTL or Relay output. The label appears in the UI20 Editor dialog box.

TTL Inputs represent the trigger configurations for the four TTL inputs. To change a configuration, double-click on the icon until the correct option (Normal Edge, Inverted Edge, or Disabled) is displayed. You can also select the configuration from the **Trigger** drop-down list box.

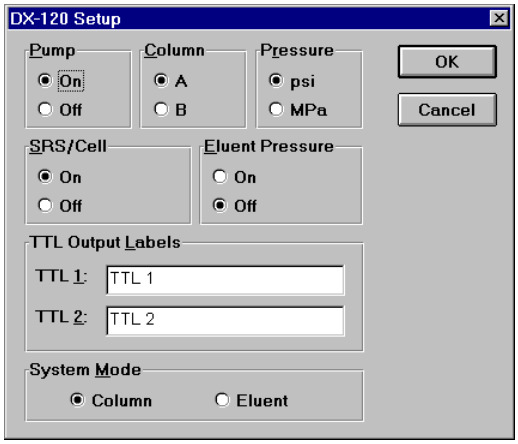
5.7.13 DX-120 Ion Chromatograph

1. If you have not previously created a DX-120 timed events program, open the DX-120 Setup dialog box by double-clicking on the DX-120 icon in the Method child window.
2. Use the controls in the DX-120 Setup dialog box to set the initial conditions (pump on or off, column selection, etc.) and click on OK. Clicking on OK accepts these selections and opens the DX-120 Editor dialog box.
3. Use the controls in the DX-120 Editor dialog box to set the conditions for each program step (up to 32 steps).

NOTE Each file must include a step for the initial conditions (INIT) and a time 0.0 step.

DX-120 Setup

The DX-120 Setup dialog box appears when you click on the Setup... command button in the DX-120 Editor dialog box, or if the pump was turned off in the last session.



Pump turns the pump On or Off. Turning off the pump deletes the DX-120 timed events list and turns off the SRS (Self-Regenerating Suppressor).

Column selects column set A or B. These controls are disabled when the Eluent System Mode is selected (see below).

Pressure sets the unit of measure for the eluent reservoir pressure to psi or MPa. This pressure reading appears in the status display in the Run program.

SRS/Cell turns the Self-Regenerating Suppressor On or Off.

Eluent Pressure turns the pressure applied to the eluent reservoir On or Off.

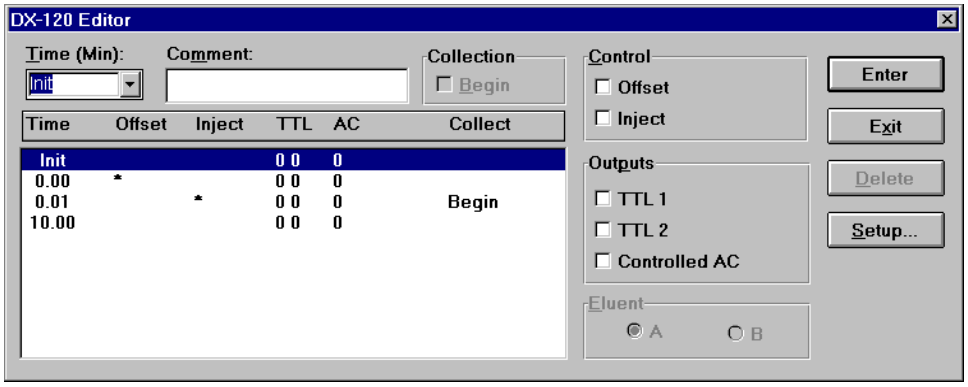
TTL Output Labels can be any desired text (up to 15 characters).

System Mode selects the mode (Column or Eluent) for a dual-column DX-120.

When you finish editing, click on **OK** to save your selections and open (or return to) the DX-120 Editor dialog box.

DX-120 Editor

NOTE Also see Section 5.7.1 for a description of features common to all module Editors.



Comment (optional) can be up to 29 characters (including spaces and punctuation). Comments can be entered for each step.

Begin Collection specifies when collection of detector data starts. This can only occur once in the timed events sequence. The default is the step at time 0.0.

Control

Offset offsets the background conductivity to zero.

Inject switches the injection valve to the inject position.

Outputs

TTL1 and **TTL2** control the TTL outputs assigned to the system for which the Method is written. These outputs provide control of accessories that need only a digital signal to trigger their operation.

Controlled AC controls the AC outlet assigned to the system for which the Method is written. The AC outlet provides control of an external accessory, such as a pre-concentration pump, that relies on/off control to trigger its operation.

Eluent switches the eluent selection valve from bottle A to bottle B.

5.7.14 AS50 Autosampler Editor

1. If you have not previously created an AS50 timed events program, open the AS50 Setup dialog box by double-clicking on the AS50 icon in the Method child window.

NOTE If the Method Type is Sample Preparation, clicking on the AS50 icon opens the AS50 Sample Preparation dialog box described later in this section.

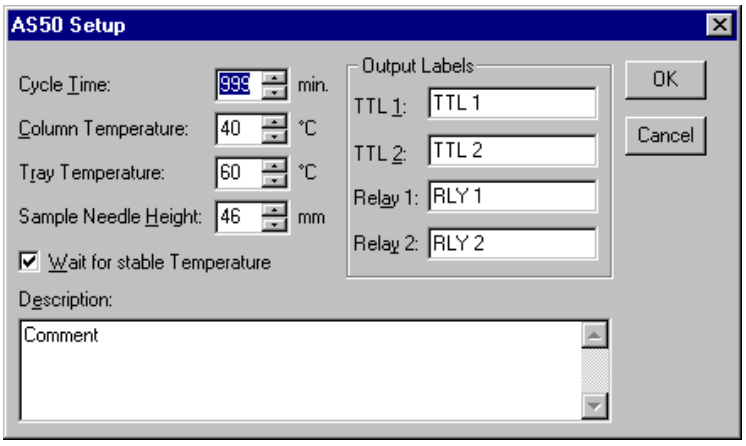
2. Use the controls in the AS50 Setup dialog box to set the initial conditions and click on OK. Clicking on OK accepts these selections and opens the AS50 Editor dialog box.

3. Use the controls in the AS50 Editor dialog box to set the conditions for each program step (up to a combined total of 100 sample preparation and timed event steps).

NOTE Each file must include a step for the initial conditions (INIT) and a time 0.0 step.

AS50 Setup

The AS50 Setup dialog box appears when you click on the Setup... command button in the AS50 Editor or AS50 Sample Preparation dialog box.



Cycle Time specifies the time interval (from 0 to 999 minutes) between the start of one Method's timed events and the start of the

next Method's timed events. The next Method's timed events are not executed until the cycle time has expired, even if the Run command occurs before that time.

Assuming that injection occurs at the start of each Method's timed events, specifying a cycle time ensures a uniform time interval between injections. Cycle Time is disabled by default.

Column Temperature can set the temperature of the thermal compartment between 10 and 80 °C (stainless steel autosampler) or 10 and 40 °C (PEEK autosampler). Use the box or arrow buttons to display the desired value. This feature is enabled only when the AS50 is equipped with the Column Temperature Control option.

Tray Temperature can be set between 4 and 60 °C or Off, using the edit box or arrow buttons. This feature is enabled only when the AS50 is equipped with the Sample Tray Temperature Control option.

Sample Needle Height sets the height of the needle (from zero to 46 mm) up from the bottom of the vial. This value is used for all sample injections. For sample preparation steps, this value is the default, unless a separate Needle Height preparation step is specified (see the section on AS50 Sample Preparation for details).

Wait for stable temperature, when checked, postpones the start of the time 0.0 step until the column temperature has stabilized.

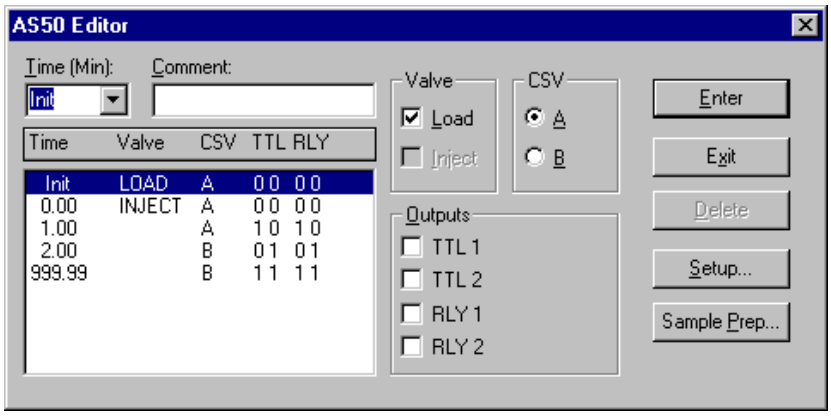
Output Labels can be up to 15 characters for any TTL or Relay output. The label appears in the AS50 Editor dialog box.

Description can be up to 319 characters. To begin a new line, press the <Ctrl> and <Enter> keys simultaneously.

When you finish editing, click on OK to save your selections and open the AS50 Editor dialog box.

AS50 Editor

NOTE See Section 5.7.1 for a description of features common to all module Editors.



Valve sets the injection valve to the load or Inject position. A timed event program can include only one Load and one Inject command; the Load command must occur before Inject. The default is to switch the valve to Load at the INIT step and to Inject at the time 0.0 step. To choose other times for switching the valve, first remove the commands from the current steps.

CSV sets the column switching valve to the A or B position.

Outputs sends a TTL or Relay output signal to a connected instrument.

Comment can be up to 29 characters, including spaces and punctuation, for each step.

Setup... opens the AS50 Setup dialog box described previously.

Sample Prep... opens the AS50 Sample Preparation dialog box, where the sample preparation conditions are specified. See the AS50 Sample Preparation section for more information.

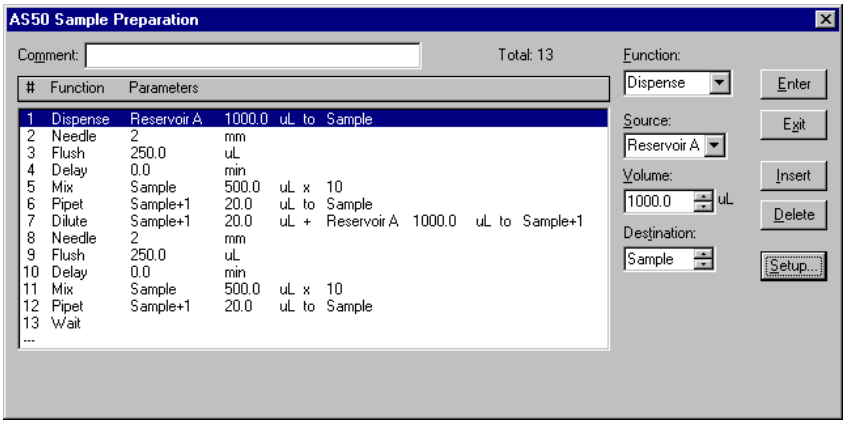
AS50 Sample Preparation

The AS50 Sample Preparation dialog box lets you define the sequence of steps that prepares the sample before injection. These steps occur before the Method's timed events begin.

The sample preparation sequence can be saved in a standard Method or in a Sample Preparation Method (*.SPR) file. A Sample Preparation Method does not include any timed events.

NOTES

1. **Each sample preparation sequence must include one (and only one) Wait step.**
2. **The Wait step cannot be deleted, but it can occur anywhere during sample preparation. The default is to include the Wait step at the end of the sequence.**
3. **The remaining steps can be any combination of the other sample preparation functions, performed in any order.**
4. **A standard PeakNet Method can include a combined total of 100 sample preparation and timed event steps.**



Function specifies the sample preparation operation to be performed by the AS50: Wait, Pipet, Mix, Flush, Delay, Needle Height, Dilute, and Dispense. When you select a function, other controls in the dialog box will be changed to function-specific controls. The functions and their controls are described below.

Wait tells the autosampler to wait for a Run command before proceeding. Each sample preparation sequence must include one (and only one) Wait step. Wait is the only function not listed in the combo box.

Pipet moves a volume of sample from one location to another.

Source is the vial from which to pick up the specified sample volume. The vial position can be specified as absolute or relative:

- To specify an absolute position, enter the vial number (1 to 100).
- To specify a relative position, select Sample (the current sample vial), Sample + 1 (one vial past the current sample vial), Sample + 2 (two vials past the current sample vial), and so on, up to Sample + 9. Some operations also let you specify Waste (for the waste vial).

Volume is the amount of sample to be pipetted.

Destination is the vial in which to add the sample volume. The vial position can be specified as absolute or relative; see the description of Source (above) for details.

Mix combines the contents of a vial by repeatedly drawing and expelling some of the vial contents.

Vial is the vial containing the sample to be mixed. The vial position can be specified as absolute or relative; see the description of Source (above) for details.

Volume is the quantity of sample to draw and then expel.

Cycles is the number of times to draw and expel the specified volume.

Flush flushes the needle with a specified volume of liquid.

Volume is the volume to be flushed.

Delay postpones processing of the next step in the sample preparation sequence for the specified number of minutes.

Delay Time is the number of minutes to wait.

Needle Height changes the default needle height used for the Pipet, Dispense, and Mix operations. The new height is used until another Needle Height step occurs.

Height is the distance in millimeters from the bottom of the vial.

Dilute (available only when the AS50 Sample Preparation option is installed) dilutes a sample with a specified volume of reagent.

Concentrate Source is the vial which contains the concentrated sample.

Concentrate Volume is the amount of concentrated sample to be diluted.

Diluent Source is the reservoir which 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.

Dispense (available only when the AS50 Sample Preparation option is installed) moves reagent from a reservoir to a vial.

Source is the reservoir from which reagent is dispensed.

Volume is the amount of reagent to dispense.

Destination is the vial in which reagent is dispensed.

The AS50 Sample Preparation dialog box also contains these command buttons:

Enter changes the highlighted step to the currently selected function.

Exit closes the AS50 Sample Preparation dialog box.

Insert inserts the currently selected function above the highlighted step.

Delete deletes the highlighted step.

Setup... opens the AS50 Setup dialog box previously described.

5.8 Data Processing

Data processing parameters specify how analytical data is processed, what information is included in the final analytical report, and whether data is stored on disk. The data processing icons in the Method window let you perform the following tasks:

 Edit data smoothing parameters

 Edit integration parameters

 Edit data events

 Edit calibration parameters

 Edit components and groups

 Edit report options

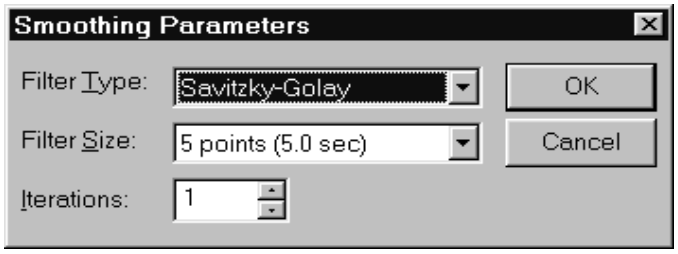
Resting the cursor on an icon displays a summary of the icon's function in the status line. To open the dialog box corresponding to the icon, click on the icon. The data processing dialog boxes are described in the following sections.

NOTE **You do not need to edit data processing parameters in order to run a Method. It is usually easier to use the Optimize program to edit the parameters graphically after a data file has been generated.**

5.8.1  Data Smoothing

Data smoothing can improve the appearance of data plots and the reproducibility of peak baselines by reducing noise through digital filtering. Smoothing affects both the display and the integration of the data plot. The digital filtering used for PeakNet's smoothing does not alter the original data because it is applied after data acquisition. The smoothing can be modified or removed at any time, so the integrity of the original data is preserved.

Use the Smoothing Parameters dialog box to select or modify the data filter applied to raw data.



Filter Type selects the algorithm to be applied to the raw data: None, Savitzky-Golay, Moving Average, or Olympic. Select None (the default) to turn off the smoothing option.

The **Savitzky-Golay** filter smoothes to a 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 basically continuous (such as a chromatogram) without significantly reducing peak heights.

The **Moving Average** filter is a simple algorithm which 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 this 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.

Filter Size selects the number of input data points (from 5 to 25) used to generate each output data point. The default is 5. The edit box also displays the corresponding filter size in seconds, based on the current data collection rate.

Use a narrow filter size if desired peaks are narrow, and a wider filter size for wider peaks. However, an excessively wide filter can significantly alter desired peaks.

Iterations selects the number of times (from 1 to 99) that the selected Filter Type is successively applied to the data. The default is 1.

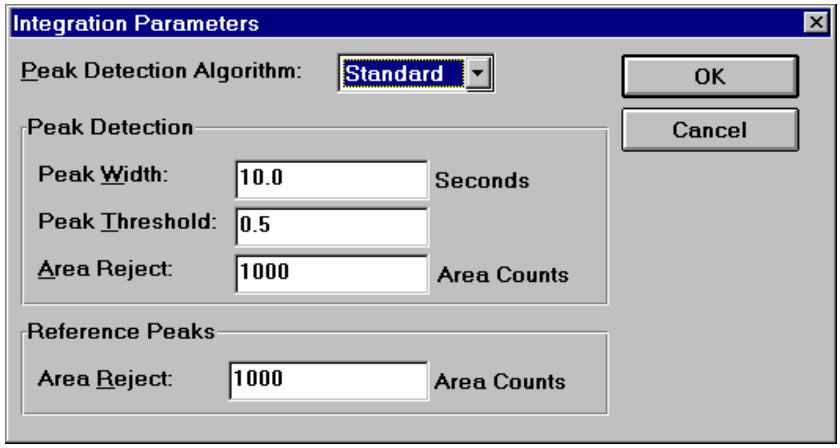
Applying a filter multiple times often provides improved noise reduction without the signal degradation that can occur with a wider filter size. However, because iterations require additional processing time, a wider filter size may be preferable if its results are acceptable.

5.8.2  Integration

Integration parameters specify how the acquired data is processed by the computer for peak detection and integration. The controls in the Integration Parameters dialog box depend on which Peak Detection Algorithm you select: Standard or Dynamic Baseline. When creating a new Method, the default algorithm is Standard for all Method Types except capillary electrophoresis. Both dialog boxes are described below.

NOTE **For a discussion of the peak detection algorithms, refer to the on-line Help topics "Integration (Standard Algorithm)" and "Integration (Dynamic Baseline Algorithm)." To learn more about the principles of peak integration, see Appendix B of this manual.**

Standard Algorithm Dialog Box



Peak Detection Algorithm specifies whether the Standard algorithm or Dynamic Baseline algorithm is applied.

Peak Detection Controls

Peak Width and the data collection rate establish how raw, digitized data points are bunched. Bunching helps the peak detection algorithm separate electronic noise from the true signal. The integration algorithm bunches 10 digital data points for each multiple of the peak width value.

A peak width of 3-5 seconds is satisfactory for most IC and HPLC applications. If narrow peaks of interest are not being detected, or if peak apex markers appear below the true peak tops, reduce the peak width. If baseline noise is being detected as peaks, increase the peak width and/or the peak area reject value.

If the peak widths are narrow at the beginning of an analysis and much wider at the end, or if an eluent change causes peaks that elute later to be narrower than ones that elute earlier, you can double or halve the bunching factor at a specified time in the analysis. See Data Events, the next section, for more information.

Peak Threshold specifies the threshold value (counts per data point interval) for peak detection.

The peak threshold is a measure of how fast the leading edge of the peak must rise before it is recognized as a peak. The larger the number (slope), the sharper the peak must be. Peaks with slopes below this threshold are not integrated or reported, but they are stored as raw data.

Basically, the peak threshold provides filtering to prevent long-term baseline drift from being detected as peaks. If drift or baseline noise is being detected as broad peaks, increase the peak detection threshold. Use the Auto Threshold feature in the Optimize program to determine the ideal peak threshold. See Appendix B for an example of how adjusting the peak width and peak threshold can affect analytical results.

Area Reject specifies the minimum area a peak must have in order to be included in the final report. This affects the report only; peaks with areas below the area reject value will still be integrated.

If small peaks of interest are not being reported, decrease the Area Reject value. If you want all detected peaks to be listed on the final report, enter a value of zero.

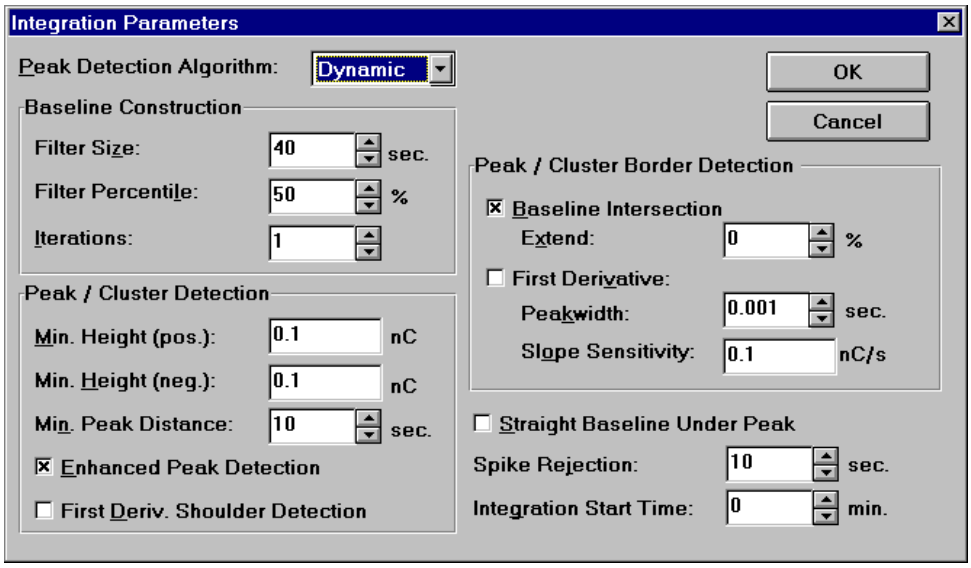
The raw data comprising rejected peaks is stored on disk along with the data for unrejected peaks. Rejected peaks can be included in a later report by processing the stored raw data again with a lower peak area reject value.

Reference Peaks Controls

Area Reject specifies the minimum area a peak must have in order to be recognized as the peak of a reference component.

A reference component helps compensate for systematic variations in retention times for each injection. The variation in retention times is used to determine the expected variation in the retention times of subsequent peaks. For long analyses, you may want to use two or more reference components.

Dynamic Baseline Algorithm Dialog Box



Peak Detection Algorithm specifies whether the Standard algorithm or Dynamic Baseline algorithm is applied. The Dynamic Algorithm requires a Data Collection Rate of 1.0 Hz or more.

Baseline Construction Controls

Filter Size sets the size (duration) of the Moving Median filter applied to the raw data to remove spikes and peaks. Select a value greater than 0 seconds but less than one-half the total run time. The filter size should be at least twice the baseline width of peaks of interest.

Filter Percentile determines which point in the sorted data set of the Moving Median filter is output as a baseline value. The default is the 50% point (the true median).

Iterations sets the number of times (from 0 to 10) that the filter is applied to the raw data. Selecting multiple iterations improves peak integration accuracy when there is a wide variety of peak widths. The

first iteration uses the Filter Percentile and subsequent iterations use only the median, because points in both positive and negative clusters are excluded in the first iteration.

Peak/Cluster Detection Controls

Min. Height (pos.) sets the minimum height a peak must have (in reference to the baseline) in order to be detected as a positive peak. The default value is 10 times the detector noise.

Min. Height (neg.) sets the minimum height a peak must have (in reference to the baseline) in order to be detected as a negative peak. The default value is 10 times the detector noise.

Min. Peak Distance sets the minimum distance between clusters (from 0.1 second to 59,999 seconds). To ensure detection of overlapping peaks, this value should be less than the distance between the peaks.

Enhanced Peak Detection separates the overlapping peaks in a cluster, using an algorithm similar to the Dynamic Baseline algorithm.

First Deriv. Shoulder Detection separates the overlapping peaks in a cluster, using the First Derivative algorithm.

Peak/Cluster Border Detection Controls

Baseline Intersection locates the cluster start and end points as the points where the raw data points and the baseline cross.

Extend extends both the cluster start and end points by the specified percentage. Select a value greater than -100% and less than 100%.

First Derivative locates the cluster start and end points at the points where the absolute value of the first derivative remains below the value of Slope Threshold for 0.5 times the Peak Width time.

Peak Width sets the expected average peak width. Select a value greater than 0.001 second but no more than the total run time.

Slope Sensitivity sets the expected slope threshold (from 0 to 1 x $10^{13)}$.

Straight Baseline Under Peak constructs a straight baseline from the start point to the end point of a cluster.

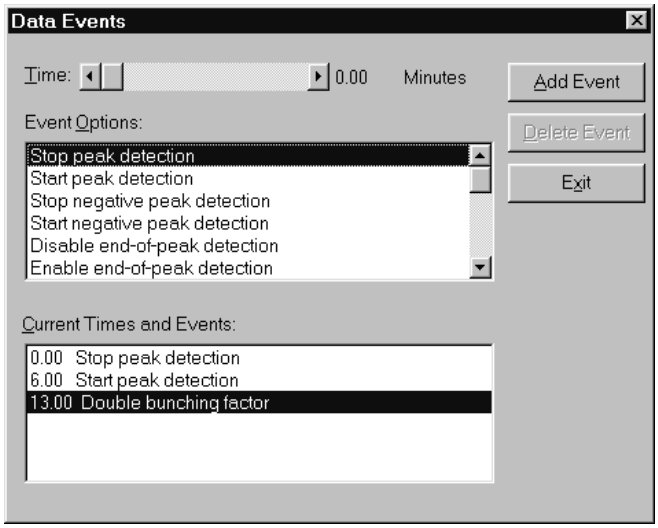
Spike Rejection will reclassify a cluster that meets the minimum height criterion (positive or negative) for less than the time specified here as a spike, rather than a cluster. Select a value greater than 0 seconds but less than the total run time.

Integration Start Time specifies the beginning of peak detection and integration. Select a value greater than 0 seconds but less than the total run time.

5.8.3 Data Events

Data Events are time-based events that affect the detection and integration of raw data. Many analyses require special treatment of unresolved peaks or baseline phenomena (for example, void volume peaks) in order to ensure that peaks are integrated correctly. In other analyses, peaks that elute later are significantly broader than earlier peaks. For these peaks, the bunching rate set at the beginning of the analysis must be changed to ensure accurate integration.

It is advisable to first run a Method **with no Data Events** to determine exactly which events are needed and when they should occur. Then, use the controls in the Data Events dialog box to create up to 100 events for each Method. If you need to edit data events, use the Optimize program, which instantly displays the effects on integration.



Time Use the scroll bar to set the time at which the selected Data Event will occur. The maximum selectable time is determined by the Data Collection Time specified for the Method.

Add Event adds the item highlighted in the Event Options window to the Current Times and Events list.

Delete Event deletes the highlighted event from the Current Times and Events list.

Exit closes the Data Events dialog box.

Event Options Use the scroll bar to view all of the Data Event options. To select an option, point and click. This highlights the event description.

Stop and Start peak detection toggle peak detection off and on. This is especially useful for preventing spurious reproducible changes (e.g., those caused by eluent changes or large pressure changes) from being detected as peaks.

Stop and Start negative peak detection turn a special negative peak detection algorithm off and on so that negative peaks can be detected.

Disable and Enable end-of-peak detection toggle this option off and on. The end of a peak is normally identified when three consecutive bunches of data fail to decline by the peak threshold value. This option is especially useful for controlling the determination of the end of a peak with a long tailing edge.

Double and Halve peak threshold multiply or divide the current peak threshold by two. Doubling the threshold is useful when an eluent change or a gradient causes an increase in the slope of the baseline, or in baseline noise. Halving the threshold is useful for finding small peaks. See Appendix B for more information.

Double bunching factor doubles the number of points averaged to make a bunch. The initial bunching factor is determined by the Peak Width value specified in the Integration parameters. In effect, each time the bunching factor is doubled, the previously set peak width value is doubled. Use double bunching when late peaks are much wider than early peaks. See Appendix B for more information.

Force baseline at start of this peak forces a baseline at the start of a peak where the peak detection software does not normally find a baseline.

Force baseline at start of all peaks forces the peak detection software to generate separate baselines, valley-to-valley, for each peak in the chromatogram.

Force common baseline following this peak forces a common baseline for all peaks following the specified peak. The peaks following this command will be separated by exponential projections or drop lines, as appropriate.

End and Don't end peaks on baseline penetration toggles this function off and on. The end of a peak is not normally detected upon baseline penetration.

Halve bunching factor divides in half the number of raw data points that are combined to form a bunched point. The initial bunching factor is determined by the Peak Width specified in the Integration parameters. Halving the bunching factor essentially halves the previously set Peak Width value.

Force exponential skim forces the baseline of a shoulder peak not normally fitting into baseline code type three or four to be determined by exponential projection. See Appendix A for more information.

Void volume treatment for this peak automatically forces a backwards horizontal baseline from the end of a peak to the data point closest to zero on the edge of a dip or negative peak. Enter the retention time of the peak requiring this treatment as the time for the event.

Disable and Enable exponential skim turn on and off the function that automatically determines if a peak is a candidate to be skimmed.

Split peak forces a detected peak to be split by drop-line integration at the selected time.

Tangent-skim riders on leading and tailing slope forces the baselines of all rider peaks in the cluster to be determined by tangential-skim projection of the host peak's leading or tailing slope. See Appendix A for more information.

Current Times and Events displays the selected Data Events.

Correcting Baselines for Void Peaks

Void peaks, those that closely follow large dips, cause the peak detection algorithms to find an inappropriate baseline (i.e., one that starts from the most negative point of the dip and ends after the void upset). Follow the steps below to correct the baseline and quantify peaks that elute just after the end of the void.

1. Click on the Data Events icon in the Method child window to open the Data Events dialog box.
2. Use the Time scroll bar to select a time within the first peak following the dip.
3. Move the Event Options scroll bar down to the Void Volume Treatment option and click on the option to highlight it.
4. Click on Add Event. The time and event description now appear in the Current Times and Events window.

5.8.4  Calibration

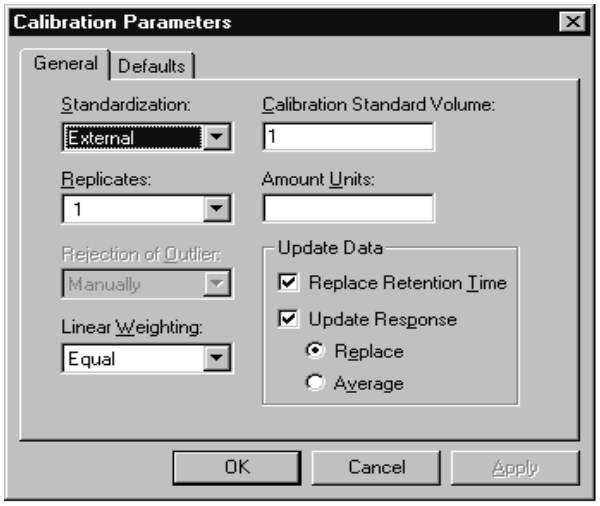
Calibration parameters determine how detected peaks are identified and quantitated. Appendix C discusses the principles of peak quantitation.

The Calibration Parameters dialog box consists of three tab pages:

- General
- Defaults
- CE Parameters

NOTE The CE Parameters tab page is available only for CE (Capillary Electrophoresis) Methods. To select the Method type, select Configuration from the View menu.

General Calibration Parameters



Standardization (**External** or **Internal**) specifies whether peaks are quantitated using internal standard or external standard calculations. See Appendix C for details.

Replicates specifies the number of replicate injections of the calibration standard for which PeakNet will store data. Calibration results will be based on the data from the replicate injections.

Rejection of Outlier can be specified if the Replicates setting is 3 or more. This option determines the method for rejecting outlying calibration points:

Manually does not reject any points automatically; points are only rejected manually.

Q-Test 90%, 95%, 99% selects a statistical Q-test to be performed on the replicate calibration data points at each level. Any points falling outside of the tolerance range are rejected.

t-Test 90%, 95%, 99% selects a statistical t-test to be performed on the calibration data points. Any points falling outside of the tolerance range are rejected.

NOTE If Replicates is 2 or less, the only Outlier Rejection option is Manually.

Linear Weighting Option determines how linear calibration curves are weighted when there are two or more calibration levels. With the **Equal** option, all replicates in each level are treated equally during calibration.

Calibration Standard Volume (for external standard calibrations only) specifies the injection volume for the standard(s). This value is a multiplication factor used to calculate external standard calculations of component amounts.

Amount Units specifies the unit of measure (such as ppm, mg/mL, or nanomoles) used to express the quantity of sample components.

Update Data specifies how to update the calibration table for each component.

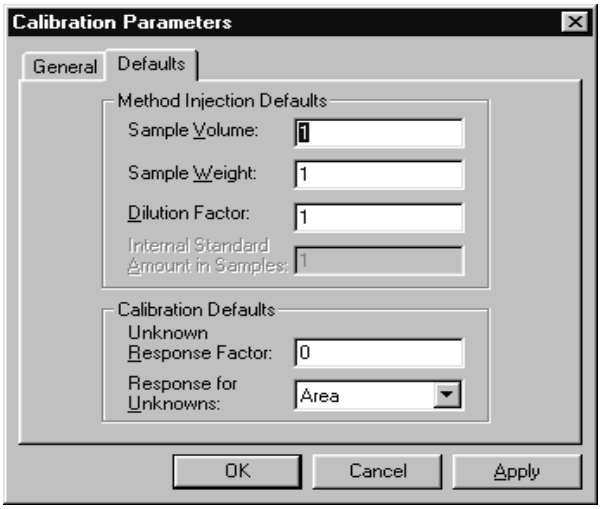
Replace Retention Time determines whether the component retention times are updated after each calibration.

Update Response specifies whether the responses are updated with the values measured for each calibration.

- If Update Response is checked and Replicates is 1, you can choose to **Replace**, or **Average** the new responses with the existing values (if any) in the calibration table of the Method.

- If Update Response is checked and Replicates is 2 or more, the component responses from each new calibration injection replace the oldest values in the calibration table.

Defaults Calibration Parameters



Method Injection Defaults

Sample Volume (for External Standard Calibrations only) enter the default Sample Volume, which is used to normalize results to the volume of standard or sample injected. (Sample volume does not affect Internal Standard Calibration, which automatically corrects for volume variations.)

Sample Weight is the weight of the sample injected.

Dilution Factor is used to normalize the results to the dilution of sample injected. (Dilution factors apply only to samples, not to standards.)

Internal Standard Amount in Sample specifies the default amount of the internal standard in the sample. (This value is not used for external standard calculations.)

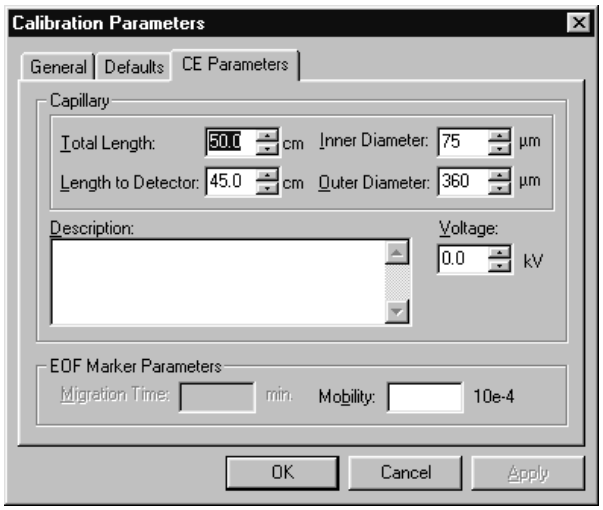
NOTE Amounts of internal standard component(s) in the calibration standards are entered separately for each calibration level in the Component Table dialog box.

Calibration Defaults

Unknown Response Factor is an optional factor that is multiplied by the response to give an approximate amount for an unknown peak.

Response for Unknowns specifies whether quantification of unidentified peaks will be based on the area or height of the peak.

CE Calibration Parameters



Total Length is the total capillary length, in centimeters.

Length to Detector is the capillary length from the inlet vial to the detector cell, in centimeters.

Inner Diameter is the capillary inner diameter, in micrometers.

Outer Diameter is the capillary outer diameter, in micrometers. This value is not used in any calculations.

Voltage is the voltage across the capillary, in kilovolts.

Description is a description of the capillary (up to 255 characters maximum). This description is printed in the Method.

EOF Marker Migration Time indicates the migration time of the EO flow marker; this value is provided for information only.

EOF Marker Mobility indicates the mobility of the EO flow marker. This value is used to calculate actual peak mobility when no marker peak is identified.

5.8.5  Component Table

For PeakNet to automatically identify and quantitate sample components, you must first create a Component Table that lists the information required for calibration calculations. After peaks have been detected and integrated, PeakNet attempts to correlate them with the Component Table entries. This process consists of three steps:

a. Identifying the reference components, if used

b. Adjusting the retention time tolerance for other peaks proportionally to the changes in retention times of the reference components

c. Assigning components to the peaks found within the adjusted tolerance

Notes on Component Identification

The peak with the greatest area that falls within the reference component's retention time tolerance is identified as the reference component.

When adjustments are made with respect to a reference component, both the retention time and the tolerance are adjusted proportionally to the change in retention of the reference component peak. If no reference component peak is found, no adjustment is made.

Once the adjusted tolerance is established, the algorithm identifies the peak closest to the adjusted retention time that is within the adjusted tolerance as the component for that retention time. If no reference component is used, the entries in the component table for retention time and tolerance are used to identify a peak with a retention time.

NOTE Component names are assigned to the component retention times in the Component Table or from the Name Peaks dialog box in Optimize.

The Component Table consists of the following tab pages:

- Identification lets you enter component names, retention times (or migration times for CE Methods) and other identification parameters.
- Quantitation lets you enter low and high amount limits for each component, and specify internal standard components.
- Calibration Standards lets you enter the amounts of each component in the calibration standard(s).
- Calibration lets you select the parameters to be used for plotting the component calibration curves.
- Check Standards lets you enter the amounts of each component in the check standard(s).

The following section describes how to edit values in the Component Table. Details about each tab page follow this section.

Setting Default Values

Brackets [ ] around a value indicate that the default setting is selected for that parameter. The controls at the bottom of a column allow you to change the default setting. If you change a default, any bracketed values are changed to the new setting. The new setting will also be used for any new components.

Selecting Cells

To select a single cell, click on the cell or move to it with the arrow keys.

To select a group of adjacent cells, hold down the mouse and drag to highlight them, or hold down the SHIFT key, click the first cell in the group and then the last cell.

To select the contents of the cell, double-click or press the F2 key.

Copying, and Pasting Cells

To copy a cell or group of cells, select the cell(s) and press CTRL+C.

To paste a cell or group of cells, first copy the desired cell(s). Then, click where the cells should be pasted and press CTRL+V. If there is any information in the cells where you are pasting, it will be replaced.

Deleting Cell Contents

To delete values from cells, select the cell or cells and press Delete.

Editing Cells

To replace the contents of the selected cell, simply type the new information into the cell.

Adding and Deleting Components

To add a component to the table, select the cell below where the new component should be added and press CTRL+Insert.

To add multiple components, select the number of rows to be added and press CTRL+Insert.

To delete a component, select any cell in the component row to be deleted and press CTRL+Delete. All entries on the line will be deleted.

To delete multiple components, select the cells in the rows to be deleted and press CTRL+Delete. All entries on the lines will be deleted.

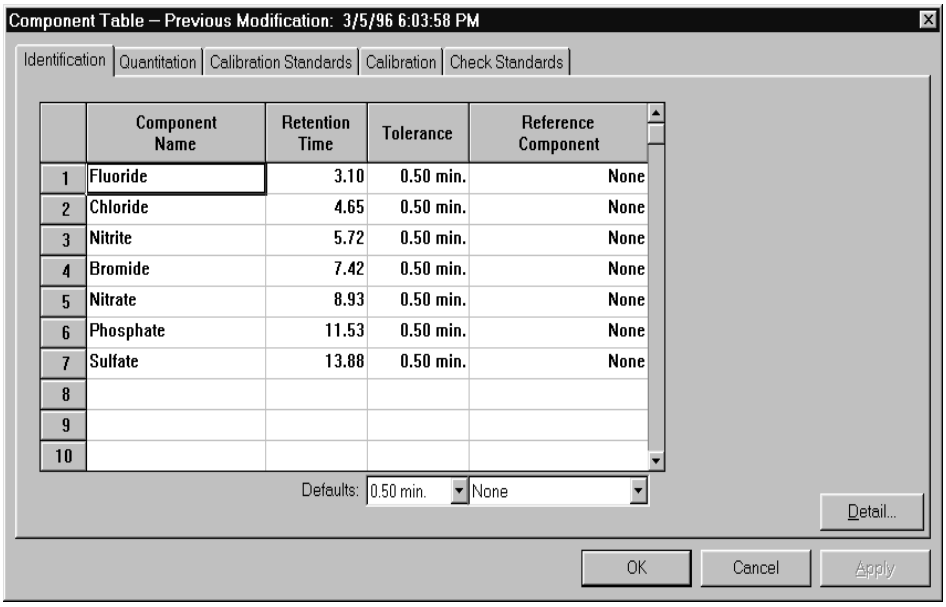
To confirm entries in a tab page:

Use one of the following methods:

- Click the Apply button.
- Select another tab page (changes are remembered when you move between tab pages and applied when the dialog box is closed by clicking the Apply or OK button.)
- Click OK to close the dialog box.

NOTE When you close the dialog box, all components in the table are resorted by retention time, and the time/date stamp (shown in the title bar) is updated.

Component Table Identification Page



NOTE For a convenient way to fill in the component identification information, as you work directly with a chromatogram, use the Name Peaks dialog box in Optimize. Information entered in the Name Peaks dialog box automatically updates the Component Table.

Component Name can be up to 32 characters. The name can be included on the chromatogram and printed in reports, if desired. The Component Table can contain 150 components.

Retention Time/Migration Time is the expected retention time or migration time (in minutes) for the component. If the retention time is unknown, enter any number greater than zero. The correct retention time can be determined later from the first calibration run, and the Component Table then updated. In subsequent calibrations, PeakNet will automatically update the retention time, if the Update Retention Time setting is selected in the Calibration Parameters dialog box.

Tolerance (min. or %) determines the amount by which the retention time or migration time of the specified peak can vary and still be identified. If more than one peak appears within the component time tolerance, the peak closest to the adjusted time is selected. It is usually best to keep the tolerance range narrow, in order to exclude unwanted peaks.

The tolerance can be expressed in one of two ways:

min. specifies the tolerance as an absolute value, in minutes.

% specifies the tolerance as a percentage of the expected retention time or migration time, in which a peak must appear before it can be identified. A 3% tolerance is usually satisfactory.

Reference Component is a component whose change in retention time is used to adjust the expected retention times of other components. When a reference component elutes earlier or later than its expected retention time, a proportional correction is made to the expected retention times of all components that use that reference.

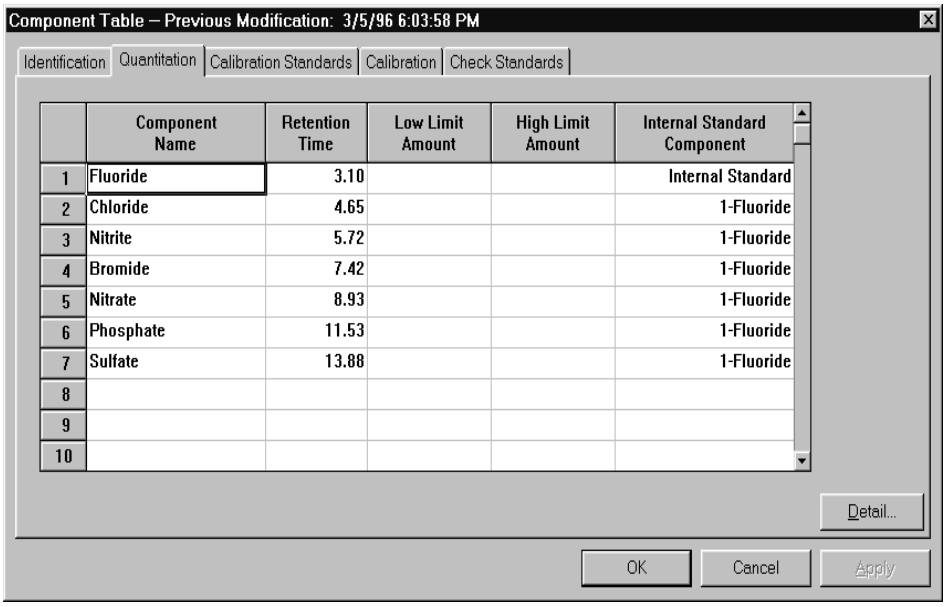
If more than one peak appears within the reference component's retention time tolerance, the peak with the greatest area is identified as the reference component. If no peak is found, the retention time tolerances of peaks which use that reference peak are not adjusted.

NOTE Reference components should be used only if retention times vary so much that peaks may be misidentified. If retention times are reproducible, select None as the reference component. If used, references should be carefully chosen.

Reference Marker (for CE Methods only) is a component with a known mobility that is used for correcting migration time variations and calculating the actual mobilities of other components and unknown peaks in a capillary electrophoresis separation. To designate a component to be used as a Reference Marker, select None. To choose a Reference Marker for a component, select a component name from the drop-down list. For components designated as Reference Markers, enter a Marker Mobility (see below).

Marker Mobility (for CE Methods only) is the mobility of the reference marker component, which is used to calculate the mobility of the components which reference that component. Enter a value from -99.999 to 99.999.

Component Table Quantitation Tab Page

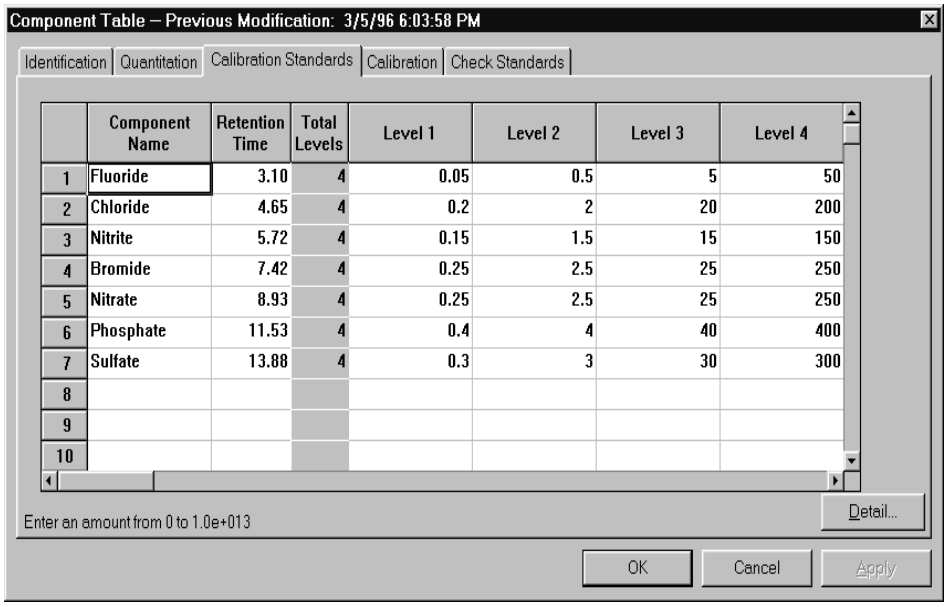


Low and High Limit Amounts specify the acceptable limits for the calculated amount of a component in an unknown sample. Amounts exceeding these limits can be annotated on reports. To do this, include a Peak Table in the report and select Limit Exceeded as one of the table variables. If the component amount is above the limit, a "+" is reported, if below, a "-" is reported.

Internal Standard Components if Internal Standardization was selected in the Calibration Parameters dialog box, designate each component as either an internal standard, or select a component name to be used as the component's internal standard.

- To designate a component as an internal standard, select Internal Standard from the drop-down list.
- For other components, select the component that should be used as the internal standard for that component. The drop-down list will display all components that were designated as Internal Standard.

Component Table Calibration Standards Tab Page



Total Levels reports the total number of used levels. Empty cells (those designated with ". . .") are not counted. This value is updated when amounts are added or deleted from the components Level 1 through Level 32 cells (see below).

Level 1 ... Level 32 specify the amount of the component in each level of calibration standard. These amounts will be used to construct the component calibration curves. When you enter an amount, the Total Levels field is updated.

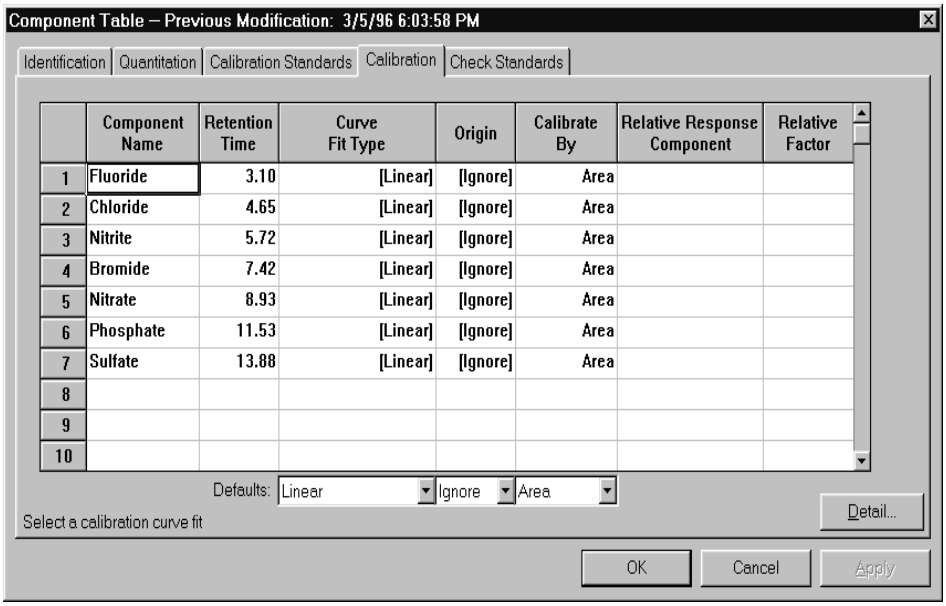
Each component can have a different number of calibration levels. The amounts entered for each level can be in any order and there can be blank entries for a component.

If all Level cells for a component are blank, the Total Levels is 0 and calibration will not be performed on that component.

Many calibrations are single-level; they use only one calibration standard. A single-level calibration assumes that the detector response for all sample components is linear over the entire amount range. If this is not the case, use a multilevel calibration.

In a multilevel calibration, several standards of different amounts are used to construct a calibration curve for each sample component. Data from each calibration run is saved until responses for each calibration level have been measured for each component. In addition, PeakNet can store responses from up to 10 replicate injections of each calibration level This calibration data is then used to construct the calibration curve for each component. The component amounts in a sample mixture can then be determined by relating the measured areas (or heights) to their corresponding calibration curve.

Component Table Calibration Tab Page



Curve Fit Type selects the fit used for each component's calibration curve. You can select different curve fits for different components. PeakNet offers the following options:

Linear fit can be used with one or more calibration levels. If only one calibration level is used, the curve is forced through the origin (zero). If more than one level is used, the calibration curve is determined by a least-squares calculation to fit a line through the calibration data points. If the Force Zero option is chosen, the K_0 term of the regression equation is set to zero.

Quadratic and **Cubic** fits can be used with multilevel calibrations only. A quadratic fit requires at least three calibration levels; a cubic fit

requires at least four levels. The calibration curve is drawn from a quadratic or cubic equation. Quadratic and cubic fits are most useful when detector response is known to "flatten out" toward one extreme of the concentration range or the other.

Point-to-point fit can be used with one or more calibration levels. If only one level is used, the line is drawn from the calibration data point on the graph through (0,0). If more than one level is used, PeakNet determines which two data points bracket the response of the unknown and then uses a straight line between the two points to interpolate the concentration of the unknown.

Relative uses the calibration equations of a selected Relative Response Component and multiplies by a Relative Factor to obtain the response factor for the component. The relative curve fit is useful in situations where it is impractical to prepare a standard for a particular component, and the response of the component, relative to a calibrated component, is known.

Average Response Factor uses a single-point, force zero, linear fit to calculate a separate response factor for each calibration point in all levels of the component. These response factors are then averaged to create the average response factor, which is used to calculate the amount of the component in samples.

Origin determines how the origin is treated in the calibration calculation.

Ignore—the origin is neither included nor forced in the regression calculation.

Force—the curve is forced through the origin of the plot by setting the K0 term (intercept) equal to 0.

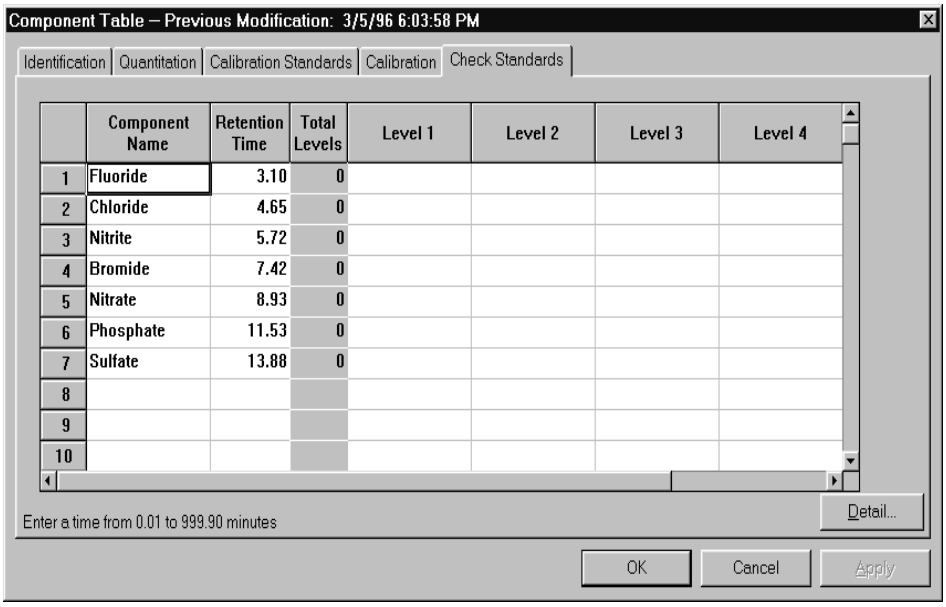
Include—adds the point (0,0) to the set of (x,y) pairs used to calculate the regression.

Calibrate By determines whether the **Area**, **Height**, or **Corr. Area** is used in the calibration calculation.

Relative Response Component specifies a component whose calibration function will be used to quantitate the current component. The component's own calibration data is not used. The Relative Response Component list will include all components, except for those that are themselves quantitated with a relative component.

Relative Factor specifies a correction factor to apply when a component is quantitated by the Relative Response technique. The factor is applied to the response factors of the relative component to determine the component's amount.

Component Table Check Standards Tab Page



NOTE When the Method is run, the Run program reports whether the check standard response falls within the confidence intervals for the calibration plot. Confidence intervals are calculated for External Standards calibrations using Linear curve fits with two or more levels. The confidence intervals for the calibration plot are calculated using a t-test at 95% confidence.

Total Levels reports the total number of used levels. Empty cells (those designated with ". . .") are not counted. This value is updated when amounts are added or deleted from the components Level 1 through Level 5 cells (see below).

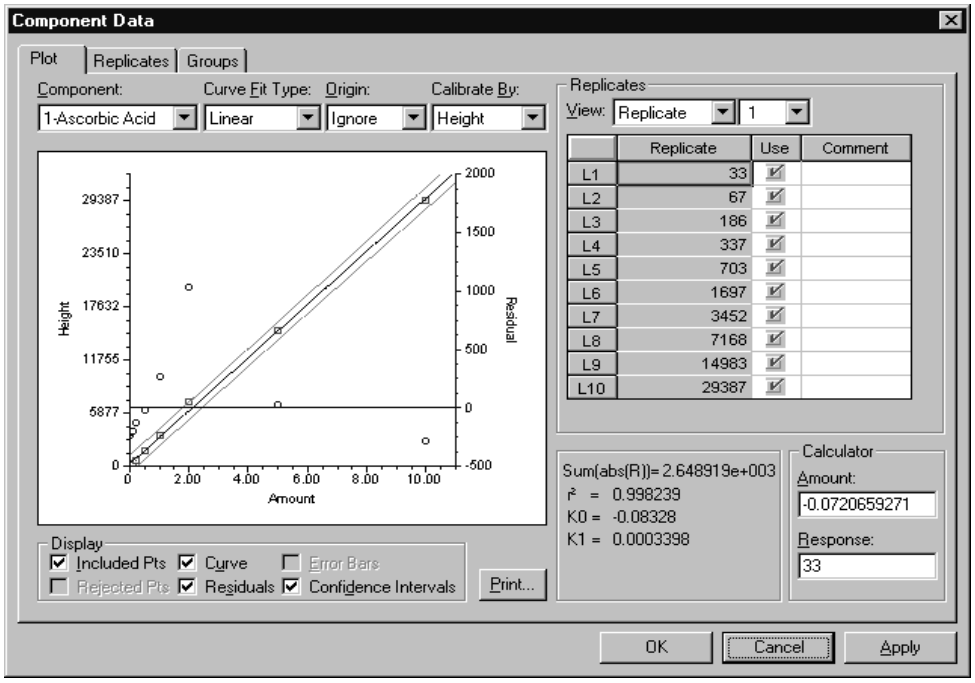
Level 1 ... Level 5 specify the amount of the component in each level of check standard. When you enter an amount, the Total Levels field is updated.

Component Data

Clicking the Detail... button or the number button next to each component on the Component Table opens the Component Data dialog box. The dialog box consists of three tab pages:

- Plot displays a plot of response vs. amount for any component of the current Method.
- Replicates displays the raw area or height calibration data for up to 10 replicate calibration injections, at each calibration level.
- Groups lets you classify components and/or unknown peaks into groups to get reports of compound classes.

Component Data Plot Tab Page



Component selects the component plot to display.

Curve Fit Type selects the curve fit to use to calculate the plot. When a new curve fit is selected the plot is updated immediately.

Origin selects how the origin is treated in the plot calculation.

Calibrate By selects whether the Area or the Height is used in the calibration plot.

NOTE The Curve Fit Type, Origin, and Calibrate By options are the same as those set in the Component Table - Calibration Tab Page. You can test new setting here, and then either select Apply or OK to save the new settings, or select Cancel to keep the original settings.

Display controls the type of information included in the plot. Check or clear the individual Display options check boxes below the plot, or point to the plot and click the right mouse button to select options from a pop-up menu.

Included Pts displays the amount, response data points for each calibration level.

Curve draws the selected Curve Fit Type.

Error Bars displays a bar between replicate values of one standard deviation or more from the average value. Narrower bars indicate closer replicate values, wider bars indicate greater deviation in replicate values.

Rejected Pts displays an X at the location of each data point not used in the plot.

Residuals displays the plot of *residual* versus amount. A residual is the difference between the actual measured Y value and the Y value that is generated by the regression calibration for a given X value. For the calibration plot, the residual is the difference between the actual response of a calibration standard and the response that would be expected based on a regression curve. The residual axis is on the right side of the plot. For each point, a circle indicates the residual value, with a vertical line indicating the difference from the ideal residual value of zero.

Confidence Intervals draws curves showing the confidence intervals for the plot. This option is available only for External Standard Linear curve fits with two or more levels. The confidence intervals are calculated using a t-test at 95% confidence.

NOTE If there are only small differences between replicate data points, or if the residuals for the data points are small, the confidence curves may be indistinguishable from the calibration curve.

Print... opens a Print dialog box for printing the plot. You can select whether to print all components or only the current component.

Replicates displays the data values (area or height) by either replicate or level.

View selects whether to list replicate data by Level or Replicate. When Level is selected, the table displays all replicate data values for the selected level. Rows are labeled R1, R2, . . . Unused (empty) Levels are not included in the list.

If **Replicate** is selected, the table displays a data value for each level of the selected replicate calibration injection. Rows are labeled L1, L2, . . .

The **Use** column, indicates which values to use in the calibration plot. The values can be manually accepted or rejected, or you can set up automatic rejection of outlying data points from the Calibration Parameters dialog box (see Section 5.8.4).

A **Comment** (up to 256 characters) is required for rejected values. For accepted values, entering a comment is optional.

Calculator lets you calculate an amount from a response, or a response from an amount, for the current component.

To calculate an amount from a response, enter the Response value and then click in the Amount box. A new amount is calculated based on the entered response. To calculate a response from an amount, enter the Amount and click in the Response box.

The following values, used to calculate component amount, are determined automatically by the Method Editor and cannot be edited.

K0 indicates the Y-intercept of the calibration curve.

K1 is the coefficient for the first-degree variable. When the fit type is linear, K1 indicates the slope of the calibration curve for the selected calibration level.

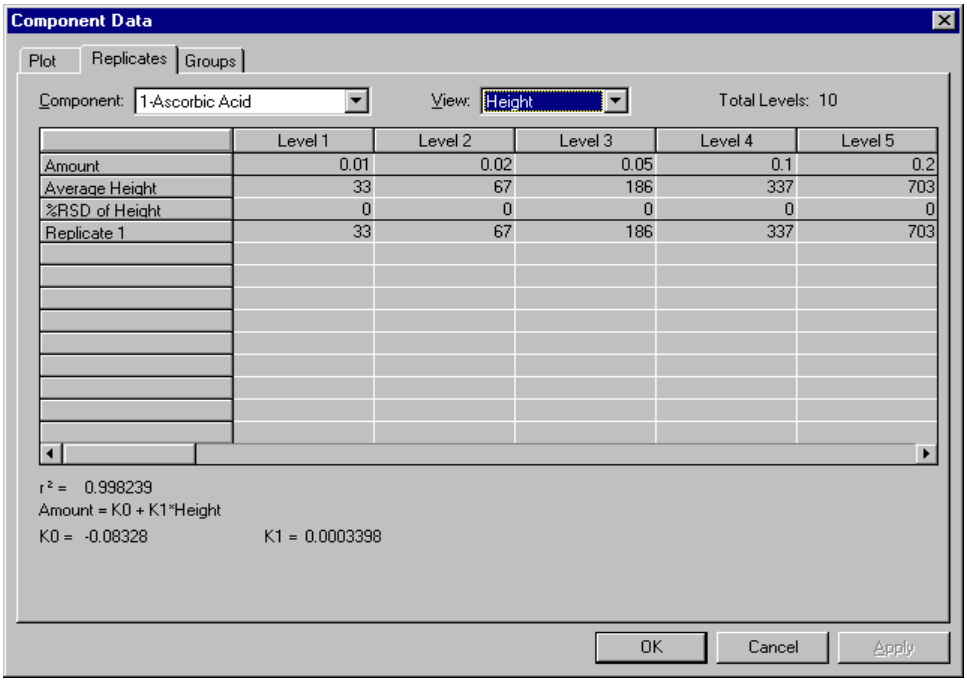
K2 is the coefficient for the second-degree variable in a quadratic fit.

K3 is the coefficient for the third-degree variable in a cubic fit.

For example, to determine the cubic fit of peak area calibration, the equation is:

$$Amount = K0 + K1 \; x \; Area + K2 \; x \; Area^2 + K3 \; x \; Area^3$$

Component Data Replicates Tab Page



Component selects the component for which to display the replicate data.

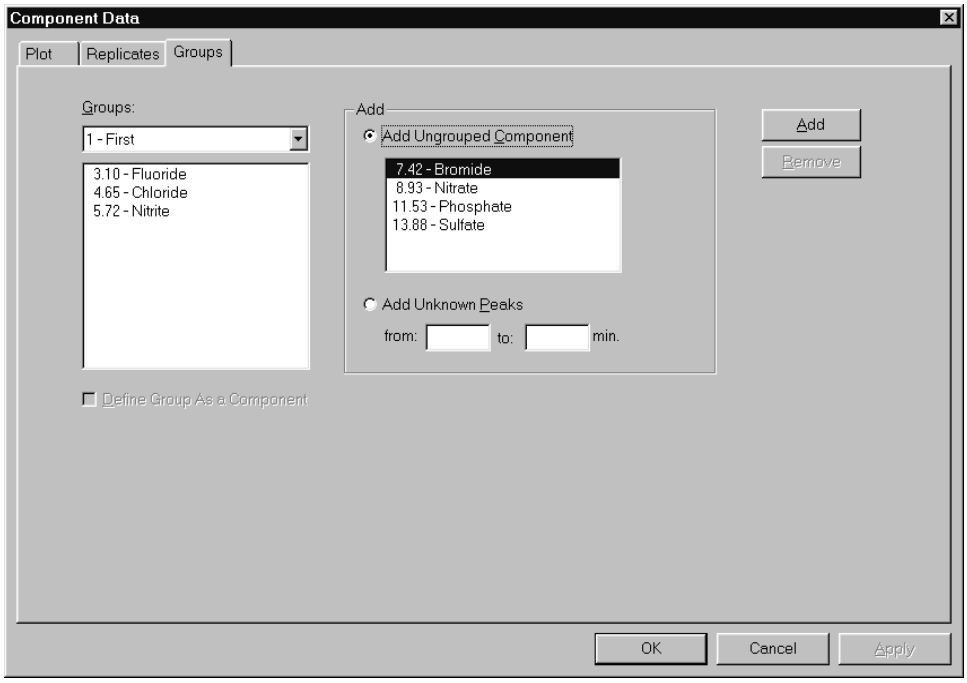
View selects whether to display the Area or Height calibration data for the selected component.

The spreadsheet shows the area or height values for the selected component. Data from up to 10 replicates and 32 levels can be displayed. Rejected calibration points are shown in strike-out font.

The equation for the calibration curve fit used to calculate the component amount is displayed at the bottom of the Replicates page. You can select the curve fit from either the Calibration tab page of the Component Table dialog box or from the Plot tab page of the Component Data dialog box.

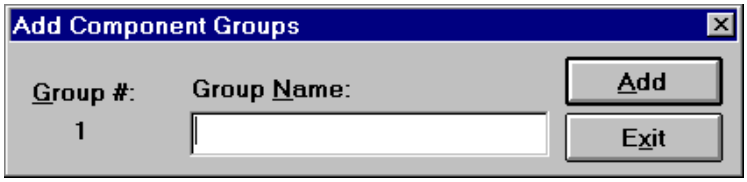
The **r2** value (Coefficient of Determination) for the component is shown at the bottom of the Replicates page. The ideal value for this coefficient is 1.0.

Component Data Groups Tab Page



New groups are created in the Add Component Groups dialog box. Use one of the following methods to open the dialog box:

- If there are no groups currently defined, select a component name from the Add Ungrouped Component list and then click the Add button, or select the Add Unknown Peaks option.
- If groups currently exist, double-click the Groups drop-down and then click the Add button.



A group may contain any number of components, and as many as five different time ranges. Enter a Group Name here and click on Add to enter the data in the Component Table. Repeat for each component group.

When you finish adding component groups, click on Exit to return to the Component Groups tab page.

Group indicates the name and number of the component group being edited. The list box directly below displays the group's components; the number preceding each component is its retention time. To see information for a different component group, click the cursor on the down-arrow beside the group name, then click on the group from the list of names now displayed. Double-clicking on an item in the Group list box transfers it to the Add Ungrouped Component list.

Add Ungrouped Component displays the names and retention times of all ungrouped components. There are two ways to add an ungrouped component to the group being edited (or to remove a component from the group being edited): double-click on the component name, or click first on the component name and then on the Add (or Remove) command button.

Add Unknown Peaks adds unknown peaks that appear within a particular time range to the component group being edited. Enter the beginning and end of the time range (in minutes) in the edit boxes here and then click on the Add command button. The word "unknowns," is displayed after the time range in the list of groups.

Define Group As a Component adds a group to the Method's Component Table. The group to be added must be made up of only unknown peaks (see Add Unknown Peaks above). The Component Table will list the group name as a single component; the retention time for the grouped component will be the average of the time ranges of the unknown peaks in the group. When a calibration standard for the group is run, the total area of all peaks in the group is entered into the Replicates table in the Component Table. The calibration curve is calculated with the group treated as a single component. When the unknown sample is run, PeakNet determines the total area of the unknown peaks in the group and determines the amount of that group in the sample based on the calibration curve.

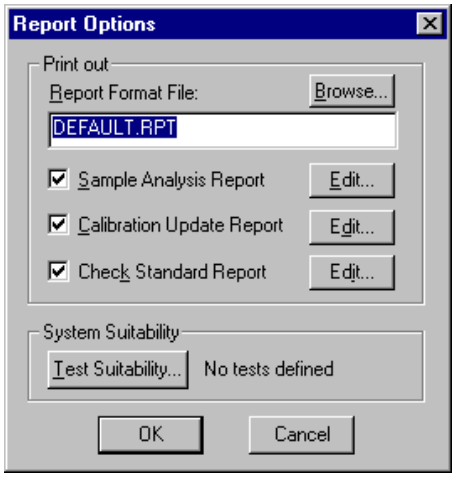
Add removes the highlighted component in the Add Ungrouped Component window and transfers it to the group being edited or, if the name of the group being edited is highlighted, clicking on Add opens the Add Component Groups dialog box.

Remove transfers a highlighted component name from the group list to the Add Ungrouped Component window. If the Group name is highlighted, clicking on Remove deletes the entire group.

5.9 Report Options

Clicking on the Report Options icon in a Method window opens the Report Options dialog box. Use the dialog box controls to:

- Access the Report Designer program to edit a Method's report formats
- Select which reports to print automatically at the end of a run
- Set up system suitability tests



Print out

Report Format File specifies the report format file associated with the Method. Click the **Browse** button to select a different format file.

When **Sample Analysis Report**, **Calibration Update Report**, and/or **Check Standard Report** are checked, the selected report(s) will print out automatically at the end of a run.

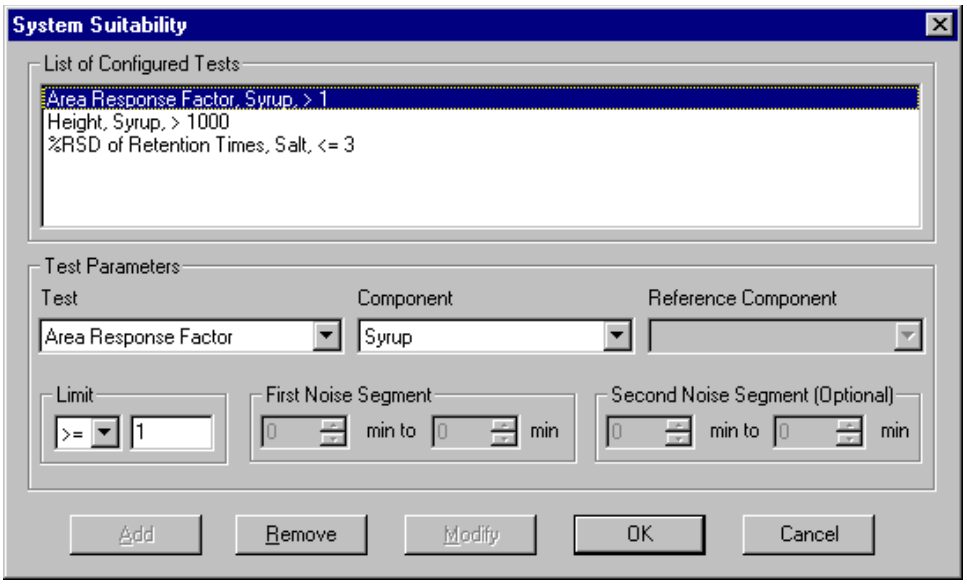
Edit... opens the corresponding report format in the Report Designer program. See the Report Designer chapter for details about editing report formats.

System Suitability

Test Suitability opens the System Suitability dialog box for configuring system suitability tests for the Method.

System Suitability Dialog Box

Use the System Suitability dialog box to define a list of tests, and their corresponding acceptability limits, which will be associated with the Method. The tests can be used to generate system suitability reports on data acquired from injections run using the Method. You define which injections to use for each test in the Schedule Editor. Tests are run from the Batch program and reported in a Summary Report when a System Suitability table is included in the report format.



List of Configured Tests shows the tests that have been configured for this Method.

Tests Parameters

Test lists all of the test types that can be configured for a Method.

Component lists the components defined in the Method's Component Table. Select the component for which the selected test should be run.

Reference Component is enabled when the selected test type is Resolution (EP) or Resolution (USP). The Resolution tests calculate the resolution of any pair of component peaks using

either the EP or the USP formulas. Select a component and a reference component for the calculation.

Limit sets the limit for a passing result on the test.

First Noise Segment and **Second Noise Segment** are enabled when the selected test type is Signal/Noise. Specify the time ranges over which the noise is to be tested.

Add adds the test defined in the Test Parameters fields to the List of Configured Tests.

Remove deletes the selected test from the List of Configured Tests.

Modify accepts changes made to the selected test's Test Parameters.

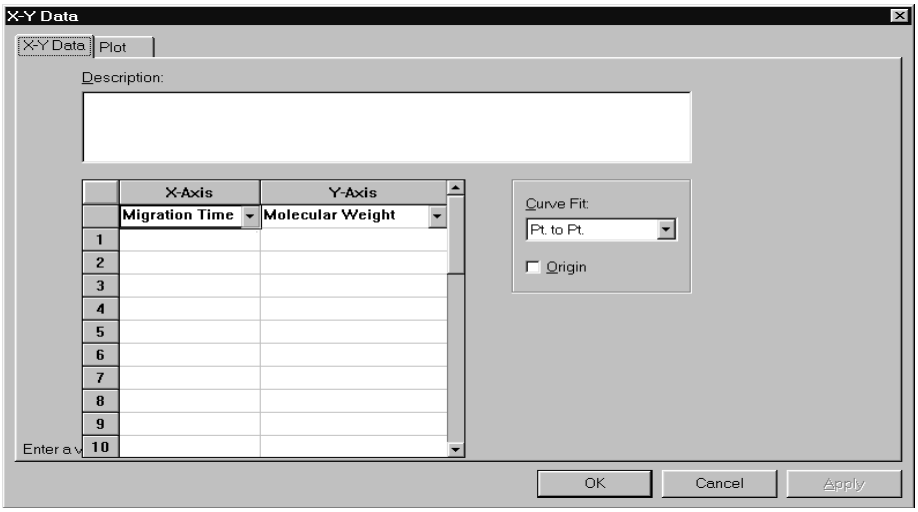
To configure a test:

1. Select the desired test from the Test drop-down list.
2. Select the component for which the test will be run. For the Resolution (EP) or Resolution (USP) tests, also select a Reference Component.
3. For a Signal/Noise test, select a First Noise Segment and optionally a Second Noise Segment.
4. Specify the test limit.
5. Click the **Add** button to add the test to the List of Configured Tests.

5.10  X-Y Data

Clicking on the X-Y Data icon in the Method child window opens the X-Y Data dialog box. Use the dialog box controls to plot calibration curves related to molecular weights and isoelectric focusing points.

X-Y Data Tab Page



1. Type a title for the plot (100 characters maximum) into the **Description** text box.

2. To select an X-axis type, Open the **X-Axis** drop-down list box and select one of the following as the X variable (the allowed ranges follow the label name).

   Migration Time: 0.01 to 999.99 minutes

   Retention Time: 0.01 to 999.99 minutes

   Mobility: -99.999 to 99.999 minutes

3. To select a Y-axis type, open the **Y-Axis** drop-down list box and select one of the following as the Y variable (the allowed ranges follow the label name).

   Molecular Weight: 10 to 99,999,999

Log Molecular Weight: 1.00 to 8.00

Number of Base Pairs: 1 to 99,999

Isoelectric Focusing Point: 0.0 to 14.0

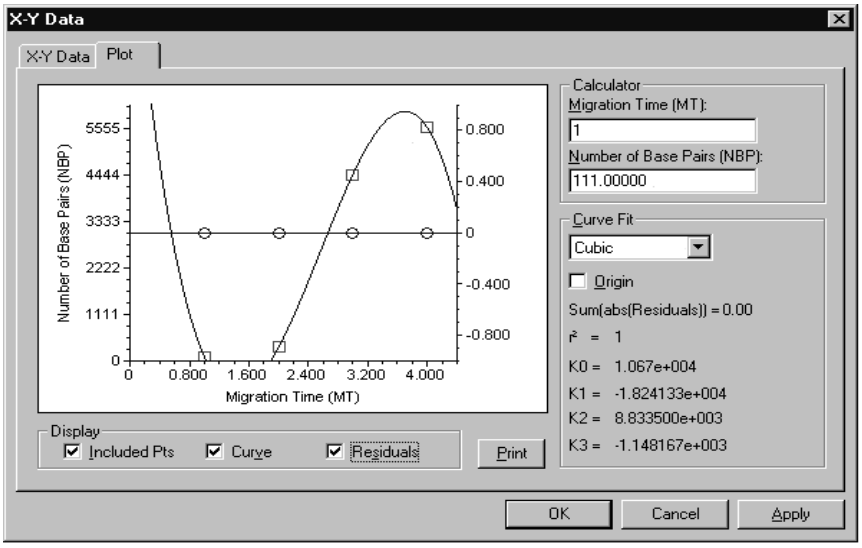
4. Type values from the allowed ranges into the cells. To be valid, every X-value must have a Y-value and vice versa.
5. Select a **Curve Fit** and select whether force the curve through the origin (check the Origin check box). If the **Origin** box is not checked, the origin is ignored and the curve is plotted using the (x,y) pairs of the data set and the normal intercept.
6. When data entry is complete, click the Plot tab to view the plot, or click OK to save the data and exit the dialog box.

Notes

- To add a blank row, click a cell in the row below where you want to insert and press Ctrl + Insert.
- To delete a row, click the row number or any cell in the row and press Ctrl + Delete.
- To copy, or paste cells, select the cell(s) and press Ctrl + C, or Ctrl + V.
- You can enter data values for multiple axis types. Entered data is kept when you switch between types.
- Entering a Molecular Weight value automatically fills in the Log Molecular Weight value and vice versa. The relationship is: Log Molecular Weight = Log10 Molecular Weight.

X-Y Data Plot Tab Page

The X-Y Data Plot tab page displays the plot of the data entered in the Data tab page and lets you calculate unknown values based on the data plot.



Display controls the type of information included in the plot. Check or clear the individual Display options check boxes below the plot, or point to the plot and click the right mouse button to select options from a pop-up menu.

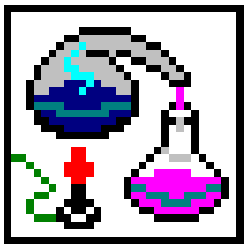
Included Pts displays the entered data points.

Curve draws the selected Curve Fit Type.

Residuals displays a plot of *residual* versus the X-axis variable (migration time, retention time, or mobility). A residual is the difference between the actual measured Y value and the Y value that is generated by the regression calibration for a given X value. The residual axis is on the right side of the plot. For each point, a circle indicates the residual value, with a vertical line indicating the difference from the ideal residual value of zero.

Calculator calculates unknown values based on the data plot and selected curve type. Enter a value in one edit box and then click in the other edit box to calculate the unknown.

6 • The ACI Method Editor



NOTE **The ACI Method Editor is used exclusively with ACI-based systems. If you have a DX-LAN system, use the Method Editor described in Chapter 5.**

The ACI Method Editor is used to create, store, and edit Method files based on the Advanced Computer Interface. Methods contain instructions that tell PeakNet how to control the analytical system, collect and process data, and generate a report after an analysis is complete. Methods include a list of the names, amounts, and retention times of the components in the standard(s) that will be used for calibration.

Each Method is stored on disk under a unique filename. A new Method can be created by recalling an existing Method, modifying it, and then saving the new Method under a different name. PeakNet supplies a default value for most Method parameters. These are useful starting points when developing a new Method.

As part of an ACI Method, you must enter and store a separate timed events file. This file lists the time-sequenced commands the ACI will execute to control your chromatograph and its accessories. The timed events file is stored under its own filename, and the name is stored in the Method file. The timed events file specified in the Method must be stored on disk before the Method can be run.

If the system includes a Dionex gradient pump, you will probably want to also create a gradient file to control the pump valves and flow rate. The gradient file is stored under its own filename, which is included in the Method. The gradient file specified in the Method must be stored on disk before the gradient can be used by the ACI Run program.

Since the files for timed events and gradients are stored separately, they can be shared by several Methods. This permits fast, easy editing of the control functions of several Methods.

NOTE The most convenient way to edit data processing parameters is through the Optimize program, which lets you work directly with the chromatogram.

6.1 Methods for a Dual-Detector System

Each chromatographic system can include up to two detectors. The Method for the first detector controls the operation of the analytical system, as well as the interpretation of the output from the first detector. The output from the second detector is interpreted by a separate Method containing only Integration Parameters, Report Parameters, Calibration, Component Table, and Data Events.

When creating separate Methods for two detectors, keep in mind the following:

- Because the detectors operate in the same chromatographic system, certain parameters for the Methods must be identical. These parameters include the ACI/System specification, the run time, the detector sampling rate, the timed events file, the gradient file, and the PED (Pulsed Electrochemical Detector) file.
- Instrument Control parameters for both Methods are stored in the Method file for Detector 1.
- Data Processing parameters may be different for each Method.

6.2 Methods Using a Dionex Gradient Pump

NOTE If a Method does not include a gradient program, you must program the pump from its front panel.

ACI Methods created for use with a gradient pump normally include both a timed events file and a gradient file. The timed events file contains timed events to control the pump motor (START/STOP) and the gradient clock (RUN/HOLD and RESET). The gradient file contains a gradient program which controls the flow rate and eluent composition delivered by the pump.

When setting up timed events for a Method with a gradient pump, remember the following:

- If you are using the valve-switching capability of the gradient pump to control the injection valve, set the pump to RUN at time zero. Make sure the gradient program includes enough time for loading the injection valve sample loop at the beginning of the program.
- If you are not using the pump to control the injection valve, keep the pump in HOLD (RUN off) at time zero, then set it to RUN when the sample is injected. In either case, it is usually best to run the system under isocratic conditions until the sample is injected.
- When successive samples are analyzed without using a Schedule, it is helpful to include both a RESET and a HOLD (RUN off) command in the last step of the timed events file. If an analysis is ended or aborted, the gradient clock will then be automatically reset to zero in preparation for the next analysis, even if no Method is downloaded between analyses.
- Each time a new gradient file is sent to the gradient pump, the timed events file for the ACI Method must include a toggle from HOLD to RUN (or from STOP to START) for the gradient pump before the new gradient program can control the pump. This is best accomplished by including a HOLD command in the INIT step of the timed events file and a RUN command in the time zero step.
- The gradient RESET command is a momentary command which resets the gradient clock to time zero. It automatically turns off 0.1 minute after it is turned on. To issue a new RESET command, toggle the command off and then on again. If RUN is on at the time of the reset, the gradient clock will continue to run and the gradient program will be repeated, starting with the time zero step.

NOTE If the last step of the timed events file does not include a RESET command for the gradient pump, the pump will continue operating according to the last step in the gradient program until a new program is downloaded.

After a gradient program is loaded into the gradient pump by the ACI Run program, the new gradient is stored in the gradient pump editing memory and the pump continues to run the current gradient program. When the pump receives an execute toggle (i.e., a HOLD/RUN toggle from the timed events file), the program stored in the editing memory is copied into the

pump's run memory, where it controls the pump. (A gradient program cannot be run until it is copied into run memory.)

NOTE For detailed programming instructions for gradient pumps, refer to the *Gradient Pump Operator's Manual* **(Doc. 032646) or** *Advanced Gradient Pump Operator's Manual* **(Doc. 034463).**

6.3 Starting the ACI Method Editor

To open the main window, click on the Method button in the PeakNet MainMenu or double-click on METACI.EXE in the directory that contains your PeakNet files. The ACI Method Editor main window will appear. The main window displays the current setting for key parameters of the ACI Method, and provides command button controls for changing these parameters.

6.4 File Menu

6.4.1 New

Use New when you want to create a new Method. The command clears from memory any Method files already loaded and returns all Settings menu parameters to their default values.

When you select New, all controls in the main window (except System) are disabled until you specify the system with which the new Method will be associated. This prevents the Method from being used with an inappropriate system configuration. After you specify the System assignment, the remaining command button controls will become active.

6.4.2 Open...

Displays a Windows common Open dialog box; select an existing Method file to open from the list.

6.4.3 Save

If the Method was previously saved, selecting the Save command rewrites it to disk under the same name as before.

If the Method was not previously saved, Save functions in the same way as the Save As... command.

6.4.4 Save As...

Save As... opens the Windows common Open dialog box. Type in a filename of no more than eight characters (letters and/or numbers, no punctuation or spaces) to identify the Method. The filename will be added to the ACI Method directory.

NOTE: If you enter a Method name which is already present in the specified directory, the existing file will be overwritten.

The ACI Method Editor automatically adds the subdirectory \METHOD and the extension ".MET" to the filename but you can change the path, if desired. Refer to Appendix E for information about the use of directories and paths for organizing your files on disk.

6.4.5 Print

Prints the Method currently being edited.

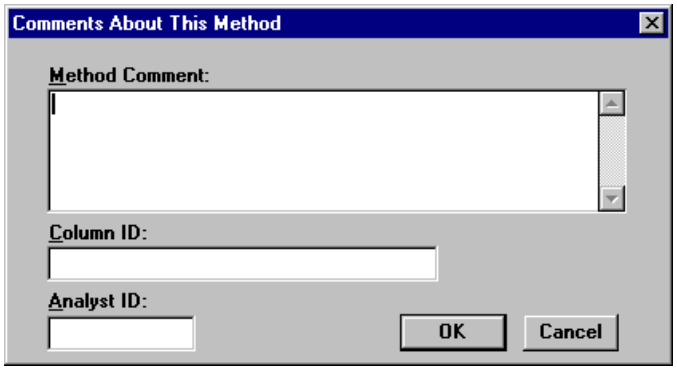
6.4.6 Exit

Closes the ACI Method Editor.

6.5 Comment Menu

6.5.1 Comment...

Enter any pertinent comments about the Method (using up to 255 characters), as well as a description of the column and the name of the analyst, in the spaces provided.



6.6 View Menu

6.6.1 MainMenu

Switch to the PeakNet MainMenu.

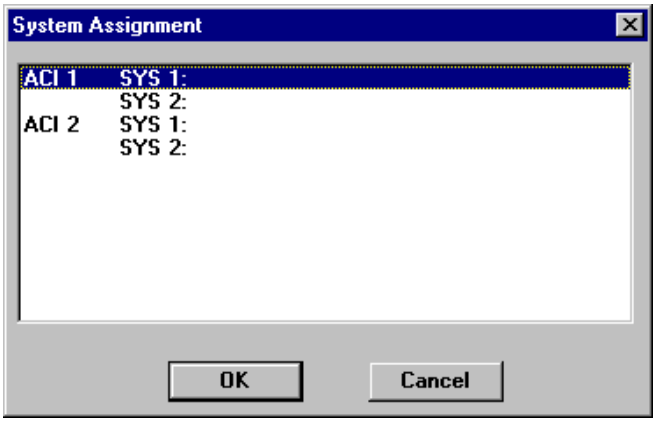
6.7 Data Acquisition Parameters

Data Acquisition parameters include all controls related to the operation of the analytical system and to data collection.

6.7.1 System

The System Assignment box shows the interface and system currently associated with an ACI Method, along with the system description stored in the configuration file(s). The list box shows all of the interfaces for which configurations are currently stored on disk. Tying the ACI Method to a specific system configuration prevents it from being used with an incorrect configuration.

When creating a new ACI Method file, remember that none of the other controls in the main window are active until the system is specified. The File menu's Save and Print commands are also inactive.



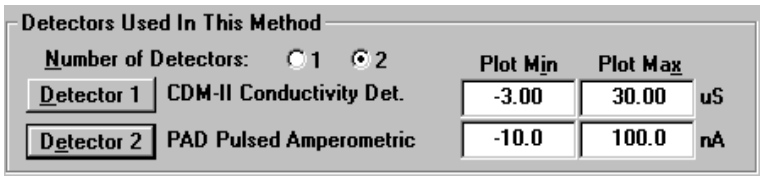
To specify the system for an ACI Method, click on the desired interface/system in the list box and then on the OK button. The selected interface and system, along with the system description, will appear to the right of the System command button.

If you have not yet configured the interface, an error message will appear when you click on the System command button. You must configure the interface, using the Configuration Editor, before you can continue.

The System command button may also be used to change the system specification for an existing ACI Method, as long as the new system has the same configuration as the one originally specified for the ACI Method. If it does not, differences in the configuration may cause errors in the Instrument Control portion of the ACI Method.

6.7.2 Detectors

Detector Selection



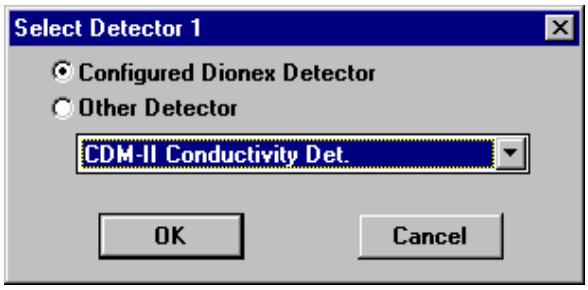
Number of Detectors specifies whether the analysis uses 1 or 2 detectors.

Plot Min and **Plot Max** are the minimum and maximum for the Y-axis of the real-time plot of the data as it is collected. The units depend on the detector selection. An inappropriate plot setting can make peaks too small to see, or else so large that the top of the peak goes off scale on the display. This setting also affects the printed output when the Autoscale options are not selected for the report.

NOTE The plot scale setting affects only the display of the data, not the collection of raw data from the detector.

Detector Assignment

Clicking on the Detector 1 or Detector 2 command button opens a Select Detector dialog box displaying the name of the currently selected detector. If this is the correct detector, click the mouse cursor on the OK button.



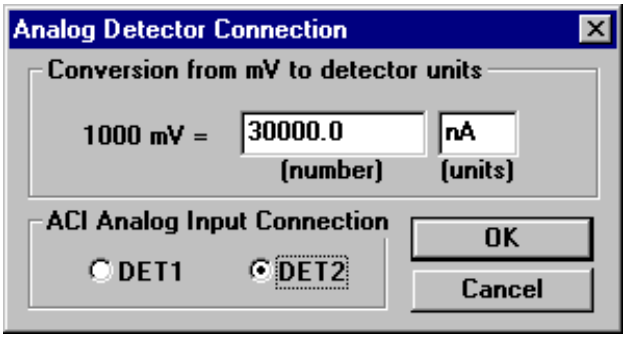
To select a different detector, click on either Configured Dionex Detector or Other Detector. Then click on the arrow at the right side of the drop-down combo box and select a name from the list of available detectors:

- If you select Configured Dionex Detector, this list will comprise detectors specified in the configuration file for the system.
- If you select Other Detector, several non-Dionex analog output detectors will be listed.

When you click on a detector name, the name immediately appears in the selected detector area in the middle of the dialog box. Click on OK to accept the selection.

If you select an analog detector (i.e., any detector except a Dionex Conductivity Detector Module, Variable Wavelength Detector Module-II, Pulsed Electrochemical Detector, or Capillary Electrophoresis System), the Analog Detector Connection dialog box appears.

The Analog Detector Connection dialog box lets you enter a formula that PeakNet uses to convert detector voltage output directly to detector units. For example, suppose you are using an absorbance detector set to 1 AU (absorbance unit) full scale, where full scale is 1000 mV. Type 1 in the "(number)" edit box and AU in the "(units)" edit box. When you click on OK, PeakNet will convert the detector output directly to AU.



ACI Analog Input Connection If you use an analog detector, you must connect the Recorder output terminal on the rear of the detector to a DET connector on the ACI rear panel. Indicate which ACI connector you used by clicking on either the DET1 or DET2 button.

Select OK to accept these selections.

6.7.3 Data Collection

Time

Enter the total period of time (0.0 to 999.9 minutes) during which data will be collected, starting with the Start Sampling command from the timed events file. This is typically the time required for all peaks in the sample to elute. The Run Time parameter also determines the range of the Time scroll bars in the Gradient and Timed Events editors.

Rate

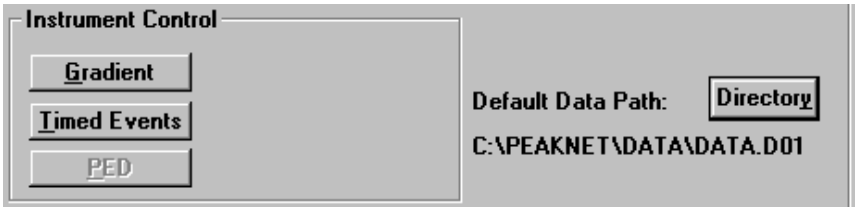
The data collection rate determines how many data points per second (i.e., samples/second) are collected and stored in ACI memory. The data collection rate can be set to 1, 2, 5, 10, 20, or 50 Hz. Five samples/second is adequate for most applications.

NOTE In a dual-detector system, both detectors must operate at the same sampling rate.

In general, the data collection rate should be set so that each peak is defined by 20-30 data points. If you expect all peaks to be relatively wide at the baseline, use a slow rate; if the peaks are less than a few seconds wide, use a fast rate. Selecting a faster rate than necessary does not improve accuracy; it simply slows down data processing and wastes memory and disk space.

See Appendix B for more information about the relationship between the data collection rate and the amount of data that can be stored. If your ACI was shipped before June 1, 1992, you may want to order a RAM upgrade kit (P/N 043592) to expand the ACI memory from 64K to 256K per system.

6.8 Instrument Control



6.8.1 Gradient

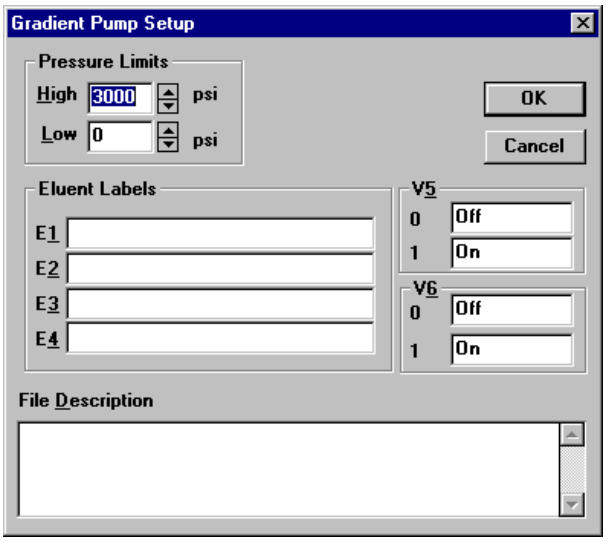
The Gradient Pump Setup and Gradient Editor dialog boxes let you create, save, and edit gradient programs for use by a Dionex gradient pump when an ACI Method is run.

When a gradient file is associated with an ACI Method, its filename and path appear next to the Gradient command button. When you click on the command button to open the Gradient Editor dialog box, any existing gradient file will be automatically loaded. If no gradient file is associated with the Method, the Gradient Pump Setup dialog box will appear.

NOTE The Gradient button is active only when the selected system includes a Dionex gradient pump in its configuration.

Gradient Pump Setup Dialog Box

These dialog box controls set the constants that are used throughout a gradient. The dialog box can also be accessed by selecting the Pump Setup command from the Edit menu in the Gradient Editor dialog box.



Pressure Limits Use the arrow buttons to select the high and low pressure limits, or else type the desired values in the edit boxes.

Piston Size is available only if you use an Advanced Gradient Pump (AGP). Click on the piston size, Microbore or Standard, that corresponds to your pump model.

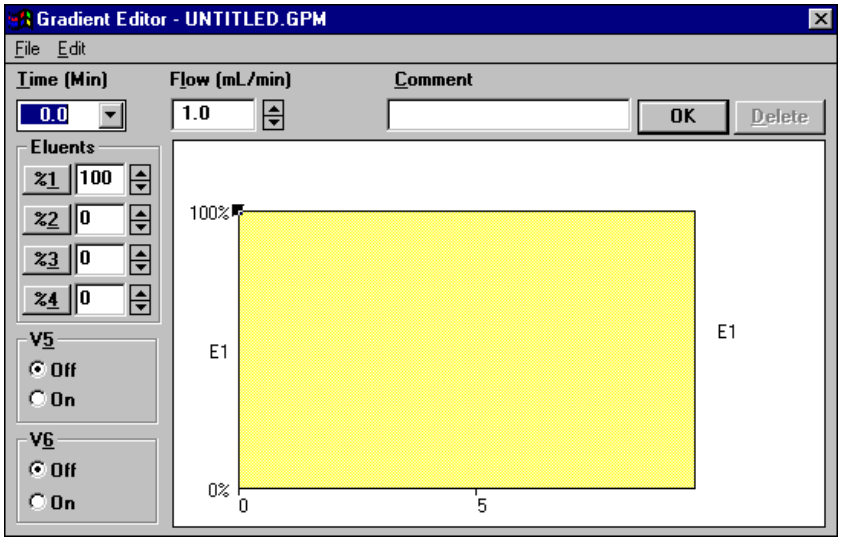
Eluent Labels Type in definitions for the eluent labels.

File Description Type in a description for the file.

V5 and V6 Type in appropriate labels for Valves 5 and 6. These on/off valves are typically used to control an air-operated injection valve and a column select valve.

Click on **OK** to save these selections.

Gradient Editor Dialog Box



File Menu

New prepares the system for creation of a new gradient file and displays the Gradient Pump Setup dialog box.

Open Gradient... displays a file Open box from which you can select and retrieve an existing gradient file from disk.

Save Gradient... saves on disk the gradient file currently being edited. Selecting the command displays a Windows common Save dialog box. If the path shown in the dialog box is the one you want, type a filename of no more than eight characters (letters and/or numbers, no punctuation or spaces). If you want a different path, type in the new path and then the filename.

NOTE **To include a different gradient file in the Method, use the File menu command Open (to retrieve the desired file from disk) or New (to create a new file). The name of the last gradient file edited using one of these commands is included in the Method, so be sure the correct gradient file is associated with an ACI Method before saving it.**

Print sends gradient program information to the printer.

Edit Menu

Pump Setup displays the Gradient Pump Setup dialog box.

Delete Step deletes the currently selected step. This command has the same function as the Delete command button.

Time (Min) lets you edit or delete existing gradient steps and add new steps. A gradient file for an Advanced Gradient Pump (AGP) can contain a maximum of 32 steps; a Gradient Pump Module (GPM) gradient file can contain up to 20 steps.

First, click on the down-arrow beside the Time edit box to display the gradient step times.

To select an existing step for editing, click on that step in the drop-down edit box.

To enter a new step, enter a new time in the edit box.

To copy an existing step, select the step, enter a new time, and press <Enter>.

When you finish, press <Tab> to move the cursor to the Eluents section.

NOTE Each gradient file must include initial conditions at time = 0.0. When the ACI is programmed with the Method by the ACI Run program, the gradient pump will begin operating according to the time zero step.

NOTE When using a concentration gradient, inject the sample at exactly the same point in the gradient each time. To do so, include several minutes of the highest-concentration eluent at the beginning of the gradient program, followed by a re-equilibration step. Inject the sample at some set time after the equilibration is complete. For more details about gradient programs, see the pump manual.

Eluents

Each eluent has the following controls:

A **Totalizer button** marked with the legend %1, %2, %3, or %4.

An **edit box** which displays the eluent percentage for the step being edited.

A **double-headed arrow** to adjust the eluent percentage.

Before a step can be entered, the percentages of the eluents must total 100%. Clicking on a Totalizer button changes the percentage of the corresponding eluent so that the sum eluent total is 100%, if possible.

Press <Tab> to move the cursor to the V5 section.

V5 and V6 Valve

Turns V5 and V6 on or off. Regardless of what function labels you create for these valves, the upper position here in the dialog box corresponds to the left light on the pump front panel and the lower position to the right light.

Flow Rate

Displays the flow rate for the currently displayed gradient step. The AGP flow rate precision is shown in hundredths of a mL/min. The GPM flow rate precision is shown in tenths of a mL/min.

Use the arrow on the right side of the display to change the flow rate.

Curve

This edit box, which is present only if you have an Advanced Gradient Pump (AGP), controls the gradient curve and offers the same configurations that are available from the AGP front panel. For an increasing eluent, curves 1 through 4 are convex, curve 5 is linear, and curves 6 through 9 are concave.

Click on the arrow to the right of the curve edit box to open the drop-down list box and click the mouse on the desired curve number. A curve is selected at the **end** of a step, not the beginning.

Comment

Type a comment of up to 28 characters, including spaces and punctuation, for each gradient step.

OK enters the parameters selected in the Gradient Editor dialog box as a step in the gradient program being edited. Clicking on OK does not save the step as part of the file.

Delete deletes the currently selected gradient step from the gradient program.

Gradient Graph

The gradient graph updates dynamically as you change eluent proportions.

To select a gradient step, click the mouse cursor on the perpendicular step line on the graph. A darkened square, called a handle, will appear at the top of the selected step line.

To change an eluent percentage, place the cursor on the step line handle; note that the cursor arrow is now an up- down arrow. Press the mouse left button and move the step line handle up or down to change the eluent percentage. Click on the Eluents totalizer buttons as required to bring the percentage for eluents to 100%, or double-click on the makeup eluent graph.

To change the time of a gradient step, first click the cursor on the step line to select it. Next, position the cursor anywhere on the step line except on the handle (the cursor arrow will change to a right-left arrow). Now you can change the step time by depressing the mouse left button and dragging the step line left or right along the time axis.

To duplicate a step at a different time, follow the procedure for changing the time of a gradient step, except now depress the <Shift> and <Alternate> keys simultaneously while dragging the time line. The position to which you drag the time line becomes a duplicate step, and the original step remains.

6.8.2 Timed Events

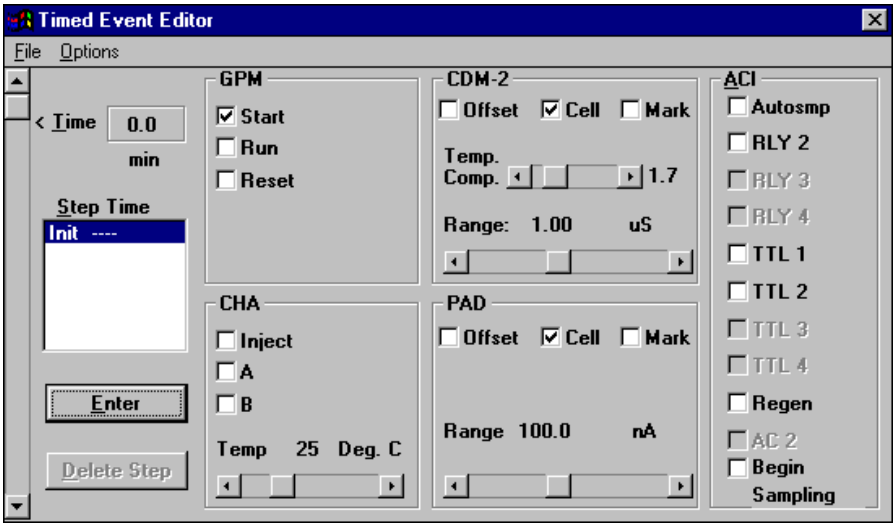
Clicking on the Timed Events command button in the Instrument Control section opens the Timed Events Editor dialog box. This editor allows you to create, save, and edit a file of timed events to control your chromatograph and its accessories.

If a timed events file is already associated with the ACI Method, the filename will appear next to the Timed Events command button and the file, if present, will be pre-loaded automatically when you click on the command button. To include a different timed events file, either retrieve the desired file from disk (using the Open command) or create a new file (using the New command). Both commands are on the File menu.

The **name** of the last timed events file edited using either the New or Open command is the one included in the ACI Method. When you edit an ACI Method, be sure the correct timed events file is associated with it.

The Dionex modules shown in the Timed Events Editor dialog box match the System configuration associated with the ACI Method. The relays, TTL control lines, and AC outlets you assigned to the specified system will also be displayed. However, if your system is configured with a relay-only Data System Model 1R or 2R, the controls portion of the Timed Events Editor dialog box will be blank except for the fields noted below. RLY x, TTL x, and, for Model 2R only, AC x, are default names. If you entered different names in the Configuration Editor, those names will be shown instead.

For detailed descriptions of the controls for an individual module, refer to the operator's manual for the module.



Enter adds the conditions selected for each module at a specified time as a step in the Timed Events table. **If the time for a new step is the same as that of an event already in the table, the new parameters will replace the old parameters.**

Time The scroll bar on the left side of the editor sets the time, in tenths of minutes, at which selected conditions will go into effect. Each time entry is a separate step in the Timed Events table. The range of the scroll bar depends upon the Run Time specified.

Step Time displays the step number and time of each entry in the Timed Events table. To select a step in the table, locate the step in the list box and click on it. The conditions currently stored for that step will be displayed on the control panel.

Every timed events file must include an initial (INIT) conditions step. The INIT step typically contains standby conditions for each module in the system. This allows you to include system equilibration conditions in each Method. The conditions in the INIT step are in effect from the time the Method is downloaded to the interface until the time the Method is started.

The conditions in the time 0.0 step go into effect as soon as the interface receives a START command. The conditions in the time 0.0 step need not match those in the INIT step.

When the next analysis starts, the time 0.0 step executes immediately after START is selected.

Delete Step removes the selected step from the Timed Events table. Select the desired step from the Step Time list box, then click on Delete. The remaining steps will be renumbered consecutively. The INIT and time 0.0 steps cannot be deleted.

ACI Controls See the *ACI Manual* (Doc. 034011) for details.

RLY x, where x is a number from 1-4, controls the relays assigned to the system for which the ACI Method is written. These relays provide contact-closure control of accessories such as a stream-select valve.

TTL x, where x is a number from 1-4, controls the TTL outputs assigned to the system for which the ACI Method is written. These outputs provide control of accessories that need only a digital signal to trigger their operation.

AC x, where x is a number from 1-2, controls the AC outlets assigned to the system for which the ACI Method is written. These outlets provide programmable AC power connections for accessories that require simple on/off control (recorder, sampling pump, etc.). Each outlet is rated for 2 amps.

Begin Sampling starts collection of detector data by the ACI. To issue a new Begin Sampling command, you must first end the current chromatogram.

File Menu

Save...

Saves on disk the timed events file currently being edited. When you select this command, a Save dialog box will appear.

Options Menu

List

Displays all the operating conditions listed in the Timed Events table, as well as the times associated with them.

EXAMPLE:

Enter a Timed Events table for a system consisting of a GPM (Gradient Pump Module), CHA (Advanced High-Pressure Chromatography Module), Conductivity Detector Module (CDM), and an ASM (Automated Sampler).

Time = Init
Flow rate = 0.5 mL/min
GPM Start
GPM Hold Gradient Clock
GPM Reset Off
Valve B = On
Inject valve = Off (Load)
Cell = On
Range = 10 µS

Time = 0.0
GPM Reset On
Relay 1 = On (trigger autosampler LOAD sequence)

Time = 1.0
CDM Offset = On

Time = 1.1
GPM Run Gradient Clock
Inject valve = On (Inject)
Mark = On

Time = 1.2
Relay 1 = Off

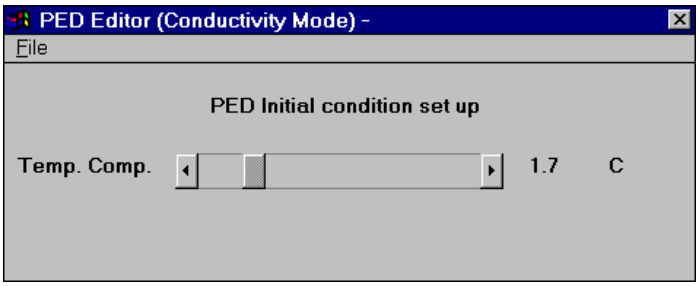
1. Click on the Timed Events command button to open the Timed Events Editor dialog box.
2. Verify that the INIT step is selected.
3. Point and click on the E1 check box in the GPM section. Point and click on the left arrow of the Flow scroll bar until the flow rate is set to 0.5 mL/min.
4. Click on Enter to enter the initial conditions step in the timed events table.
5. Using the Time scroll bar, set the time to 0.0.

6. Repeat Step 3 to set the Time 0.0 conditions, then click on the Relay 1 check box in the ACI section. Click on Enter to enter the time 0.0 conditions as Step 1 in the timed events table.
7. Using the Time scroll bar, set the time to 1.0. Click on the Offset check box in the CDM section, and then on Enter.
8. Repeat Step 7 to enter the remaining timed events.
9. Verify that the conditions for each step are correct by selecting each step from the list box and examining the conditions as they appear on the control panel.
10. Select Save (from the File menu) to save the timed events file. Type the filename AS5A in the filename box and click on Save. The extension ".TE" is added to the filename automatically and the file is added to the Method being edited. Add the file to the directory of your choice.

6.8.3 PED Editor

Click on the PED command button to open the PED Editor. The dialog box controls depend on which PED Mode is selected.

Conductivity Mode



File Menu

New prepares the system for creation of a new file.

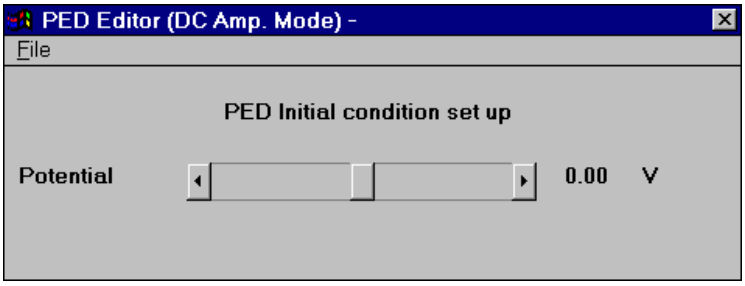
Open... displays a file box from which you can select and retrieve an existing file from disk.

Save... displays a Save dialog box, so that you can save on disk the PED file currently being edited. Type a filename of no more

than eight characters (letters and/or numbers, no punctuation or spaces).

The dialog box scroll bar adjusts the detector temperature compensation factor to correct for changes in response caused by temperature variation in the mobile phase. For more information, see the *PED Operator's Manual* (Doc. 034177).

DC Amperometry Mode



File Menu

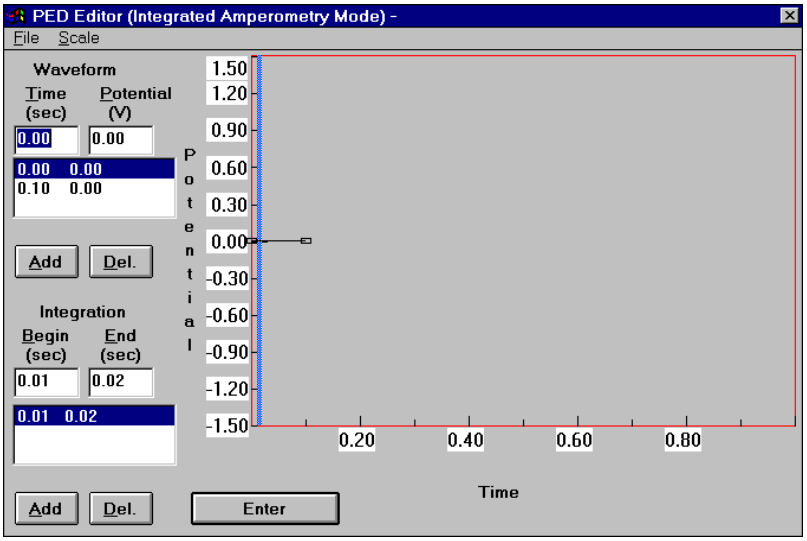
New prepares the system for creation of a new file.

Open... presents a file box which allows you to select and retrieve an existing file from disk.

Save... displays a Save dialog box, so that you can save on disk the PED file currently being edited. Type a filename of no more than eight characters (letters and/or numbers, no punctuation or spaces).

The DC Amperometry Mode can be used for DC amperometry or cyclic voltammetry. The dialog box scroll bar lets you select a potential for a new program or edit a potential in an existing program. For more information, see the *PED Operator's Manual* (Doc. 034177).

Integrated Amperometry Mode



File Menu

New prepares the system for creation of a new file.

Open... presents a file box in which you can select and retrieve an existing file from disk.

Save... saves on disk the PED file currently being edited and opens a Save dialog box. Type in a filename of no more than eight characters (letters and/or numbers, no punctuation or spaces).

Print sends the current file to the printer.

Scale Menu

To view graph scales, click on the desired menu option.

Creating a Program

Integrated Amperometry Mode can be used for integrated amperometry or pulsed amperometry. To create a program, you must first enter both a time/potential program and an integration period. The repeating sequence of potentials applied to the cell working electrode is defined by points selected on the displayed graph.

Step 1 of every program is at time zero. Since this cannot be changed, the first value you will enter is the first potential. Enter the remaining times and potentials in sequence until the program is completed; for each step, enter first the time and then the potential. Enter a program as follows:

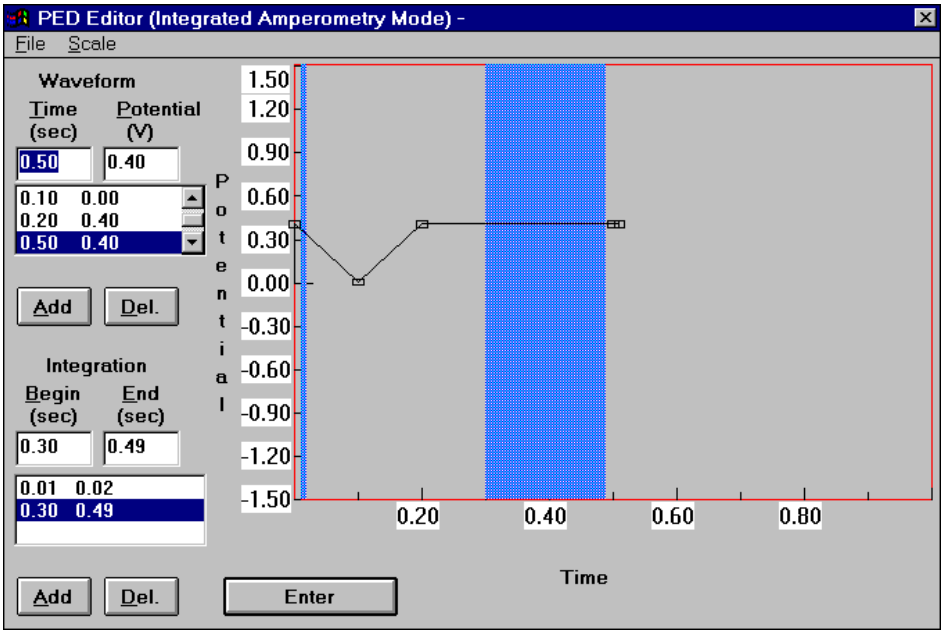
Waveform

1. Enter the potential for the first step of the program in the Potential dialog box (the Waveform Time is always 0 for the first entry). Click on the Add command button below the Waveform list box to enter the value.
2. Enter the time for the second step in the Time edit box. Use the <Tab> key to move to, and highlight, the Potential edit box and then enter your second step Potential value. Click the mouse cursor on the Add button to enter the values. (If you prefer, use the I-bar cursor to enter values in the edit boxes rather than highlighting with the <Tab> key.)
3. Enter the remaining times and potentials in sequence until the program is complete.

Integration

Enter the Integration beginning time and ending time in the Integration dialog boxes, and then click on the Add command button.

The integration period appears as a shaded region on the screen waveform graph.



Editing a Program

1. Select a line in the list box for editing.
2. Change the value(s) as desired in the edit box(es).
3. Click the mouse cursor on the Enter command button.

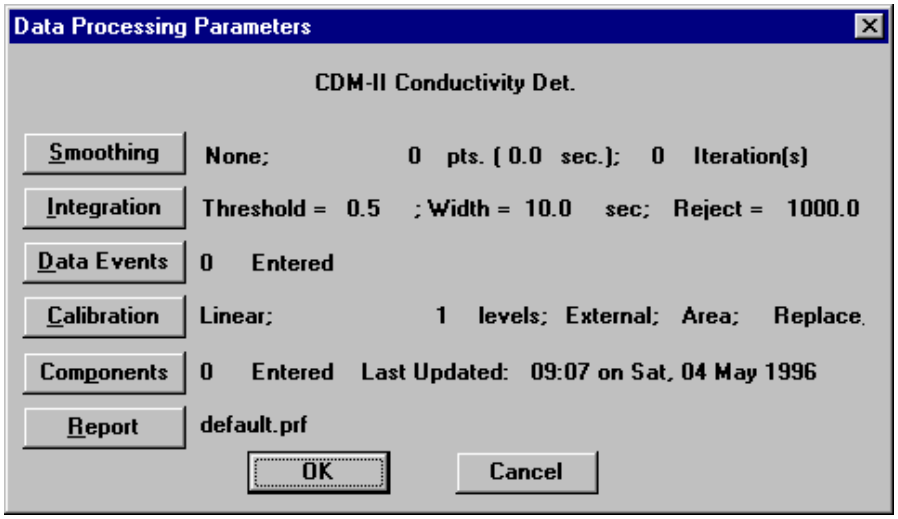
6.9 Data Processing Parameters

Data processing parameters specify how the data from an analysis is processed, what information is included in the final analytical report, and whether the data is stored on disk.

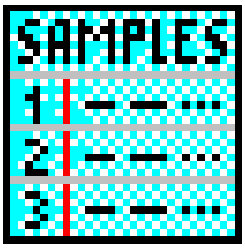
Click on the Detector 1 or Detector 2 command button in the ACI Method Editor main window to open the Data Processing Parameters dialog box. The six command buttons in the dialog box correspond to the six types of data processing parameters; click on the desired command button to open a a dialog box in which you set these parameters.

The ACI Method Editor Data Processing dialog boxes are the same as the Data Processing dialog boxes described in the Method Editor chapter. See Section 5.8 for details about each dialog box.

NOTE The easiest way to edit Data Events is through the Optimize program, where the effects on integration are displayed instantly.



7 • The Schedule Editor



The Schedule Editor is used to create, edit, and save Schedules, which consist of one or more Methods linked so that they automatically perform a series of analyses. A typical Schedule might include one or more calibration runs, analyses of several samples, a column change and an equilibration, followed by new calibration runs and more samples. Each Schedule step specifies the Method, data filename, and other parameters used to analyze a single injection. A Schedule may be repeated from 1 to 999 times. You can also use the Schedule Editor to specify groups of data files to be reprocessed by the Batch program.

The Run (or ACI Run) program performs this sequence of events for each Schedule step:

(a) Run retrieves the Schedule file from disk and uses the Method specified in the Schedule to analyze the injection for that step.

(b) Raw data is processed according to the data processing parameters selected for the Method.

(c) Run saves the data and prints any reports specified in the Method.

(d) Run updates the data filename in the Schedule file with the raw data filename it actually used.

(e) Once all modules reach the last timed event ***and*** Run completes data collection from all detectors (or Advanced Computer Interfaces) used in the Method, Run loads the Method for the next injection and transfers it to the modules in the system.

NOTE You may open the Schedule Editor and view the updated file while a Schedule step is running. However, do not save this file to the hard disk; doing so would overwrite the Schedule file updated by Run.

7.1 Starting the Schedule Editor

To open the Schedule Editor's main window, click on the Schedule button in the PeakNet MainMenu or double-click on SCHEDDX.EXE in the directory that contains the PeakNet program files. The main window contains a blank spreadsheet in which each row represents one injection.

7.1.1 The Toolbar

Click on a toolbar button to quickly implement frequently used menu commands and controls for the Schedule Editor. Click on the buttons for the PeakNet MainMenu and Help to display those programs.

From left to right, the toolbar button functions are:

1. New
2. Open
3. Save
4. Print
5. Cut
6. Copy
7. Paste
8. Fill
9. Comments
10. AutoCopy
11. Increment
12. Help
13. Switch to MainMenu

7.2 File Menu

7.2.1 New

Click on the New toolbar button (or select the menu command) to create a new Schedule. A dialog box lets you choose to create a standard, AS50, or AS3500 Schedule.

7.2.2 Open...

Click on the Open toolbar button (or select the menu command) to display a Windows common Open dialog box. From the dialog box, select an existing Schedule to display in the main window.

7.2.3 Close

Closes the Schedule in the active child window.

7.2.4 Save

Click on the Save toolbar button (or select the menu command) to rewrite a previously saved Schedule to the disk under the same name.

If the Schedule was not previously saved, Save functions in the same way as the Save As... command.

7.2.5 Save As...

Save As... opens the Windows common Save As dialog box. Type in a filename of no more than eight characters (letters and/or numbers, no punctuation or spaces) to identify the Schedule. If you do not enter an extension, the Schedule Editor automatically adds the extension ".SCH" to the filename.

Unless you specify otherwise, the filename is added to the ...\SCHEDULE subdirectory.

7.2.6 Import ASCII File...

Bring a specially formatted ASCII source file into a new Schedule, or append it to the current Schedule.

To create the ASCII source file:

The ASCII file can be created in any text editor, or generated by a database, such as a LIMS.

When you save the file, add the .SCH extension (for a standard PeakNet Schedule), .SAS extension (for an AS50 Autosampler Schedule), or .AS3 extension (for an AS3500 Autosampler Schedule) to the file name.

The file must:

- Have one line for each line that is to be created or updated in the Schedule
- Have each line end with carriage return and linefeed characters
- Have each input field separated from the next by a comma

Each line includes the following input fields:

Standard PeakNet Schedule:

```
Sample Name,Sample Type,Level,Method,Data
File,Volume,Dilution,Weight,Int. Std.,Comment
```

AS50 Schedule:

```
Vial #,Inj/Vial,Sample Name,Sample
Type,Level,Method, Sample Prep.,Data
File,Volume,Dilution,Weight,Int. Std.,Comment,Inj.
Type,Syr. Spd.,Cut Vol.
```

AS3500 Schedule:

```
Vial #, Inj. Vol.,Inj/Vial,Sample Name,Sample
Type,Level,Method,Data File,Dilution,Weight,Int.
Std.,Template,Column Oven,Column Oven
Temp,Cooler,Cooler Temp,Cycle Time,Flush
Volume,Viscosity,Prep. Viscosity,Injection
Type,Needle Height
```

Example for a standard schedule:

Sample 1,0,C:\peaknet\one.met,C:\peaknet\one.dxd,1

Sample X,1,8,C:\peaknet\x.met,C:\peaknet\x.dxd,5,2,3,2,some comment

Sample Y,2,5,C:\peaknet\test.met,C:\peaknet\y.dxd

When the ASCII field is imported into the Schedule Editor, empty fields are either assigned default values (if they are number fields), or are left blank (if they are text fields).

Value Ranges for Schedule Fields

Field	Value Range	Default
Vial # (AS50)	1..100	1
Vial # (AS3500)	A01-A40, B01-B40, C01-C40	A01
Sample Type	0 (Sample) 1 (Calibration Standard) 2 (Check Standard)	0
Level	1..32	1
Volume (standard)	> 0, < 10.E12	1
Volume (AS50)	1.0..99.9, 100..1000	100
Volume (AS3500)	0..1500	10
Inj/Vial	1..99	1
Dilution	> 0, < 10.E12	1
Weight	> 0, < 10.E12	1
Int.Std.	> 0, < 10.E12	1
Injection Type (AS50)	0 (Full-loop), 1 (Partial-loop), or 2 (Partial-loop, Limited Sample)	0
Injection Type (AS3500)	0 (Push), 1 (Pull), or 2 (full)	0

Field	Value Range	Default
Syringe Speed (AS50)	1..5	3
Cut Volume (AS50)	0..30	0
Column Oven	0 (off) or 1 (on)	0
Column Temp	15..80	18
Cooler	0 (off) or 1 (on)	0
Cooler Temp	0..35	0
Cycle Time	0.00..655.35	0
Flush Volume	200..5000	400
Viscosity	0 (Normal), 1 (Medium) or 2 (Viscous)	0
Prep. Viscosity	0 (Normal), 1 (Medium) or 2 (Viscous)	0
Injection Type	0 (Push), 1 (Pull), or 2 (Full)	0
Needle Height	0.0..20.0	2

To import the source file:

1. Create the ASCII source file (see above).
2. Do one of the following:
   - To import the ASCII file into a new Schedule file, click the New toolbar button to open a blank Schedule.
   - To add the Schedule lines in the ASCII source file to the end of an existing Schedule, open the existing Schedule.
3. Select Import ASCII File... .
4. Select the ASCII source file that is to be converted to a Schedule.
5. Click Open.

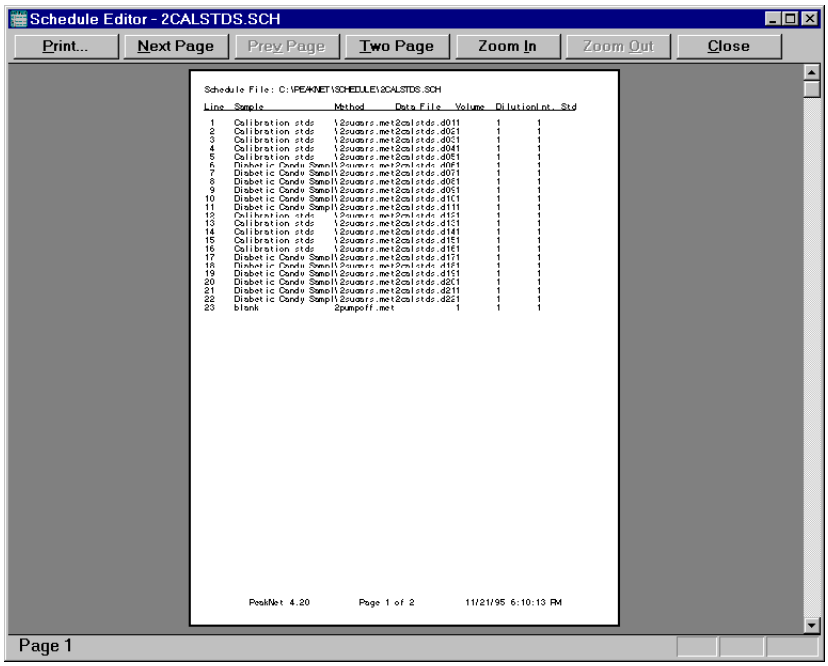
7.2.7 Print...

Click on the Print toolbar button (or select the menu command) to print the current Schedule.

7.2.8 Print Preview

Displays full pages of the current Schedule as they will look when printed, in the Print Preview window.

If the number of columns for each row of the printout is wider than a single page on the printer, the Schedule will be displayed as a series of pages numbered from left to right, top to bottom. A header with the Schedule file name and a footer with the page number will be printed on each page. The system number, default Schedule path, default data path, and any comments included in the Schedule will be printed after the last row of Schedule data.



Click on the command buttons below the title bar in the Print Preview window to modify the display:

Next Page displays the next page of the Schedule.

Prev Page displays the previous page of the Schedule.

One Page switches from a two-page display (the default) to a one-page display of the last left-hand page displayed.

Two Pages reverts to the default view.

Zoom In switches from a full-page view to a magnified view. (This does not affect the printing size.)

Zoom Out switches from a magnified view to a full-page view. (This does not affect the printing size.)

To print from the Print Preview window, click on the **Print** command button.

To exit the Print Preview window without printing, click on the **Close** command button.

7.2.9 Print Setup...

Displays the Windows common Print Setup dialog box for the current printer. Use the dialog box controls to select the printer settings (print quality, paper size, etc.) or to change the printer.

7.2.10 Most Recently Used

Opens one of the last four Schedules used when you click on its name here.

7.2.11 Exit

Closes the Schedule Editor.

7.3 Edit Menu

The Schedule Editor features true spreadsheet functionality: lines or blocks of information can be easily cut, copied, and pasted using standard Windows conventions.

NOTE Clicking the right mouse button anywhere on the Schedule spreadsheet displays the Edit menu for the Schedule spreadsheet.

7.3.1 Cut

Click on the cell(s) to be cut, then click on the Cut toolbar button (or select the menu command) to cut information from the spreadsheet and transfer it to the Windows Clipboard.

7.3.2 Copy

Click on the cell(s) to be copied, then click on the Copy toolbar button (or select the menu command) to copy entries from any group of consecutive rows to another location in the spreadsheet.

7.3.3 Paste

Click on the Paste toolbar button (or select the menu command) to paste the contents of the Windows Clipboard at the insertion point.

7.3.4 Delete Rows

Deletes one or more injections from a Schedule.

Highlight at least one cell in each row to be deleted, then select the Delete Rows command or press the <Ctrl> and <Delete> keys. All rows containing a highlighted cell will be deleted.

7.3.5 Insert Rows

Inserts one or more blank lines between two existing injections in a Schedule.

- To insert one row, highlight any cell of the row where you want the new row to appear.
- To insert more than one row, highlight two or more adjacent cells in the same column. The number of highlighted cells determines the number of new rows added to the spreadsheet.

After highlighting the cell(s), select the Insert Rows command. When the new row is inserted, the row previously at that location, as well as all subsequent rows, will be renumbered.

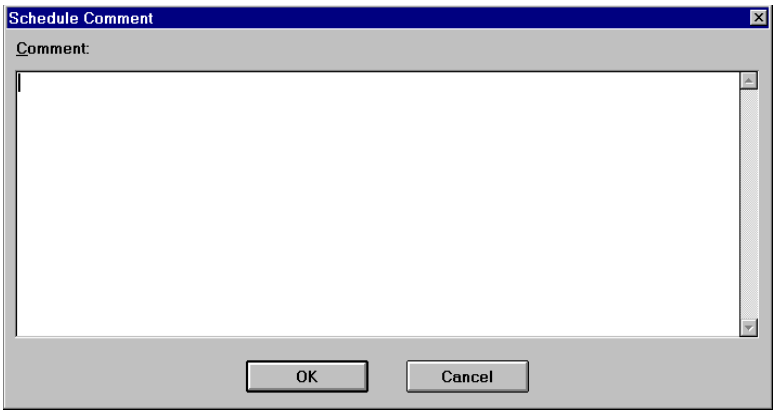
7.3.6 Fill

Click on the Fill toolbar button (or select the menu command) to copy the contents of the cells in the top row of a selected block into other cells in the block. This overwrites any data already in the selected block.

The Fill option is automatically enabled when you select at least two cells in the Schedule spreadsheet; it is automatically disabled after the copy operation is completed.

7.3.7 Comments...

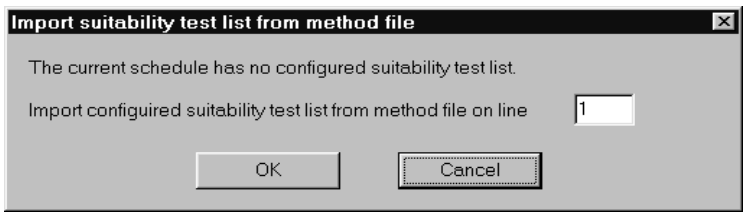
Click on the Comments toolbar button (or select the menu command) to open the Comment dialog box. In the space provided, enter any remarks (up to 255 characters) about the Schedule that you want to have saved as part of the file.



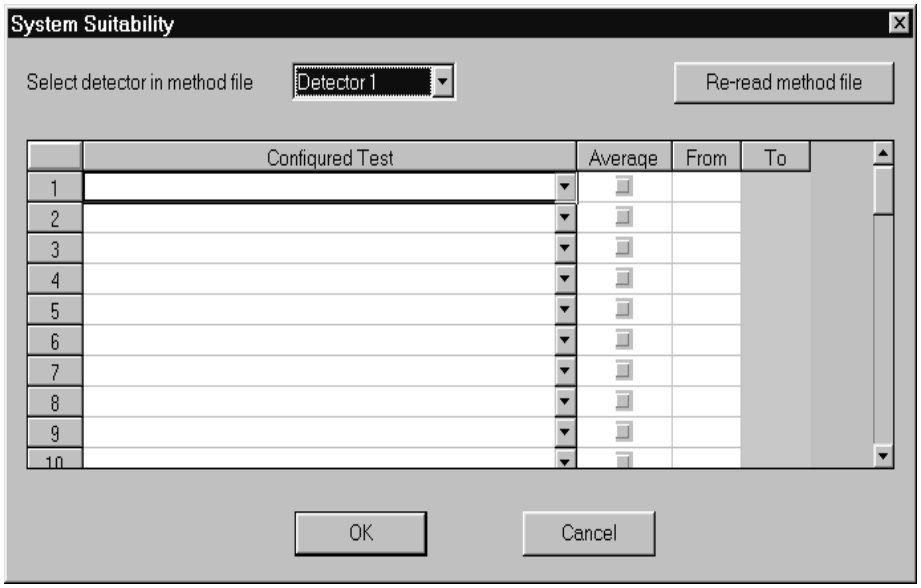
7.3.8 System Suitability

Displays the System Suitability dialog box for specifying system suitability tests to be run on Schedule injections. You run the tests using the Batch program and the results are reported in a System Suitability Table in the Summary Report.

If the Schedule does not already have tests specified, a message box appears asking you to specify the Method from which to import configured tests. Enter the Schedule line number that contains the Method.



The System Suitability dialog box appears:



Select detector in method file lets you select which detector to use. A different group of tests is defined for each configured detector in the Method.

Configured Test Select a test from the drop-down list. The list will show all tests that were defined in the Method (for the selected detector).

Average lets you select a range of injections and then average the results. Averaging is not available if the test requires multiple injections (for example, the %RSD test).

From, To Specify the Schedule line(s) on which to run the test. Some tests require a range, others can be run on a single injection. The To column must not be less than the From.

Notes for the Signal/Noise test:

To use the same injection for the signal and noise values, enter a line number in the To column and leave the From column blank.

To use a different injection for each value, enter the line number for the Signal in the To column and enter the line number for the Noise in the From column.

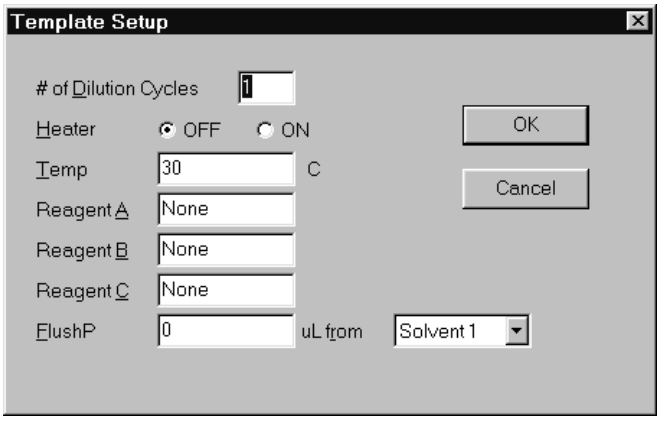
If Average is checked, the From column sets the end of the range, not the injection to use for the Noise value.

Re-read method file lets you re-import the list of tests from the Method. This is useful if the list of defined tests in the Method has changed, or if you want to clear the current test configurations from the dialog box. A message appears, warning you that the current tests will be deleted.

7.3.9 Template (AS3500 Schedules only)

Opens the AS3500 Template Editor dialog box. If the current line in the Schedule does not already have a template specified, the Template Setup dialog box opens on top of the Template Editor.

The Template Setup dialog box is used to set parameters that stay constant throughout an AS3500 sample preparation procedure.



# of Dilution Cycles determines how many times (1-4) the fixed sequence of 10 preparation steps will be performed.

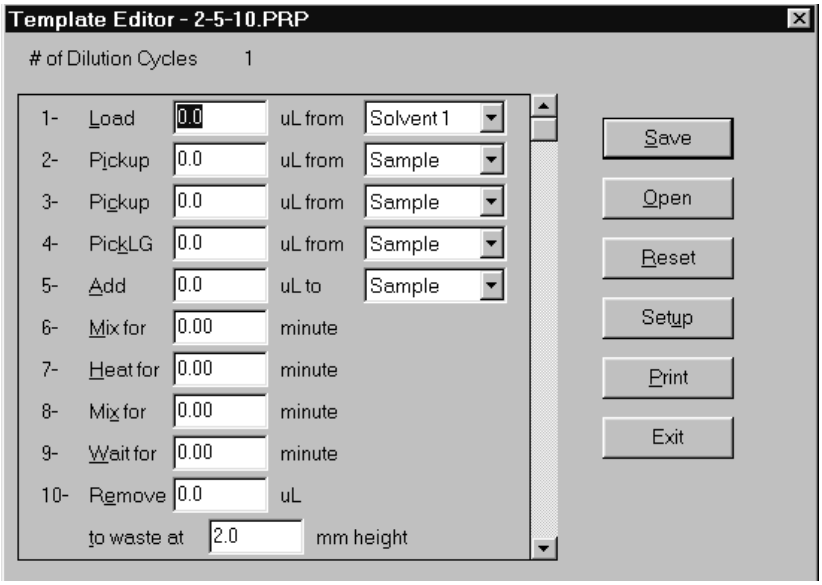
Heater turns on and off the vial heater in the vortex mixer.

Temp sets the temperature of the vial heater as an integer from 30 to 100°C.

Reagent designates a vial position (A01-C40, or NONE) as a reagent resource for the preparation procedure. Liquid can be drawn from a reagent vial, but not added to it.

FlushP µL from sets the solvent volume and solvent reservoir used to flush the sample preparation syringe between sample preparation procedures.

The Template Editor dialog box is used to edit the steps of a Sample Preparation Template.



# of Dilution Cycles indicates how many times (1-4) the fixed sequence of 10 preparation steps will be performed. The number of cycles is set in the Template Setup dialog box.

When more than one dilution cycle is selected, scroll down to view steps beyond the first 10.

Preparation Steps in the large list box can be edited, but their order cannot be changed. A step can be skipped by entering a value of 0; other entries are automatically checked for errors when the template is saved.

Load pre-loads the preparation loop with the indicated volume of the selected solvent.

Pickup loads the indicated volume of liquid from the selected vial into the preparation loop, using the small syringe.

PickLG loads the indicated volume of liquid from the selected vial into the preparation loop, using the large syringe.

Add dispenses the indicated volume of liquid from the preparation loop into the selected vial. The vial position is selected relative to the sample vial for which the template is used.

Mix spins the vial in the vortex mixer for the indicated period.

Heat heats the vial for the indicated period while in the vortex mixer. Time is measured from the end of the first mixing period.

Wait leaves the vial resting in the sample tray for the indicated period.

Remove draws the indicated volume of liquid from the vial at the indicated needle height and sends it to waste.

Save accesses a File Save dialog box which writes the template to disk as a file with the extension *.PRP.

Open accesses a File Open dialog box for retrieving an existing template from disk.

Reset clears all template editing and resets all template parameters (including Template Setup parameters) to their default values.

Setup accesses the Template Setup dialog box.

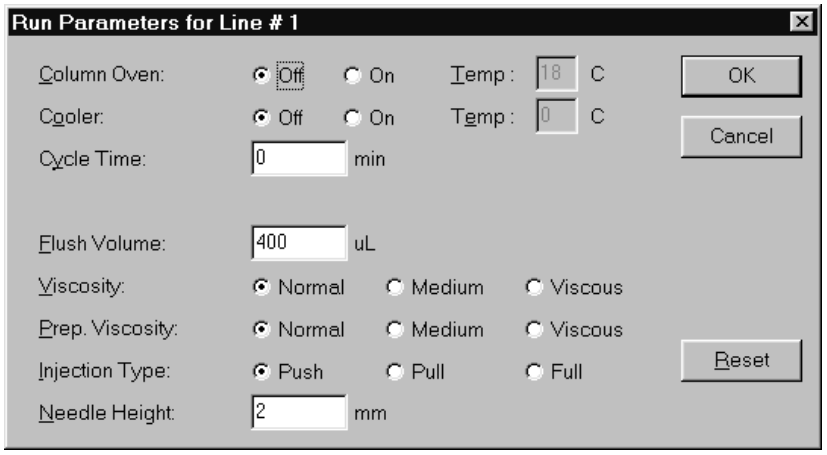
Print prints the sample preparation parameters as currently edited.

Exit closes the Template Editor dialog box.

7.3.10 Run Parameters (AS3500 Schedules only)

Opens the Run Parameters dialog box to set conditions which are held constant throughout an analysis. Run Parameters can be different for each line of the Schedule. The default values apply to a line unless you edit them or copy the Run Parameters from another line.

To edit the Run Parameters for a line, select the line in the Schedule and select Run Parameters... from the Edit menu. The Run Parameters dialog box appears.



Column Oven and Sample Cooler control the temperature of those options, if installed in the AS3500 Autosampler. If either is installed and its Run Parameter is on, the Run Program will wait for it to reach its temperature set point before starting the analysis.

Cycle Time sets how long the AS3500 will wait between loading samples. If you leave this at the default value of 0, the Run program downloads a cycle time to the AS3500 that starts the next run when the current run is complete.

Flush Volume sets the volume of flush solvent used to rinse the sample path between injections.

Viscosity controls the rate of syringe draw. For most liquids, Normal provides good precision and minimizes loading time. For viscous liquids, Medium or Viscous allows time for fluid to flow and provides better precision than Normal.

Prep Viscosity controls the Sample Prep syringe as above, if the Sample Preparation option is installed.

Injection Type controls whether the loop is partially loaded by drawing the sample into it (Pull) or pushing the sample into it (Push), or whether the loop is fully loaded (Full).

Full tends to provide the best precision, but does not allow easy variation of injection volume. Push provides better precision than Pull, but takes more time.

The sample volume required depends on the selected injection type, as shown below.

- Pull Loop: Volume Pulled = Injection Volume + 1.1 µL
- Push Loop: Volume Pulled = Injection Volume + 15 µL
- Full Loop: Volume Pulled = 1.3 x Loop Size + 70 µL

Needle Height controls the distance between the tip of the sampling needle and the outside of the vial bottom when a sample is being drawn or dispensed.

CAUTION: Setting too short a needle height for the vials used can damage the needle.

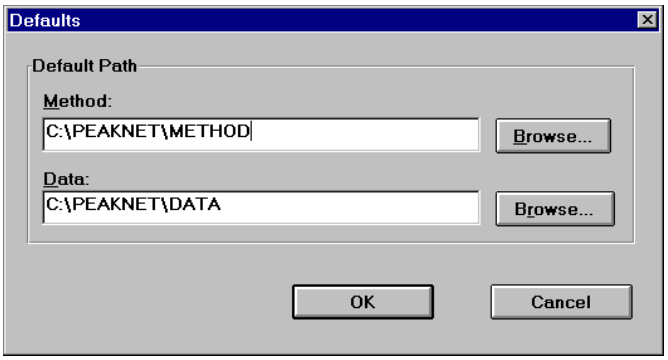
Reset sets all Run Parameters back to defaults.

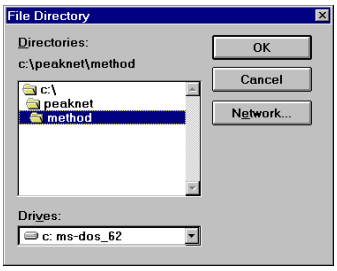
7.4 Options Menu

7.4.1 Defaults...

Type in a default path name for the Method file and/or data file in the space provided in this dialog box, or click on the **Browse...** command button to open a File Directory dialog box from which you can select a different path.

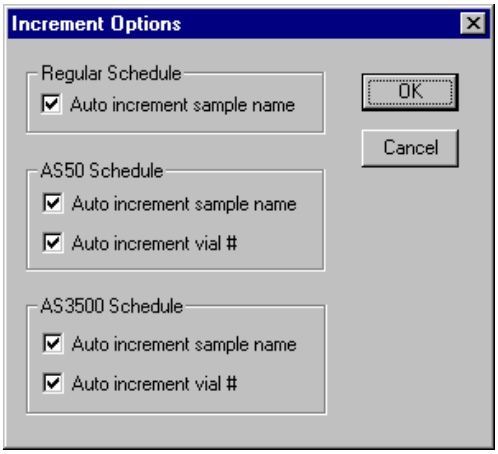
Each Schedule stores a separate set of default paths. Method and data file paths are not listed in the Schedule spreadsheet or the body of the printout unless they differ from these defaults. (The default paths are listed below the body of the Schedule printout.)





7.4.2 Increment Options...

Click on the check box to enable or disable automatic incrementing of a number appearing at the end of the sample name. For AS50 and AS3500 Schedules, you can also select to increment the vial number. Automatic incrementing takes effect only when the Increment command is enabled (see Section 8.4.4).



7.4.3 AutoCopy

Click on the AutoCopy toolbar button (or select the menu command) to enable or disable this mode. When enabled, AutoCopy fills in a blank line with entries from the previous line. The Increment Option (if enabled) will be applied.

1. Verify that AutoCopy is enabled (there should be a check mark before the menu command).
2. Select a cell in the row above the first blank line.
3. Using the mouse, <Tab> key, or arrow key, move the cursor from the last data-containing row of the Schedule spreadsheet to a blank row immediately below it. (A “blank” row is one without a sample name, Method name, or data file name.)

7.4.4 Increment

Click on the Increment toolbar button (or select the menu command) to enable or disable automatic incrementing.

The incrementing affects the number that appears after the sample name (and/or the vial number for AS50 and AS3500 Schedules), when a row of the spreadsheet is copied to a new location. For example, if you copy Sample 1 to a new location, the entry will automatically be renamed Sample 2. If you copy the sample again, it will automatically be renamed Sample 3, and so on.

7.4.5 Calc. Dilution (AS3500 Schedules only)

Calculate the dilution factor for a vial, based on the dilution factor and template settings of the vial in the previous line of the Schedule.

Position the cursor in the Dilution cell and select Calc. Dilution from the Options menu. PeakNet calculates the dilution factor and enters it into the cell.

The dilution factor is calculated as follows:

*Dil2 = Vol2/Vol1 * Dil1*

where:

Dil2 is the dilution factor to be calculated

Vol2 is the **Add to** volume specified in the template

Vol1 is the first **Pickup volume** specified in the template

Dil1 is the dilution factor of the first **Pickup vial**

7.5 View Menu

7.5.1 Toolbar

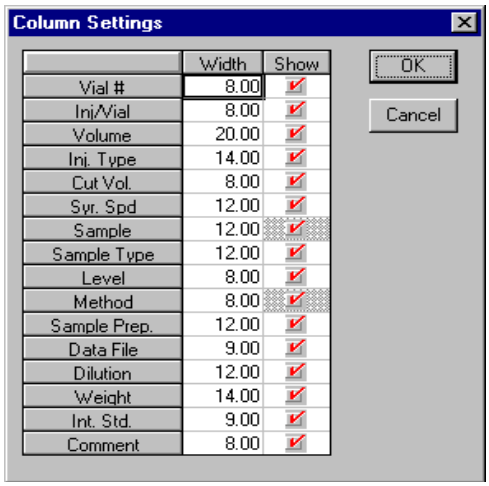
Shows or hides the toolbar.

7.5.2 Status Bar

Shows or hides the status bar.

7.5.3 Columns...

Specify the width of data columns in the spreadsheet (in number of characters) and select which columns to show or hide. The Column Settings dialog box for a standard Schedule is shown here.



When it is not necessary to precisely define column width, you can quickly resize columns as follows:

1. Position the cursor over the column border to be moved. The cursor will change to a column-adjustment cursor with a left-right arrow.

2. Press and hold the mouse button and drag the border to its new location.

7.5.4 Size Column to Content

Automatically size a column to fit the longest entry in the column, whether that is the column header or data in a cell.

There is a second way to access this command: clicking the right mouse button anywhere on the Schedule spreadsheet displays a menu that includes Size Column to Content.

7.5.5 Font...

Opens the Windows common Font dialog box, which lists all the typefaces and sizes supported by the printer currently installed in the Control Panel.

7.5.6 MainMenu

Displays the PeakNet MainMenu.

7.6 Window Menu

7.6.1 Tile

Resizes and positions all open child windows so that each is fully visible.

7.6.2 Cascade

Arranges child windows in an overlapping fashion so that each title bar is visible.

7.6.3 Arrange Icons

Automatically arranges icons neatly at the bottom of the window.

7.6.4 Open Windows List

Makes an open window active.

7.7 Schedule Editor Spreadsheet

A Schedule spreadsheet can contain instructions for up to 999 injections. The last line in the spreadsheet that includes a Method filename is considered the last Schedule step; therefore, subsequent lines will not be saved.

To enter information in the spreadsheet, select a blank cell and type directly into the cell. (To have the status bar display a summary of what type of information to enter, position the cursor over the cell.) When you finish typing, do one of the following:

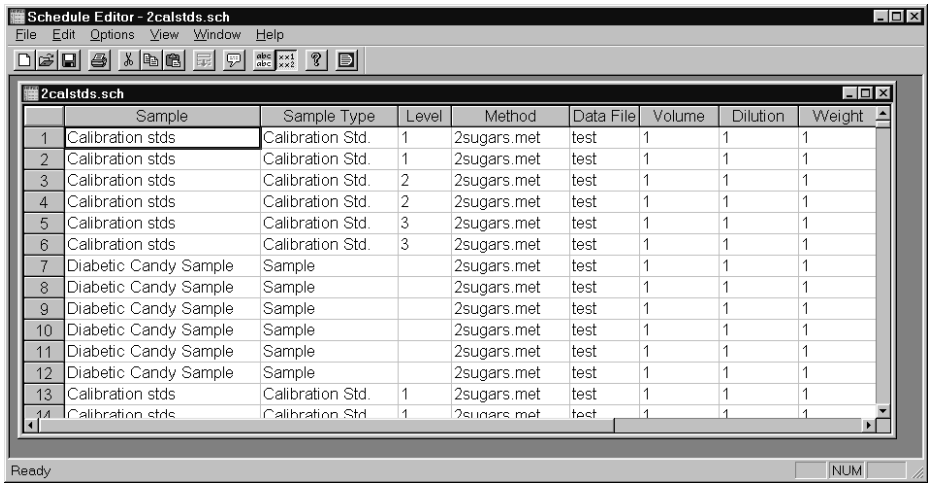
- Press <Enter> to leave the current cell highlighted.
- Press <Tab> to highlight the next cell.

  If the last cell in a row is highlighted and AutoCopy mode is enabled, pressing <Tab> copies the entries of the current row to the next row **if** it is blank.
- Press <Esc> to abandon editing and leave the cell blank.

To edit the contents of a spreadsheet cell, do one of the following:

- To overwrite the current entry, begin typing in the cell.
- To delete the current entry, press the <Delete> or backspace key.
- To modify the current entry, position the cursor in the correct location and then type and delete characters as required.

7.7.1 Schedule Parameters



	Sample	Sample Type	Level	Method	Data File	Volume	Dilution	Weight
1	Calibration stds	Calibration Std.	1	2sugars.met	test	1	1	1
2	Calibration stds	Calibration Std.	1	2sugars.met	test	1	1	1
3	Calibration stds	Calibration Std.	2	2sugars.met	test	1	1	1
4	Calibration stds	Calibration Std.	2	2sugars.met	test	1	1	1
5	Calibration stds	Calibration Std.	3	2sugars.met	test	1	1	1
6	Calibration stds	Calibration Std.	3	2sugars.met	test	1	1	1
7	Diabetic Candy Sample	Sample		2sugars.met	test	1	1	1
8	Diabetic Candy Sample	Sample		2sugars.met	test	1	1	1
9	Diabetic Candy Sample	Sample		2sugars.met	test	1	1	1
10	Diabetic Candy Sample	Sample		2sugars.met	test	1	1	1
11	Diabetic Candy Sample	Sample		2sugars.met	test	1	1	1
12	Diabetic Candy Sample	Sample		2sugars.met	test	1	1	1
13	Calibration stds	Calibration Std.	1	2sugars.met	test	1	1	1
14	Calibration stds	Calibration Std.	1	2sugars.met	test	1	1	1

NOTE See the following sections for descriptions of the parameters for AS50 and AS3500 Schedules.

Sample

Type in a name (up to 31 characters) that identifies the sample.

Sample Type

Specifies whether the injection is a Sample, Calibration Standard, or Check Standard. If the Sample Type is Calibration Standard, the Run or ACI Run program will use sample data to calculate the response factors for each sample component and update the Method's Component Table. All peak heights, areas, and retention times will also be updated.

NOTE In previous versions of PeakNet, a special sample name, AUTOCALx, where x is the calibration level, was used to trigger automatic calibration. Older Schedules that use the AUTOCAL nomenclature will still work as before.

Level

When the Sample Type is Calibration Standard or Check Standard, this field specifies the calibration level of the injection. You specify the amount of each component in a particular calibration level in the Method's Component Table.

Method

Double-click on an empty Method cell to open the Windows common Open dialog box. When you select the Method to be used to analyze the sample, the filename will be entered in the empty Method cell. (The Method must be stored on disk before it can be executed as part of a Schedule.)

The path for the filename is not displayed, unless it is different from the default path (see Section 8.4.1).

Data File

Type in a filename under which raw data from the analysis should be stored on disk. PeakNet automatically adds a letter and number identification code to the end of the name you enter, and then adds a .DXD extension. See Data File Naming for details.

PeakNet uses the following conventions for naming data files when they are created during Method and Schedule runs:

- The extension .dxd is always added
- To ensure that existing data files are never overwritten, an identifying letter and number combination is added to data file names. The following naming scheme is used:

  [user assigned name]~xxxyyy.dxd

where:

[user-assigned name] is the name entered into the Data File column of the Schedule, or the name specified at the time a Method is run.

xxx is a series of letters starting with aaa that increments each time a Method or Schedule is loaded.

yyy is a series of numbers starting with 001 that increments each time the Method is run.

Examples:

- Create a Schedule that has 10 lines, and enter a data file name of sample data. The following data files are created when the Schedule is run:

  sample data~aaa001.dxd - sample data~aaa010.dxd

- Load and run the same Schedule, but stop the Schedule after five runs. The following data files are created:

  sample data~aab001.dxd - sample data~aab005.dxd

- Load and run the same Schedule, and allow it to finish. The following data files are created:

  sample data~aac001.dxd - sample data~aac005.dxd

  sample data~aab006.dxd - sample data~aab010.dxd

- Create a Schedule that has 10 lines; name the first five data files standard and the last five sample. The following data files are created:

  standard~aaa001.dxd - standard~aaa005.dxd

  sample~aaa006.dxd - sample~aaa010.dxd

If you do not enter a path for the filename, raw data will be stored in the default data directory specified in the PEAKNET.INI file. If you do enter a path, the Run and ACI Run programs will use that path, rather than ...\DATA. The path for the filename is not displayed, unless it is different from the default path (see Section 8.4.1).

You can override the default path when Run or ACI Run loads the Schedule.

To simply the management of data files, use a new subdirectory for each new Schedule. For information about how to organize files on disk, see Appendix E.

Volume

If desired, enter the volume of sample injected so that the calculated concentrations will be corrected for differences in sample volumes. When injecting the same sample volume each time, use the value 1. **This parameter applies only to Methods using external standard calibration.**

Dilution

The dilution factor provides a mathematical correction (diluent volume/sample volume) for dilution effects. For a dilution of 1:10, enter 10. If there was no dilution, use the value 1. **This parameter is ignored for calibration standards.**

Weight

Enter the weight of the sample. If there is no variation, use the default value of 1.

Int. Std.

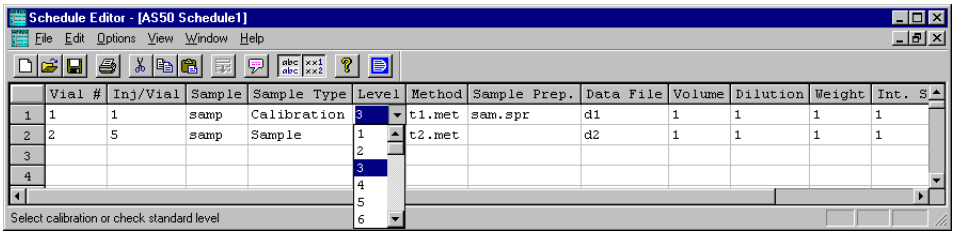
Enter the amount of the internal standard added to each standard or sample. If there is no variation, use the value 1. If there is a variation, enter the value. This value will be compared to the one in the Component Table. **This value is used in internal standard calculations only.**

Comment

Enter a descriptive comment (up to 127 characters) about the current injection. The comment will be saved with the data file and printed below the header of the injection reports.

7.7.2 AS50 Schedule Parameters

In addition to the Schedule parameters described in Section 7.7.1, the following parameters are included in an AS50 Schedule.



Vial

Is the sample vial number (1 through 100). Vials may be sampled in any desired sequence.

Sample Prep.

Is the name of the Sample Preparation Method (*.SPR) to be run. When a Sample Preparation Method is specified, any sample preparation steps in the standard Method are ignored.

Volume

Controls the volume of sample injected. This value will be automatically taken into account during External Standard Calibration calculations. If no entry is made in this column, the default value of 100 µL is used.

The following value ranges are allowed:

- 1.0 - 99.9 µL (in increments of 0.1)
- 100 - 1000 µL (in increments of 1)

Inj/Vial

Is the number of injections to be made from a vial; up to 99 injections are allowed.

Inj. Type

Specifies whether the injection type is full-loop, partial-loop, or partial-loop, limited sample.

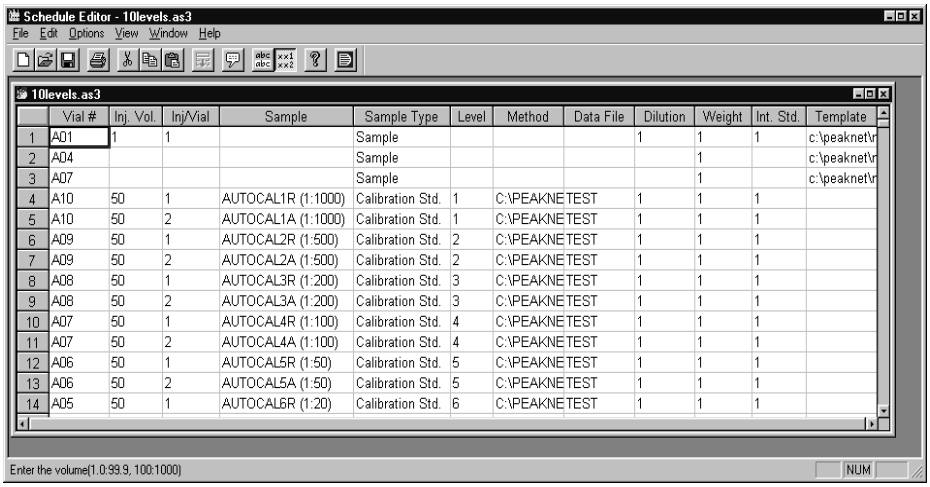
Syr. Spd.

Is the speed of the sample syringe (1 - 5). The default value of 5 (fastest) corresponds to the speed that should be used with water. More viscous liquids require slower speeds.

Cut. Vol.

Is the volume (up to 30 µL) to be discarded from each end of the sample at injection.

7.7.3 AS3500 Schedule Parameters



	Vial #	Inj. Vol.	Inj/Vial	Sample	Sample Type	Level	Method	Data File	Dilution	Weight	Int. Std.	Template
1	A01	1	1		Sample				1	1	1	c:\peaknet\r
2	A04				Sample					1		c:\peaknet\r
3	A07				Sample					1		c:\peaknet\r
4	A10	50	1	AUTOCAL1R (1:1000)	Calibration Std.	1	C:\PEAKNET	EST	1	1	1	
5	A10	50	2	AUTOCAL1A (1:1000)	Calibration Std.	1	C:\PEAKNET	EST	1	1	1	
6	A09	50	1	AUTOCAL2R (1:500)	Calibration Std.	2	C:\PEAKNET	EST	1	1	1	
7	A09	50	2	AUTOCAL2A (1:500)	Calibration Std.	2	C:\PEAKNET	EST	1	1	1	
8	A08	50	1	AUTOCAL3R (1:200)	Calibration Std.	3	C:\PEAKNET	EST	1	1	1	
9	A08	50	2	AUTOCAL3A (1:200)	Calibration Std.	3	C:\PEAKNET	EST	1	1	1	
10	A07	50	1	AUTOCAL4R (1:100)	Calibration Std.	4	C:\PEAKNET	EST	1	1	1	
11	A07	50	2	AUTOCAL4A (1:100)	Calibration Std.	4	C:\PEAKNET	EST	1	1	1	
12	A06	50	1	AUTOCAL5R (1:50)	Calibration Std.	5	C:\PEAKNET	EST	1	1	1	
13	A06	50	2	AUTOCAL5A (1:50)	Calibration Std.	5	C:\PEAKNET	EST	1	1	1	
14	A05	50	1	AUTOCAL6R (1:20)	Calibration Std.	6	C:\PEAKNET	EST	1	1	1	

In addition to the Schedule parameters described in Section 7.7.1, the following parameters are included in an AS3500 Schedule.

Vial

Is the vial number (A01-A40, B01-B40, or C01-C40). Vials may be sampled in any desired sequence. The letter specifies the AS3500 sample-vial tray; the number indicates the vial position within that tray.

Inj. Vol.

Controls the volume of sample injected. This value will be automatically taken into account during External Standard Calibration calculations. If no entry is made in this column, the default value of 10 µL is used.

The following value ranges are allowed for the **full loop** and **variable volume** (either **Pull-Loop** or **PushLoop**) modes:

- Full loop mode: 5, 10, 20, 50, 100, 200, 500, and 100 µL
- Pull-Loop mode range: 1 to 1500 µL
- PushLoop mode range: 0.1 to 10 µL (in increments of 0.1), or 1 to 200 µL

You can set the mode for each Schedule line in the Run Parameter dialog box (see Section 7.3.10).

Inj/Vial

Is the number of injections to be made from a vial; up to 99 injections are allowed.

Dilution

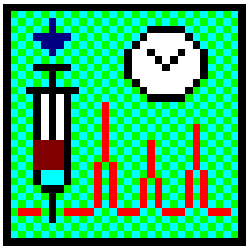
Specifies the dilution factor of the sample. For example, if the sample was diluted to 10 times its volume, enter 10. To calculate the dilution due to a sample preparation procedure in the previous line, select Calc. Dilution from the Options menu.

Template

Lets you specify a sample preparation template for processing the current vial. No injection is made on a sample schedule line that includes a template; repeat the vial number on a subsequent line if you want it to be injected. See the description of the Edit menu's Template... command (Section 7.3.9) for information about creating a sample preparation template.

You can select a Template from a directory by double-clicking on a cell in the Template column.

8 • The Run Program



NOTE Run is used exclusively with DX-LAN systems. ACI-based systems use the ACI Run program described in Chapter 10.

Run conducts the analyses specified in Methods, Schedules, and Sample Tables. Run can perform module status display, Method and Schedule loading, real-time data display, data reduction, report printing, data storage, module Direct Control, and modification of a running Method.

Run can monitor up to eight systems simultaneously, controlling multiple DX-500 instrument systems via the DX-LAN interface. Run controls the optional AS3500 Autosampler through the RS-232 interface.

Before opening Run for the first time, use the Configuration Editor to configure the system. The configuration specifications will be stored in the PEAKNET.CFG file. Each time Run is opened, it must access this file in order to communicate with modules in the system.

8.1 OLE Automation

OLE automation capability allows instrument systems that include hardware and/or software from more than one vendor to be controlled by a single program. This allows remote control of systems over a network and facilitates the export of data to other applications. You must have Windows programming knowledge in order to write OLE links to Run and implement OLE. The following tasks can be performed via OLE automation:

- Load Methods and Schedules
- Start, stop, and abort Methods and Schedules
- Check the status of a PeakNet system and/or modules

For complete Windows programming information, see the OLE automation topic in the PeakNet on-line Help.

NOTE Dionex cannot provide assistance to programmers attempting to use OLE links, and assumes no liability for any errors or problems resulting from the use of these formats.

8.2 Starting the Run Program

To open Run's main window, click on the Run button in the PeakNet MainMenu or double-click on RUNDX.EXE in the directory that contains the PeakNet program files.

8.2.1 Toolbar

Click on a toolbar button to quickly implement frequently used Run menu commands and controls. Click on the buttons for the PeakNet MainMenu and Help to display those programs.

From left to right, the toolbar button functions are:

1. Load Method
2. Load Schedule
3. Baseline
4. Start
5. Modify
6. End
7. Abort
8. Direct Control
9. Help
10. Switch to MainMenu

8.3 File Menu

8.3.1 Load Method...

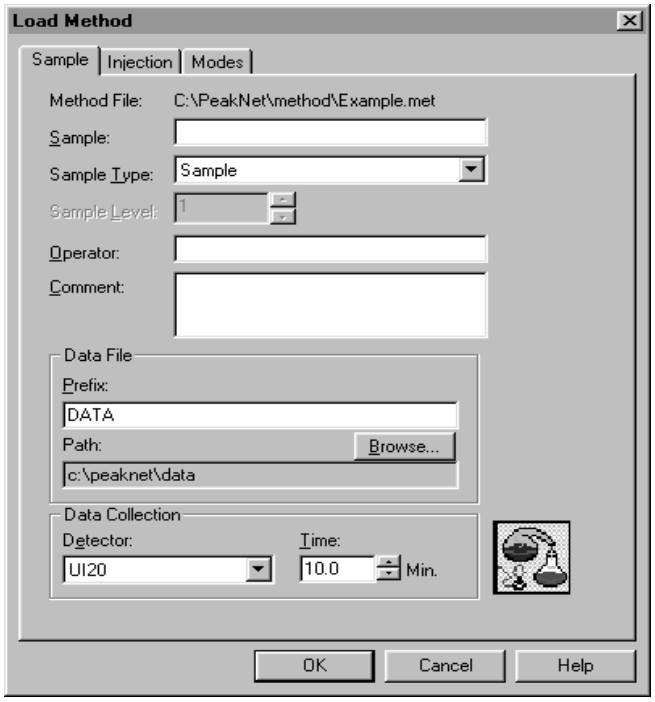
NOTE If the Method was recently loaded, you may be able to select it from the Most Recently Used list on the File menu.

Before loading a Method, activate the system you plan to load, either by clicking on the system name in the Window menu or by clicking on the title bar of the system window.

Next, click on the Load Method toolbar button (or select this menu command) to display the Open dialog box. Select a Method file from the dialog box, then click on OK to display the Load Method dialog box.

Select Method parameters from the dialog box's three tab pages: Sample, Injection, and Modes.

Load Method - Sample Tab Page



Sample specifies a name (up to 30 characters) that identifies the sample.

Sample Type specifies the type of injection: Sample, Calibration Std., or Check Std. If Calibration Standard is selected, the response values from the analysis are entered automatically into the Method's component table.

Sample Level for Calibration Standard or Check Standard injections, enter the level number of the standard.

Operator specifies an operator's name (up to 19 characters).

Comment lets you enter a description (up to 127 characters) about the current injection. These comments are saved with the data file and printed below the header of reports.

Data File lets you enter a name for the file in which to save raw data for the injection. If you do not want to save raw data, leave this space blank. To save raw data, type in a **File Prefix**. PeakNet automatically adds a letter/number identifier code and the extension .DXD when the data is stored on disk.

The following naming scheme is used:

[user assigned name]~xxxyyy.dxd

where:

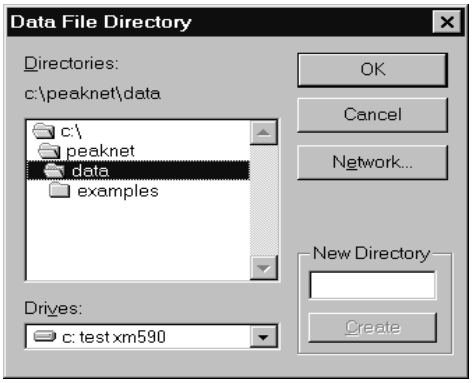
[user assigned name] is the name entered Data File Prefix field.

xxx is a series of letters, starting with aaa, that increments each time a Method or Schedule is loaded.

yyy is a series of numbers, starting with 001, that increments each time the Method is run.

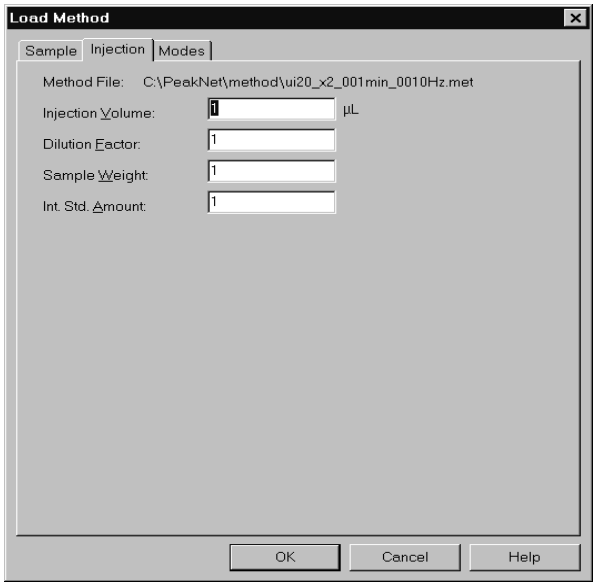
Unless you select a different pathname, data will be stored in the same directory as other PeakNet data files.

To save the file in a different directory, click on the **Browse...** command button and select a directory from the following dialog box. To create a new directory for the file, type the directory name in the New Directory box and click on the **Create** button. The new directory is created under the current directory.



Detector From the list boxes, select any detector used in the Method, as well as a Time period for data collection (up to 999.9 minutes). For a UI20 Universal Interface, this time will be applied to both channels.

Load Method - Injection Tab Page



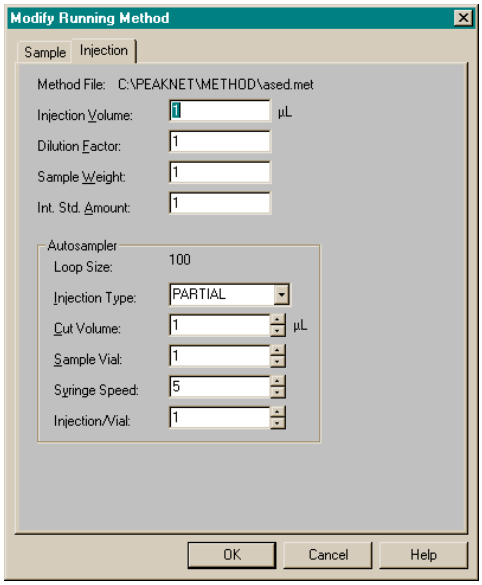
Injection Volume Enter the volume of sample injected (using the same unit as the calibration standards), so that the calculated amount can be corrected for differences in sample volumes. *Note: Injection Volume is used only in external standard calculations.*

Dilution Factor provides a mathematical correction for dilution effects. For example, enter 10 for a dilution of 1 to 10. If there was no dilution, use the value 1. *Note: Dilution Factor is used in external and internal standard calculations, but is ignored for calibration standards.*

Sample Weight Enter the weight of the sample.

Int. Std. Amount Enter the amount of the internal standard (if one is used) so that the sample amount can be corrected for differences in the internal standard amount. *Note: If there is no internal calibration standard, this parameter is ignored.*

When a system includes an AS50 Autosampler, the Injection tab page includes an Autosampler group box.



Loop Size indicates the sample loop volume. This value is determined by the parameters you select on the AS50 **PLUMBING CONFIGURATION** screen.

Injection Type This parameter is automatically selected, depending on the settings of other parameters:

Full is selected when the Injection Volume is greater than the Loop Size.

Partial is selected when the Cut Volume (see below) is greater than 0.

Partial Injection, Limited Sample is selected when the Injection Volume is less than the Loop Size and the Cut Volume is zero.

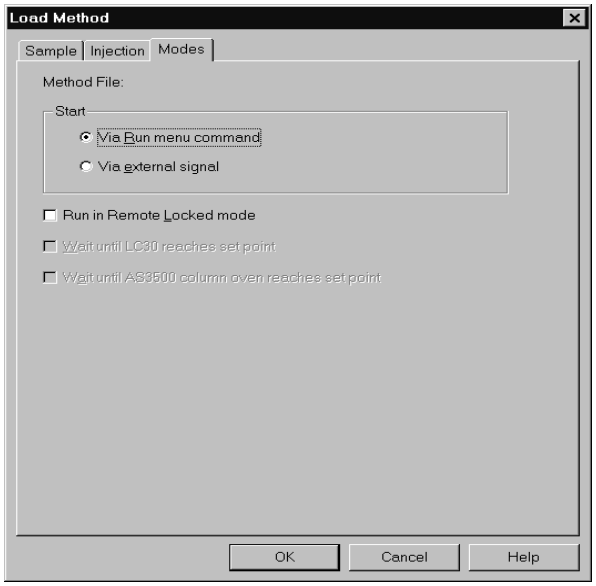
Cut Volume specifies the volume (0 to 30 µL) to cut from each side of the sample during injection.

Sample Vial selects the vial (1 - 100) to run.

Syringe Speed sets the speed of the sample syringe (1 - 5). Select the default value (5) for water; more viscous liquids require slower speeds.

Injection/Vial specifies the number of injections to perform on the vial.

Load Method - Modes Tab Page



Start determines how the Method is started:

Select **Via Run menu command** to start the timed events for the loaded Method by selecting the Run Start... command.

When you select **Via external signal**, you do not have to start the timed events for the loaded Method; the modules will start timed events when they receive a signal from the front panel or from a remote device. This permits an instrument to signal the modules that the next sample has been injected and is ready for analysis. When you select Via external signal, the Run Start... command remains enabled so that you can modify Method parameters before the next remote start.

Click on a check box to select the corresponding Start Option:

Select **Run in Remote Locked mode** to prevent front panel operation while a run is in progress. This ensures that the original, unaltered Method is used for the run and stored with the data file. This option is disabled when a run is in progress.

Select **Wait until LC30 reaches set point** to ensure that a run does not begin until the LC30 Chromatography Oven temperature matches the value set in the GP50 or GP40 Gradient Editor.

Select **Wait until AS3500 column oven reaches set point** to defer the start until the AS3500 Autosampler temperature matches the value set in the Run Parameters for the current line in the 3500 Editor.

After you select a Method, Run retrieves the system information from the Method file. If this information does not match the selected system, a message box suggests what to do. If the systems match, Run downloads the module timed events to each module and saves the data reduction parameters in memory.

The Start command is enabled only after the Method is successfully loaded. When the Method is loaded, the injection number in the Module Control Bar is set to 1. When the Method ends, Run increments the injection number by 1.

The next time the Run program is opened, it “remembers” the Method and automatically restores the Method and all previously collected data.

8.3.2 Load Schedule...

Before loading a Schedule, activate the system you plan to load the Schedule to, either by clicking on the system name in the Window menu or by clicking on the title bar of the system window.

Next, click on the Schedule toolbar button (or select this menu command) to display an Open dialog box with a list of all available Schedule files in the default Schedule directory. The file types are *.SCH, *.SAS (if an AS50 Autosampler is configured), or *.AS3 (if an AS3500 Autosampler is configured).

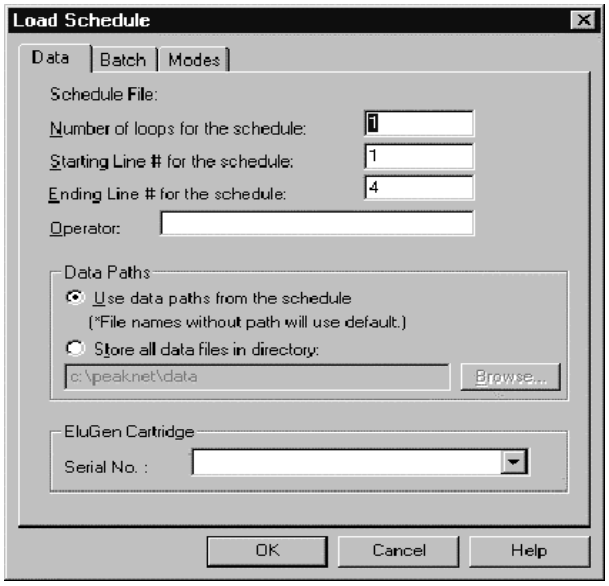
NOTE For important information about autosampler Schedules, see the subsections entitled AS50 Autosampler Schedules and AS3500 Autosampler Schedules.

Select a Schedule from the list in the Open dialog box and click on **OK**. Run then retrieves the system information from the Schedule file.

If the required modules are present, the Load Schedule dialog box appears. The dialog box contains three tab pages: Data, Batch, and Modes. Use the tab page controls to specify the Schedule conditions.

Run then retrieves the Method information from the Schedule and downloads the timed events to all modules. Clicking on OK from either the Load Method or Load Schedule dialog box also enables the Start... command.

Load Schedule - Data Tab Page



Number of loops for the Schedule is the number of times the Schedule is to be run. Enter a value from 1 to 99, or enter -1 to run the Schedule continuously. (The looping option is disabled when an AS3500 Autosampler is configured.)

Starting Line # for the Schedule is the Schedule line number at which analyses begin. This option enables you to start or resume at any line number. Each time raw data is stored, the extension of the data filename is indexed to match the injection number, starting with the number entered here.

After a Schedule is loaded, the starting line number is displayed in brackets next to the Method name. The line number is incremented each time Run begins the next injection.

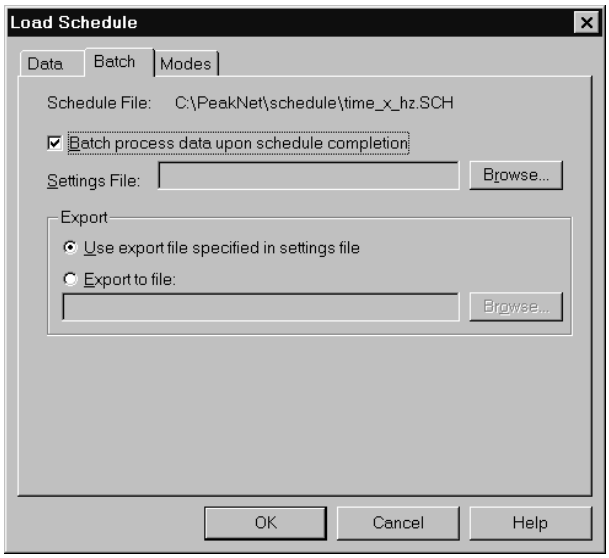
Ending Line # for the Schedule is the Schedule line number at which analyses end.

Operator is the operator's name. Type up to 19 characters here.

Clicking on **Use data paths from the Schedule** automatically stores data files in the file paths previously entered in the Schedule. To change the data path, or to specify a new data path if the Schedule does not include one, click on **Store all data files in**

directory and type in the desired data path or else click on the **Browse...** command button and select a path from the dialog box that appears.

Load Schedule - Batch Tab Page

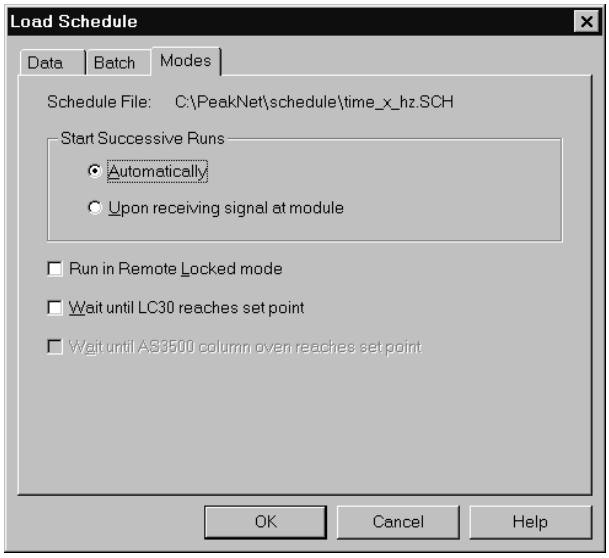


Select **Batch process data upon Schedule completion** to have the Batch program automatically started after the Schedule has run.

Settings File is the name of the batch settings file.

Use export file specified in settings file exports reprocessed data to the destination specified in the settings file. To select a different destination, click on **Export to file** and either type in the desired file name or click on the **Browse...** command button and specify a different file from the dialog box that appears.

Load Schedule - Modes Tab Page



Start Successive Runs determines how the next analysis in the Schedule is started:

Select **Automatically** (the default setting) to automatically start the timed events for the next Method as soon as the data reduction process from the preceding analysis is completed. The Run menu's Start command... will be enabled as soon as you click on OK and exit this dialog box. **This option is disabled when an AS3500 Schedule is loaded.**

Select **Upon receiving signal at module** to defer the start of the timed events from the next Method until the module receives a signal from the front panel or a remote device. For example, this enables the AS3500 to signal the module that the next sample has been loaded and injected and is ready for analysis.

Before selecting **Upon receiving signal at module**, review the following considerations:

- To remotely start all modules in a system, all RUN TTL INs must be wired correctly; otherwise, the Run program may never finish the run.
- When the system status is **Ended**, Run has to detect all of the modules in the system that have been changed to

RESET/HOLD before it can update the system status to **Waiting for external start**. Once this occurs, the system can be remotely started again.

- When the Method is started via an external signal, the system status will remain on **Ended** when data collection is complete. To remotely start the system again, you must RESET/HOLD all of the modules in the system by triggering the TTL input for RUN/HOLD. This will update the system status to **Waiting for external start**.
- If you select Direct Control for a module when the system status is **Waiting for external start** a message appears informing you that the run may not start correctly while the system is in Direct Control. If you choose OK to go to Direct Control mode, exit this mode before the next start signal occurs, or manually start the run at the appropriate time (for example, when the baseline is stable).
- If you are using Direct Control when the system status is **Waiting for external start**, click the Apply button to implement Direct Control commands. If you click OK or Cancel, the following message appears:

  "Because the system is waiting for an external start, exiting Direct Control will restore initial conditions."

  Selecting OK in the message box exits the Direct Control mode. Any current Direct Control settings are canceled and the initial conditions of the Method are restored. Selecting Cancel returns you to Direct Control and maintains the current Direct Control settings.

AS3500 Autosampler Schedules

The only start option for an AS3500 Schedule (*.AS3) is **Upon receiving signal at module**. You must start an AS3500 Schedule from the Run menu using the Start AS3500... command. (This replaces the usual Start... command when an AS3500 Schedule is loaded.) When you select Start AS3500..., the autosampler remotely starts the DX-500 modules.

NOTE When you select an *.AS3 Schedule, the Run program converts it, line by line, to an *.SCH Schedule before downloading it to the modules. This incremental conversion allows you to edit lines in the *.AS3 Schedule that have not yet run.

The conversion begins when Run creates a *.SCH file that includes the information from line #1 of the loaded *.AS3 file up to the line number specified in **Starting Line # for the Schedule** in the Load Schedule dialog box.

Although multiple injections per vial are listed on a single line in the *.AS3 Schedule file, they are listed on separate lines in the *.SCH file (i.e., a single line of information is “expanded” into multiple lines). For example, if line #1 specifies 3 injections per vial, Run creates three separate lines in the *.SCH file. Therefore, the number of lines in the *.SCH file equals the total number of injections in the run. The results of each injection are stored in a separate raw data file.

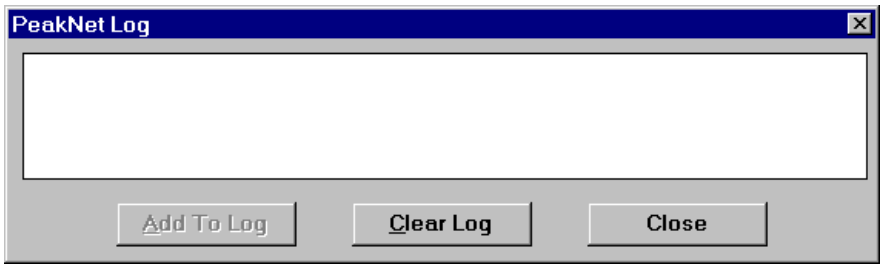
When Run reaches the end of the *.SCH file, it returns to the *.AS3 file and checks the next line. If there is only one injection, Run adds the line to the *.SCH file; if there is more than one injection, Run expands each injection into its own line in the *.SCH file. This series of events continues until the last line in the *.AS3 file is finished.

8.3.3 Save Method

Writes the current Method to disk under the current file name.

8.3.4 Edit Log...

Lets you add a comment to the PEAKNET.LOG file, or erase the contents of the file. PEAKNET.LOG is the file in which PeakNet records significant system events. For more information about event logging, refer to the PeakNet on-line Help program.



Type your comment (up to 128 characters) into the edit box. Click on **Add to Log** to write the comment into the PEAKNET.LOG file. The comment will be preceded by the date and time of the entry, along with the label "User Comment," as in this example:

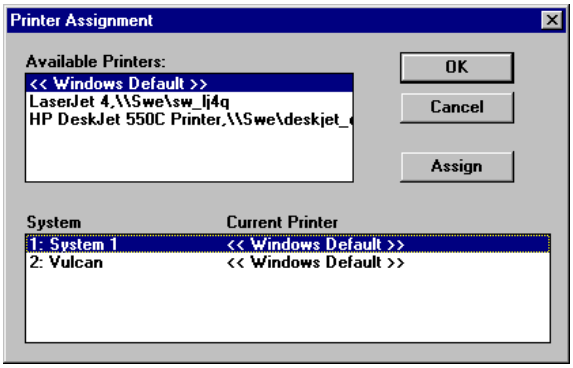
12/01/97 09:46:27 AM User Comment - Restarted system with new buffers.

Clear Log erases the contents of PEAKNET.LOG. This deletes all information except the header, which is always retained.

Click on **Close** to exit the dialog box.

8.3.5 Printers...

Lets you assign a specific printer to each configured instrument system, so that printouts from multiple systems are not interleaved.



To assign a printer to a system:

1. Select a **System** from the list box.
2. Select an **Available Printer** from the list box.
3. Click on **Assign**.
4. Repeat Steps 1-3 as needed.
5. When you finish, click on **OK** or press <Enter>.

8.3.6 Most Recently Used

Open one of the last four Method or Schedule files used by the currently active system by clicking on its name here.

8.3.7 Exit

Closes Run, after saving the loaded Method and any data that was collected. When Run is reopened, it will load the same version of the Method and restore the collected data.

NOTE Run uses the previously loaded Method even if you have edited the Method (using the Method Editor) since the last time Run was opened.

If you close Run while a Schedule is running, Run saves all the Schedule parameters ***unless*** an AS3500 Autosampler is configured. Because Run will not automatically reload an *.AS3 Schedule, you must reload it manually. Run will then start from the first injection.

8.4 Run Menu

8.4.1 Baseline

This command toggles the display of the baseline for all detectors in the Real-Time Plot area of the system window. The Baseline command is disabled while a Method or Schedule is running.

Once the Baseline command is selected, Run monitors the baseline continuously until one of the following occurs: you load a Method, start a loaded Method, or close the Run program. If baseline monitoring continues for more than 10 minutes, Run shifts the display forward so that only the most recent 10 minutes are visible.

To check baseline stability after a Method is loaded, select the Baseline command. The plot scale specified in the Method will be used. The time axis is fixed at 10 minutes and cannot be changed. The Y scale will be the same as the real-time plot scale in the Method.

NOTE Baseline data cannot be saved.

8.4.2 Start.../Start AS3500...

NOTE The Start... command is replaced by Start AS3500... when an AS3500 Schedule (*.AS3) is loaded. The Start... commands are enabled only after a Method has been loaded; once a run begins, they are disabled.

To start a run, click on the Start toolbar button (or select the menu command).

If you are starting a Schedule, a confirmation dialog box appears. Click OK or press <Enter> to start the run.

If you are starting a Method, the Start Method dialog box appears. The tab page controls are the same as those in the Load Method dialog box (see Section 8.3.1).

If it is not necessary to change any parameters in the Start Method dialog box, click on OK or press <Enter> to start a run. However, if you are running multiple samples with the same Method, you can use the Start Method dialog box to change the parameters for a sample(s) without reloading the Method.

The following series of events occurs during a run:

(a) The timed events for all modules begin to run, and Run displays the real-time status of each module in the Module Status Display area of the system window (see Section 8.7).

(b) As data collection begins, Run displays real-time plots in the Real-Time Plot area of the system window.

(c) At the completion of data collection and timed events for all modules, Run saves the raw data and prints any reports requested in the Method. The modules remain in the last timed event conditions for the Method.

(d) If a Schedule is running, Run loads the Method for the next injection and transfers it to the modules in the system.

NOTE You may open the Schedule Editor and view the updated file while a Schedule is running. However, do not save this file to the hard disk; doing so can overwrite updates to the Schedule file made by the Run program.

8.4.3 Modify...

Click on the Modify toolbar button (or select the menu command) to edit parameters for the Method that is currently loaded. The Modify Method dialog box contains the same controls as those in the Load Method dialog box previously described.

8.4.4 End...

Click on the End toolbar button (or select the menu command) to finish a run early and keep the data from the run.

End... terminates the running Method **and** the Schedule for all modules of the specified system. It quickly executes the last timed events and leaves the system operating under the conditions specified in the last timed event.

If the Method includes a print parameter, the result report for the analysis up to the point of interruption will be printed and the raw data saved.

The injection number displayed in the Control Bar will be incremented by one.

After using the End... command, restart a Schedule as follows:

- If no AS3500 Autosampler is configured, select the Start... command again. Run will restart from the current injection number.
- If an AS3500 Autosampler is configured, you must reload the Schedule because Run does not automatically reload *.AS3 Schedules. Run will restart from the line number specified in the Load Schedule dialog box.

8.4.5 Abort...

Click on the Abort toolbar button (or select the menu command) to finish a run early and discard the data.

Abort terminates execution of both the Method **and** Schedule for all modules of the specified system. Abort... quickly executes the last timed events and leaves the system operating under the conditions specified in the last timed events step.

Selecting Abort... does not change the injection number displayed in the Control Bar.

After using the Abort... command, restart a Schedule as follows:

- If no AS3500 Autosampler is configured, select the Start... command again. Run will restart from the current injection number.
- If an AS3500 Autosampler is configured, you must reload the Schedule because Run does not automatically reload *.AS3 Schedules. Run will restart from the line number specified in the Load Schedule dialog box.

8.4.6 Priority...

Lets you interrupt a currently running AS50 Autosampler Schedule (*.SAS) to run an unscheduled (priority) Method on a vial. A priority Method is treated as the next Method in the Schedule. This means that it is overlapped with the currently running Method; the priority Method's sample preparation sequence is completed while the current Method's timed events are being run. In addition, the next vial's Method is overlapped with the priority Method.

The Priority... command is enabled under certain conditions.

- The Priority... command is enabled only while an AS50 Schedule is running. When you select Priority... and begin running a priority Method, the command is disabled.
- The Priority... command is enabled once more when the priority Method has finished running, but before the Schedule has finished. This allows you to initiate priority Methods multiple times during a single Schedule run.

To run a priority Method:

1. Select the Priority... command.
2. The Open Method dialog box appears. Select the Method to be run and click OK.
3. The Modify Running Method dialog box appears. The parameters are the same as those in the Load Method dialog box, except the Modes tab page is not included.

4. Select the desired parameters.
5. Click OK to load the priority Method and start the run.

8.4.7 Direct Control

Click on the Direct Control toolbar button (or select the menu command) to activate Direct Control of module(s) in the system. See Section 8.8 for a description of each module's Direct Control parameters.

8.4.8 Method Control

To edit timed events for a module after a Method has started running, click on the module name from the cascade menu here, or click on the module's icon in the system window.

8.5 View Menu

8.5.1 Overlay

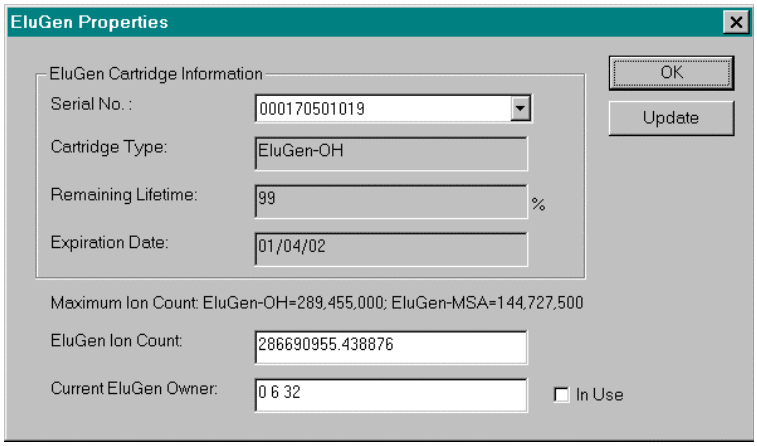
Displays the real-time plots on a single set of axes. Only the maximum value for each detector is displayed on the Y axis; the major Y-tick label is displayed. The longest run time will be displayed on the X axis.

A check mark before the Overlay command indicates that it is active; clicking on Overlay again deactivates it.

8.5.2 EluGen Properties

Displays information about all EluGen cartridges that have been configured in PeakNet. This menu item appears only if the current system includes an Eluent Generator.

NOTE Information about the cartridge currently being used by the EG40 also appears in the Module Status Display.



Serial Number is the unique 12-digit number that identifies each EluGen cartridge. When the dialog box opens, the list box displays the serial number of the cartridge in use by the EG40. To view properties for a different cartridge, select its serial number from the list box.

Cartridge Type indicates whether the cartridge is an EluGen-OH or EluGen-MSA.

Remaining Lifetime reports the number of ions remaining in the EluGen cartridge. The ion quantity is counted down in 1% increments. At 10%, Run displays a warning each time an EG40 Method or Schedule is loaded. After 0%, Run can no longer load an EG40 Method or Schedule until the cartridge is replaced.

Expiration Date is the date on which the EluGen cartridge will expire. One month before expiration, Run displays a warning each time an EG40 Method is loaded. On the expiration date, Run displays a message that the cartridge has expired. Although PeakNet allows the use of an expired cartridge, performance will be impaired until a new cartridge is installed.

EluGen Ion Count displays the cartridges latest ion count.

Current EluGen Owner is the unique ID of the EG40 module that currently owns the cartridge.

In Use is selected when the EG40 module is using the EluGen cartridge. This occurs between the time a method or sequence is loaded and the method or sequence is finished running. If you selects a cartridge via direct control, the cartridge is in use until you choose another cartridge

8.5.3 Toolbar

Shows or hides the toolbar.

8.5.4 Status Bar

Shows or hides the status bar.

8.5.5 Confirmations

Shows or hides the dialog boxes which confirm start, end, and abort operations.

8.5.6 MainMenu

Click on the MainMenu toolbar button (or select the menu command) to display the PeakNet MainMenu.

8.6 Window Menu

8.6.1 Monitor

Open a child window for monitoring the instrument(s) attached to the system selected from this list.

Each time you open Run, it checks the PEAKNET.CFG file for all configured systems and then lists the system names and numbers on the Window menu. If a system is open, its menu listing is disabled. If a system is closed, its menu listing is enabled; to open the system, click on the menu listing.

8.6.2 Tile Horizontally

Resizes and positions all open windows horizontally (one above another) so that each is fully visible.

8.6.3 Tile Vertically

Resizes and positions all open windows vertically (side-by-side) so that each is fully visible.

8.6.4 Cascade

Arranges windows in an overlapping fashion so that each title bar is visible.

8.6.5 Arrange Icons

Automatically arranges icons neatly at the bottom of the screen.

8.6.6 Open Windows List

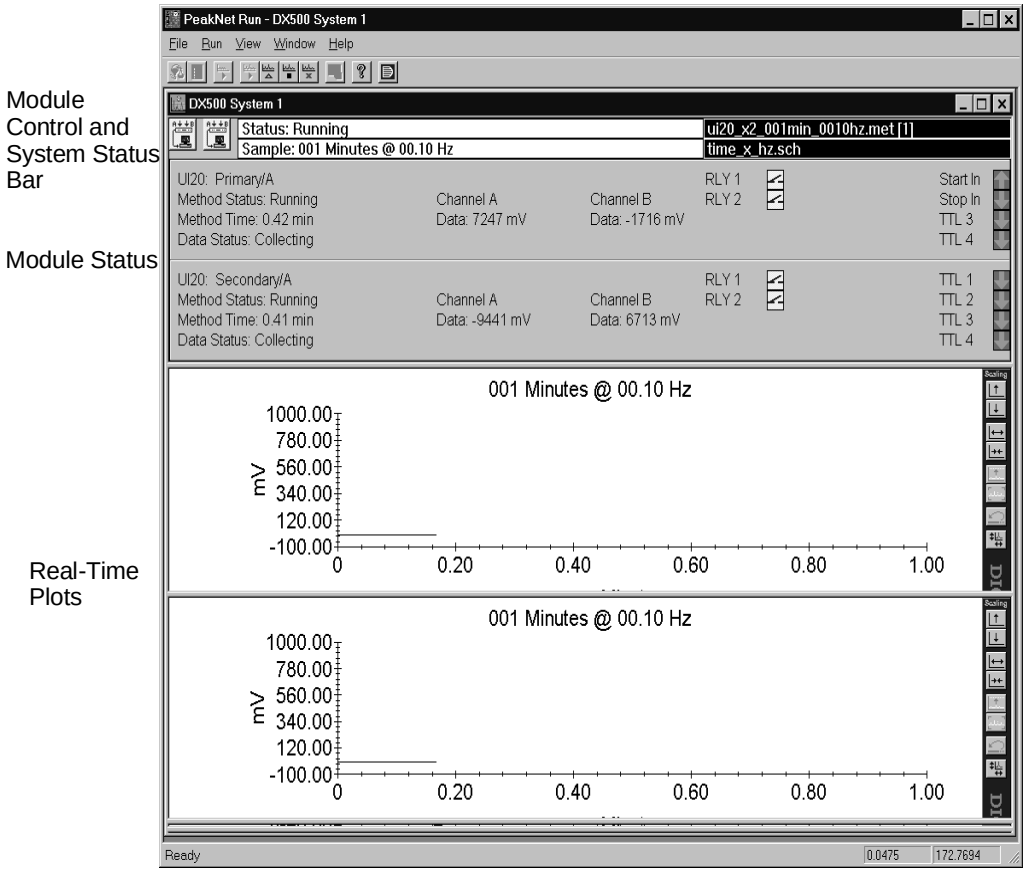
Makes an open window active when its name is selected from this list.

8.7 The System Window

Each time the Run program is loaded, it checks the PEAKNET.CFG file for all configured systems and then opens an individual window for each system detected on the DX-LAN network. The system name assigned in the Configuration Editor appears in the title bar of each system window.

A system window consists of three main areas:

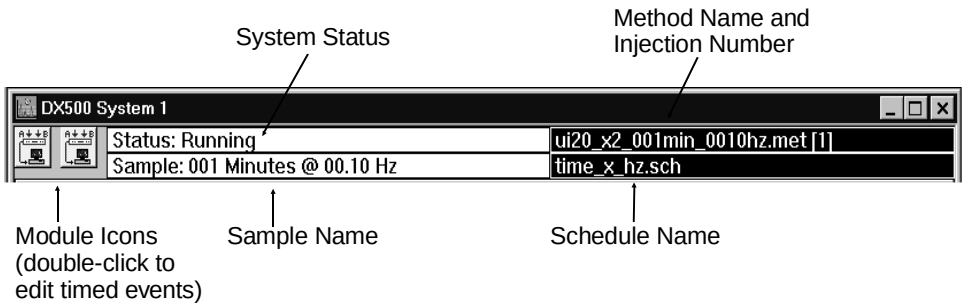
- Module Control and System Status Bar
- Module Status Display
- Detector Real-Time Plot(s)



Run also attempts to communicate with each module listed as installed in the PEAKNET.CFG file; if a module responds, its icon is displayed in the

Run system window. Run updates the status of all modules every 5 seconds. If a module does not respond (usually because it was powered down), its icon is not displayed.

8.7.1 The Module Control and System Status Bar



Before any Methods have been loaded, the Control Bar displays icons for all the active modules defined in the system configuration. After a Method has been loaded, Run will rearrange the icons to match their order of definition in the Method. If a particular module is not defined in the Method, its icon is not displayed.

NOTE The UI20 Universal Interface is represented by only one icon, even if both UI20 channels are configured.

Double-click a module's icon to edit the timed events for the module.

The center of the Control Bar displays the system status and the name of the sample being run.

The system status may be any of the following:

- **Not Loaded**—A Method has not yet been loaded.
- **Ready—**A Method is loaded and the system is ready to begin running when you click on the Start toolbar button (or select the command from the Run menu.
- **Waiting for external start**—The remote start option has been selected. A Method is loaded, but the system waits for an external signal before starting the modules.

- **Running**—The system has been started and a Method is running.

Ended—All modules in the system have finished running the Method and collecting data, and the data has been processed.

The right side of the Control Bar displays the Method name, if a Method has been loaded, followed by the injection number in brackets. If a Schedule has been loaded, its name appears below this.

8.7.2 The Module Status Display

The Module Status Display provides an overview of the status of all active modules. Before a Method is loaded, this area shows the status of *all* configured and detected modules. After a Method is loaded, it shows the status of only those modules defined in the Method.

All information obtainable from a module's front panel is presented in the Module Status Display: settings for flow rate, pressure limits, detection mode, etc. Most information appears as text, but graphics indicate the status of the TTL inputs, the relay contact closures, and the absorbance detector lamp.

There are two ways to adjust the viewing area:

- Position the cursor on top of the splitter bar between the Module Status Display and the Real-Time Plot. The cursor will change to a resizing cursor with an up-down arrow. Press and hold the mouse button and drag the splitter bar up or down to change the size of the viewing area.
- Use the vertical scroll bar on the right side of the Module Status Display.

Module Method Status The possible conditions for DX-500 modules are listed below.

- **Not Loaded**—The Run program is communicating with the system, but no Method is currently loaded.
- **Holding**—A Method is currently loaded, but timed events have not started. TTL and relay outputs are set to the initial conditions for the timed events in the current Method.

- **Running—**Timed events and/or data acquisition are in progress. TTL and relay outputs are controlled by the timed events in the current Method.
- **Ended—**Timed events and/or data acquisition are complete, but Run is still collecting and processing data for all modules in the system. TTL and relay outputs are set to the End conditions for the timed events in the current Method.
- **WAITING FOR EXTERNAL START**—A Method has been loaded to all modules in a system with an AS3500 Autosampler and the system is ready to be started via a remote signal.

Operational states for the DX-120 Ion Chromatograph and UI20 Universal Interface are as follows:

- **Not Loaded**—The module has been powered up but no Method has been loaded. (If you select the Clear All option in the UI20 diagnostics, the UI20 returns to the Not Loaded state.)
- **Ready—**A Method is loaded, but has not started running. TTL and relay outputs are set to the initial conditions. The Wait TTL input can be asserted.
- **Waiting**—(UI20 only) A Run command or input has been received and the Wait TTL input is enabled and asserted. TTL and relay outputs are at the initial conditions.
- **Running**—Timed events and/or data acquisition are in progress. TTL and relay outputs are controlled by the timed events in the current Method.
- **Ended**—Timed events and data acquisition are completed, but the Run program has not finished collecting and processing data for all of the modules in the system. TTL and relay outputs are set to the End conditions for the timed events in the current Method.
- **Done**—The Run program has uploaded and processed data for all of the modules, or else the Method has been aborted and the data has been discarded. The UI20 can accept a Run signal as either a TTL input or button event. TTL and relay outputs are set to the End conditions for the timed events in the current Method. A Run command will cause the UI20 to set the output to the initial conditions and begin Method execution.

- **Direct Control**—Run is directly controlling the UI20 TTLs, relay outputs, and voltage range. Run must download a Method to the UI20 before Direct Control is enabled.

Method Time indicates the elapsed time since the Method began running.

8.7.3 The Real-Time Plot

The Real-Time Plot area is blank until a Method is loaded. After a Method is loaded, a detector window containing a graph appears and, as data collection progresses, data is drawn on the graph.

The Real-Time Plot can simultaneously display up to four detector signals. Each detector window is labeled with the X axis and Y axis, the detector name in the upper right corner, and the appropriate unit of measurement in the upper left corner. If the Gradient Overlay option is selected, the eluent names are listed along the right side of the window.

The Scaling Toolbox at the right of each plot allows you to zoom in or out of portions of the plot.

To adjust other plot features, double-click anywhere on the plot to open the Plot dialog box.

NOTE For details about the Scaling Toolbox and the Plot dialog box, see Chapter 11.

8.8 Direct Control

With Direct Control, you can issue instantaneous commands from the computer to a module and have each command carried out immediately, if desired, or you can enter parameters for one or more modules and, when ready, issue a single command to begin carrying out commands for these modules. Any Method currently being run by the module must be ended or aborted before you select Direct Control.

Direct Control parameters are set from the tab page for each module. There are two ways to display a tab page:

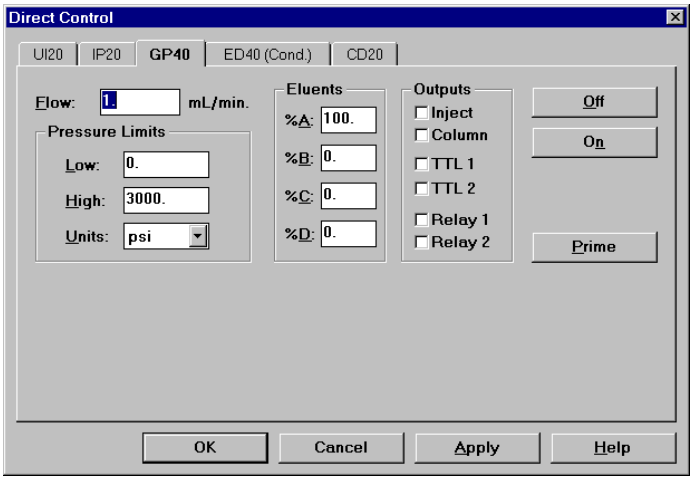
- Click on the Direct Control toolbar button.
- Select the Direct Control command from the Run menu.

Run will display the last active page, unless the program has been closed. If necessary, click on the tab for a different module. Change the controls for the module as desired, then select the tab page for other modules as required.

PeakNet supports Direct Control for the instruments listed below. For more information about operating parameters, refer to the user's manual for each instrument.

- GP40 Gradient Pump
- GP50 Gradient Pump
- IP20 Isocratic Pump
- IP25 Isocratic Pump
- EG40 Eluent Generator
- AD20 Absorbance Detector
- AD25 Absorbance Detector
- CD20 Conductivity Detector
- ED40 Electrochemical Detector
- UI20 Universal Interface
- DX-120 Ion Chromatograph
- IC20 Ion Chromatograph
- AS50 Autosampler

8.8.1 GP40 Direct Control



Flow Enter 0, a flow rate of 0.04 to 10.00 mL/min for a pump with standard heads, or 0.10 to 2.50 mL/min for the microbore version.

Pressure Limits Enter the Low and High pressure limits in the edit boxes. Click on the adjacent drop-down list box to select the Units (psi, MPa, or bar). The pressure limit ranges are 0 to 5000 psi, 0 to 34.02 MPa, and 0 to 340.20 bar.

Enter the eluent percentages in the **%A**, **%B**, **%C**, and **%D** edit boxes. The total of all eluents must equal 100% before you can enter a set of Direct Control conditions.

The **Outputs** group box lists the TTL and relay outputs. Click on the appropriate check box to turn a TTL or relay output on or off.

Off turns off the pump, **On** turns on the pump, and **Prime** primes the pump.

Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

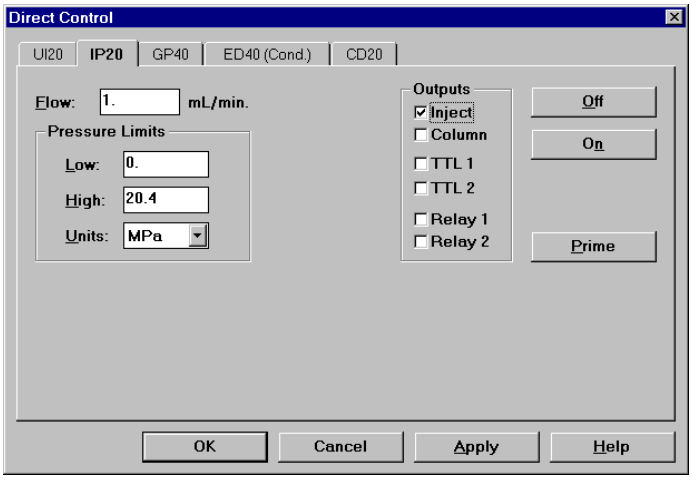
Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.2 GP50 Direct Control

Controls in the GP50 Direct Control dialog box are identical to those for the GP40; refer to the preceding section for a description.

8.8.3 IP20 Direct Control



Flow Enter 0, a flow rate of 0.04 to 10.00 mL/min for a pump with standard heads, or 0.10 to 2.50 mL/min for the microbore version.

Pressure Limits Enter the Low and High pressure limits in the edit boxes. Click on the adjacent drop-down list box to select the Units (psi, MPa, or bar). The pressure limit ranges are 0 to 5000 psi, 0 to 34.02 MPa, and 0 to 340.20 bar.

The **Outputs** group box lists the TTL and relay outputs. Click on the appropriate check box to turn a TTL or relay output on or off.

Off turns off the pump, **On** turns on the pump, and **Prime** primes the pump.

Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

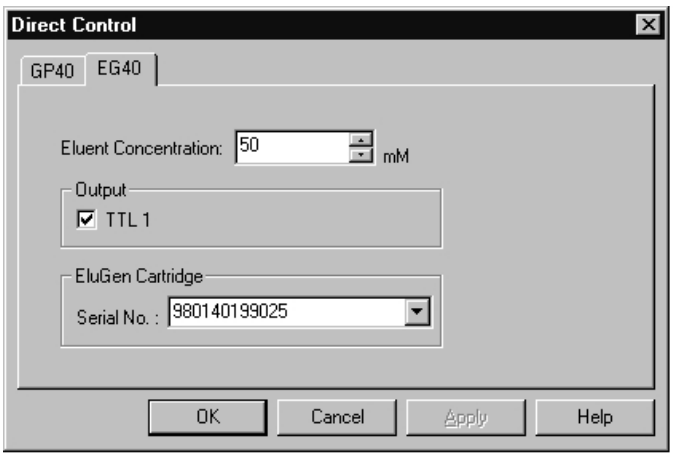
Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.4 IP25 Direct Control

Controls in the IP25 Direct Control dialog box are identical to those for the IP20; refer to the preceding section for a description.

8.8.5 EG40 Direct Control



Eluent Concentration Select a concentration of 0.10 to 100 mm. If the pump flow rate is more than 3 mL/min or less than 0.1 mL/min, Run will set the eluent concentration to zero. After setting the flow rate to within the proper range, reset the eluent concentration.

The **Output** group box lists the TTL output. Click on the check box to turn the output on or off. Unless you created a custom label in the Method Editor, the TTL is listed here by number.

EluGen Cartridge indicates the serial number of the cartridge in use by the EG40. To view the serial number for a different cartridge, select the number from the list box.

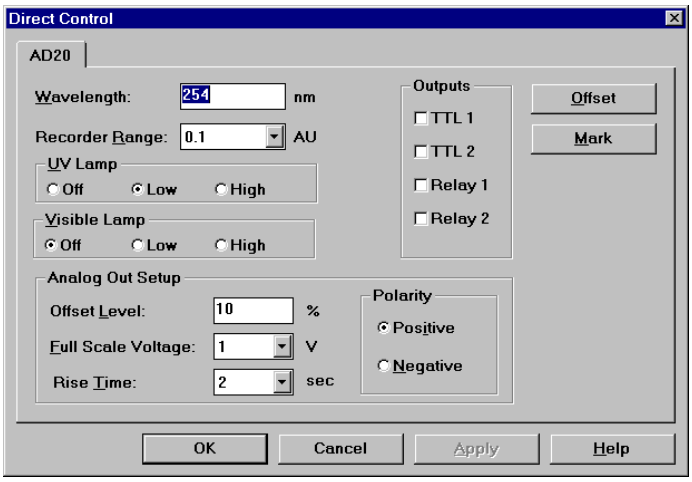
Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.6 AD20 Direct Control



Wavelength Enter a wavelength of 190 to 380 nm for the UV lamp, or 381 to 800 nm for the Vis lamp.

Recorder Range If the detector's recorder output is being used, select the desired full-scale range. The limits are 0.02 and 2.0 AU.

Set **UV Lamp** or **Vis Lamp** to Off, Low, or High by clicking on the corresponding option button.

The **Outputs** group box lists the TTL and relay outputs. Click on the appropriate check box to turn a TTL or relay output on or off.

Offset Level Enter a value of from 0 to 100% in the edit box.

Full-Scale Voltage Select a recorder full-scale voltage of 0.01, 0.1, or 1.0 volt from the list box.

Rise Time Select a filter rise time of 0.05 to 10.0 seconds from the list box.

Set the **Polarity** to positive or negative by clicking on the corresponding option button.

Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

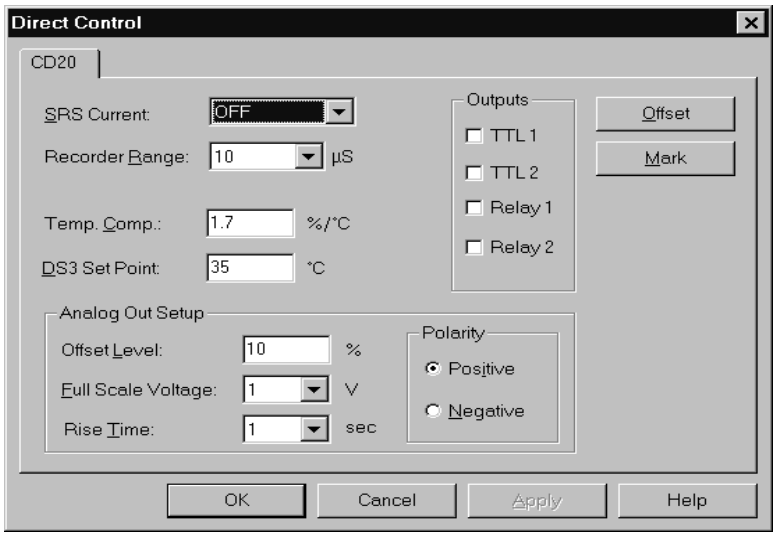
Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.7 AD25 Direct Control

Controls in the AD25 Direct Control dialog box are identical to those for the AD20, except that the lamp controls are Off and On only; refer to the preceding section for a description

8.8.8 CD20 Direct Control



SRS Current selects the Self-Regenerating Suppressor current.

Recorder Range If the detector's analog recorder output is being used, select a full-scale range between 0.01 and 3000 µS from the drop-down list box.

Temp. Comp. Enter a temperature compensation value of 0.0 to 3.0 %/°C in the edit box.

DS3 Set Point (available only when a DS3 is connected to the system) selects the temperature set point for the DS3.

Oven Temp (available only when an LC25 oven is connected to the system) selects the temperature for the LC25 oven.

The **Outputs** group box lists the TTL and relay outputs. Click on the appropriate check box to turn a TTL or relay output on or off.

Offset Level Enter a value of from 0 to 100% in the edit box.

Full-Scale Voltage Select a recorder full-scale voltage of 0.01, 0.1, or 1.0 volt from the list box.

Rise Time Select a filter rise time of 0.05 to 10.0 seconds from the list box.

Set the **Polarity** to positive or negative by clicking on the corresponding option button.

Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

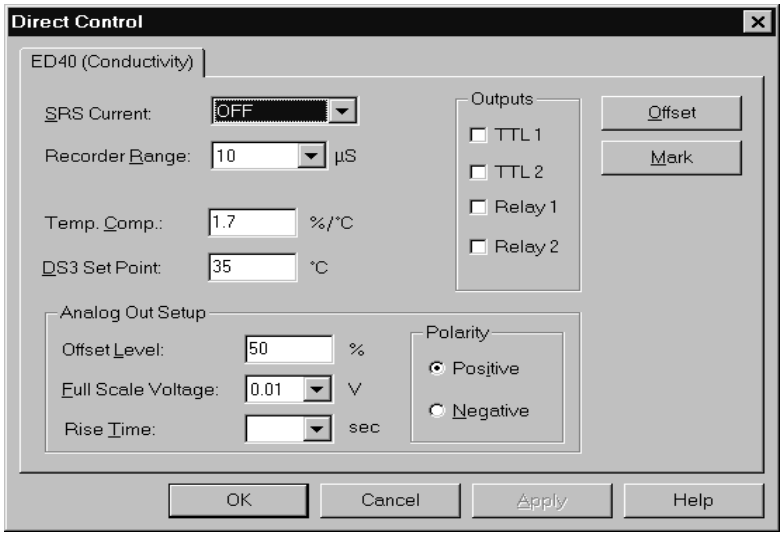
Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

ED40 Direct Control

There are three ED40 Direct Control tab pages, since each detection mode requires different controls. After checking the Method for the selected detection mode, Run automatically displays the correct Direct Control tab page. If no Method has been loaded yet, Run checks for the operating mode selected from the ED40 front panel and then displays the correct tab page.

8.8.9 ED40 (Conductivity) Direct Control



SRS Current selects the Self-Regenerating Suppressor current.

Recorder Range If the detector's analog recorder output is being used, select a full-scale range between 0.01 and 3000 µS from the drop-down list box.

Temp. Comp. Enter a temperature compensation value of 0.0 to 3.0 %/°C in the edit box.

DS3 Set Point (available only when a DS3 is connected to the system) selects the temperature set point for the DS3.

Oven Temp (available only when an LC25 oven is connected to the system) selects the temperature for the LC25 oven.

The **Outputs** group box lists the TTL and relay outputs. Click on the appropriate check box to turn a TTL or relay output on or off.

Offset Level Enter a value of from 0 to 100% in the edit box.

Full-Scale Voltage Select a recorder full-scale voltage of 0.01, 0.1, or 1.0 volt from the list box.

Rise Time Select a filter rise time of 0.05 to 10.0 seconds from the list box.

Set the **Polarity** to positive or negative by clicking on the corresponding option button.

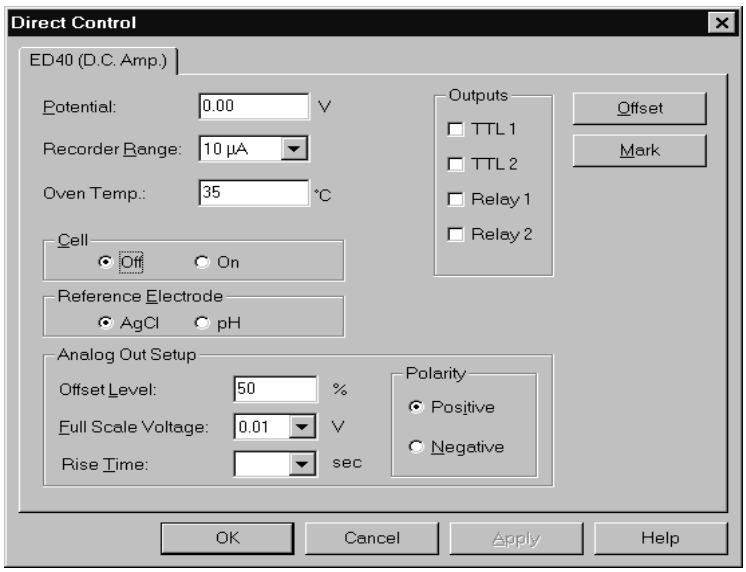
Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.10 ED40 (D.C. Amp.) Direct Control



Potential Enter the voltage (-2.04 to +2.04 volts) to apply to the cell.

Recorder Range If the analog recorder output of the detector is being used, select a full-scale range of 0.05 to 300 µA from the drop-down list box.

Oven Temp (available only when an LC25 oven is connected to the system) selects the temperature for the LC25 oven.

Turn the **Cell Off** or **On** by clicking on the corresponding option button. The cell must be On before data collection can begin.

Reference Electrode Select the AgCl or pH electrode by clicking on the corresponding option button.

The **Outputs** group box lists the TTL and relay outputs. Click on the appropriate check box to turn a TTL or relay output on or off.

Offset Level Enter a value of from 0 to 100% in the edit box.

Full-Scale Voltage Select a recorder full-scale voltage of 0.01, 0.1, or 1.0 volt from the list box.

Rise Time Select a filter rise time of 0.05 to 10.0 seconds from the list box.

Set the **Polarity** to positive or negative by clicking on the corresponding option button.

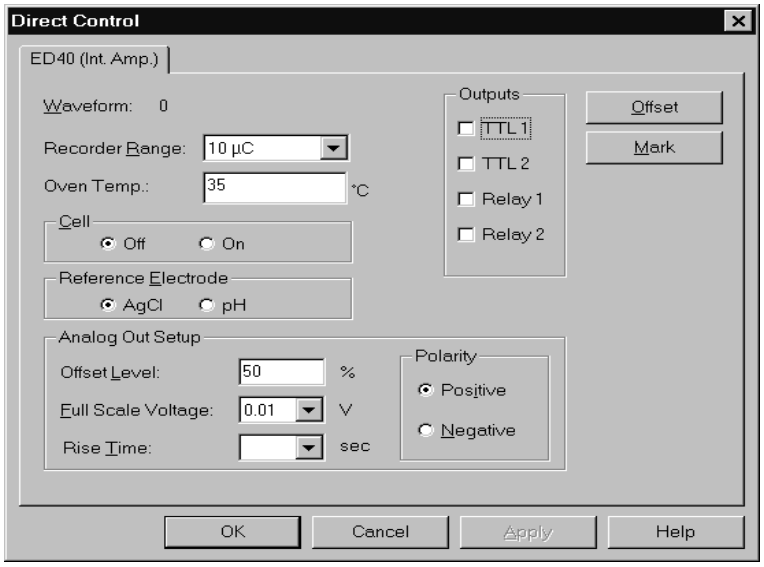
Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.11 ED40 (Int. Amp.) Direct Control



Waveform The waveform setting is zero and cannot be edited. Waveform can only be changed by downloading a new Method.

Recorder Range If the analog recorder output of the detector is being used, select a full-scale range between 50 pC and 200 µC from the drop-down list box.

Oven Temp (available only when an LC25 oven is connected to the system) selects the temperature for the LC25 oven.

Turn the **Cell Off** or **On** by clicking on the corresponding option button. The cell must be On before data collection can begin.

Reference Electrode Select the AgCl or pH electrode by clicking on the corresponding option button.

The **Outputs** group box lists the TTL and relay outputs. Click on the appropriate check box to turn a TTL or relay output on or off.

Offset Level Enter a value of from 0 to 100% in the edit box.

Full-Scale Voltage Select a recorder full-scale voltage of 0.01, 0.1, or 1.0 volt from the list box.

Rise Time Select a filter rise time of 0.05 to 10.0 seconds from the list box.

Set the **Polarity** to positive or negative by clicking on the corresponding option button.

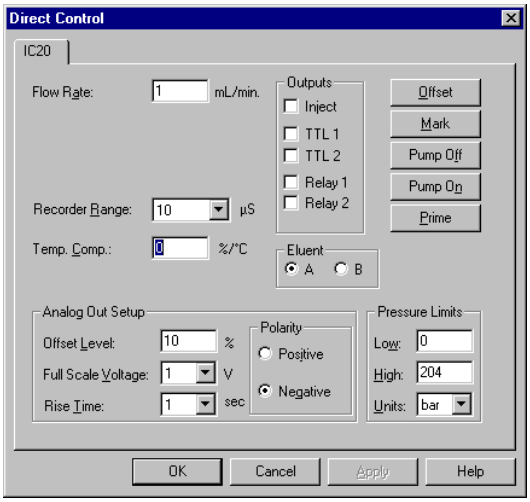
Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.12 IC20 Direct Control



Flow Rate Enter 0, a flow rate of 0.04 to 10.00 mL/min for a pump with standard bore heads, or 0.10 to 2.50 mL/min for the microbore version.

The **Outputs** group box lists the TTL and relay outputs. Click on the appropriate check box to turn a TTL or relay output on or off.

Recorder Range If the detector's recorder output is being used, select the desired full-scale range. The limits are 0.01 and 3000 AU.

Temp. Comp. Enter a temperature compensation value of 0.0 to 3.0 %/°C in the edit box.

Eluent selects eluent A or B.

Offset Level Enter a value of from 0 to 100% in the edit box.

Full-Scale Voltage Select a recorder full-scale voltage of 0.01, 0.1, or 1.0 volt from the list box.

Rise Time Select a filter rise time of 0.05 to 10.0 seconds from the list box.

Set the **Polarity** to positive or negative by clicking on the corresponding option button.

Pressure Limits Enter the Low and High pressure limits in the edit boxes. Click on the adjacent drop-down list box to select the Units

(psi, MPa, or bar). The pressure limit ranges are 0 to 5000 psi, 0 to 34.4 MPa, and 0 to 344.7 bar.

Pump Off turns off the pump, **Pump On** turns on the pump, and **Prime** primes the pump.

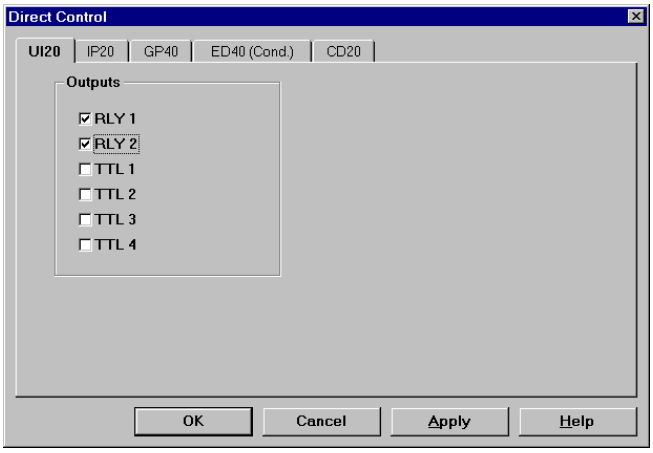
Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.13 UI20 Direct Control



NOTE Run must download a Method to the UI20 Universal Interface before the Direct Control mode of operation is enabled.

Outputs lists the relay and TTL outputs. Click on the appropriate check box to turn a relay or TTL output on or off. Relays and TTLs are listed by number unless you created custom labels in the Method Editor. This example tab page displays custom labels for Relay 1, Relay 2, and TTL1.

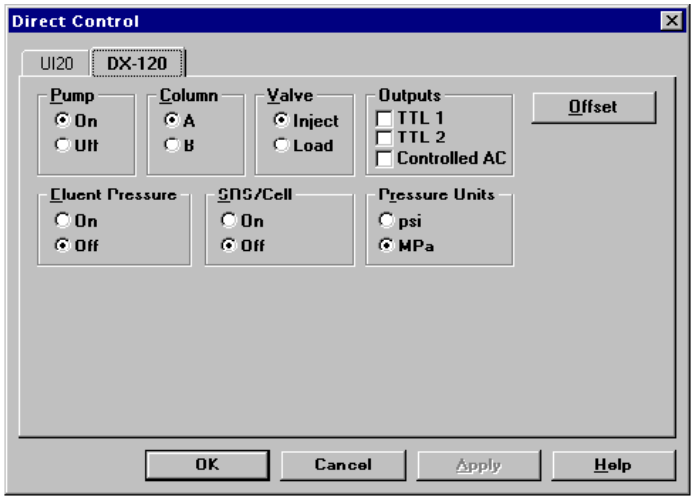
Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.14 DX-120 Direct Control



Pump turns the pump on or off. Turning off the pump deletes the timed events list, turns off the SRS, and disables the SRS/Cell and Column/Eluent controls.

NOTE The next section contains either Column or Eluent controls, depending on which System Mode is selected in the DX-120 Setup dialog box. The Column/Eluent controls are disabled if the DX-120 is in rinse mode when the Direct Control dialog box is opened.

Column selects column A or B. (The Column controls are enabled only for the dual-column DX-120.)

Eluent selects eluent A or B.

Valve selects the inject or load position for the injection valve.

Eluent Pressure turns the eluent reservoir pressure on or off.

SRS/Cell turns the SRS on or off. (These controls are disabled if an SRS is not connected to the currently-selected column when this dialog box is opened.)

Pressure Units selects psi or MPa for the pump pressure shown on the Run program status display and the DX-120 front panel.

Outputs lists the two TTL outputs and the controlled AC outlet. Click on the appropriate check box to turn an output on or off. Unless you created custom labels in the Method Editor, the outputs are listed here by number.

Offset offsets the current detector value to zero.

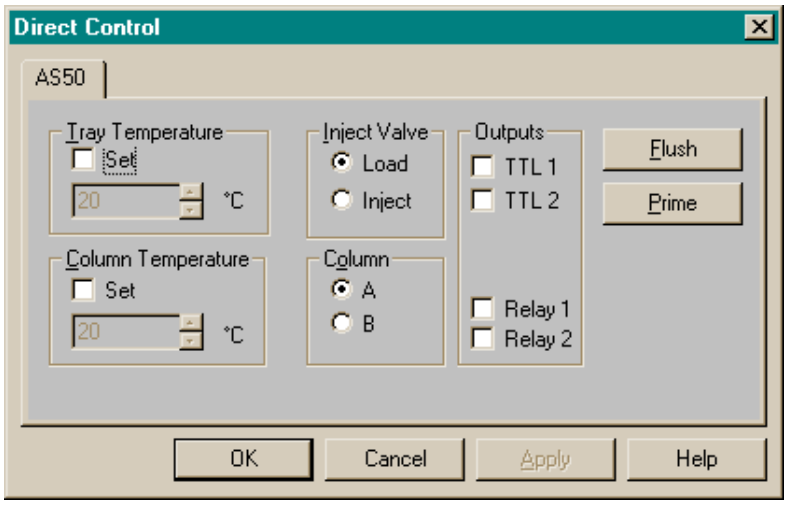
Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

8.8.15 AS50 Direct Control



Tray Temperature controls the sample tray temperature, if the AS50 Sample Tray Temperature Control option is installed.

Click the **Set** check box to turn the control on and off. Select a temperature of 0 to 60 °C from the list box.

Column Temperature sets the temperature in the thermal compartment, if the AS50 Column Temperature Control option is installed.

Click the **Set** check box to turn the control on and off. Select a temperature between 10 and 80 °C (heat/cool) or between 20 and 99 °C (heat only) from the list box.

Inject Valve sets the injection valve to the inject or load position.

Column selects column A or B.

Outputs lists the two TTL and relay outputs. Click on the appropriate check box to turn an output on or off. Unless you created custom labels in the Method Editor, the outputs are listed here by number.

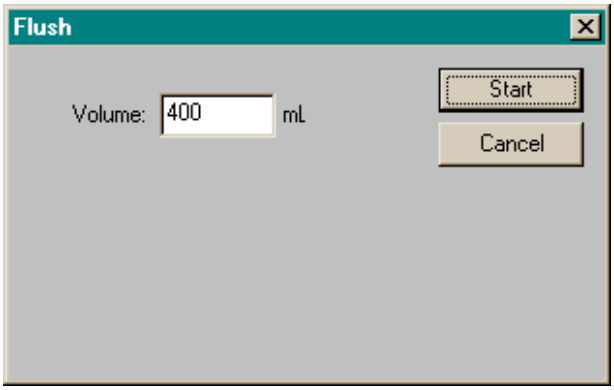
Click on **OK** to send the commands to the module and close the dialog box.

Click on **Cancel** to abandon the editing changes.

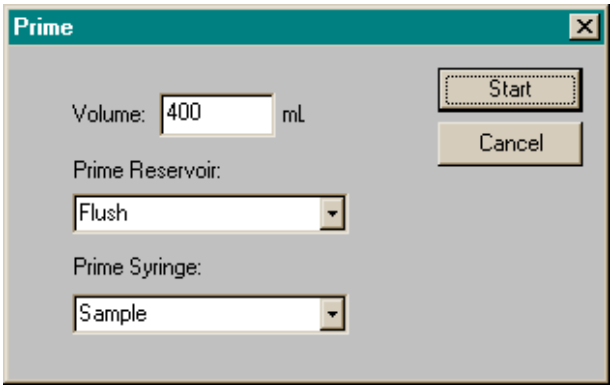
Click on **Apply** to send the commands to the module, leaving the dialog box open.

Click on **Help** to access the PeakNet on-line Help.

Flush opens the following dialog box. Specify the volume of fluid (100 to 5000 µL) that will be taken from the flush reservoir to flush the inject port. Click the **Start** button to begin the operation.



Prime opens the following dialog box, where you specify the parameters for priming the sample and reagent lines.



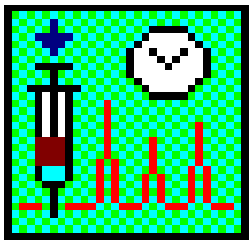
Volume specifies the volume of fluid (100 to 5000 µL) that is used to prime the lines.

Prime Reservoir selects the reservoir (Flush, A, B, C, or D) that is the source. Unless the AS50 Sample Preparation option is installed, the selected reservoir is always Flush.

Prime Syringe selects the syringe (Sample or Prep) that is used. Unless the AS50 Sample Preparation option is installed, the selected syringe is always Sample.

Click the **Start** button to initiate priming. The needle is moved to the wash port and the specified volume of liquid is dispensed. The inject port is not flushed during priming.

9 • The ACI Run Program



NOTE **ACI Run is used exclusively with ACI-based systems. DX-LAN systems use the Run program described in Chapter 8.**

The ACI Run program conducts the analyses specified in ACI Methods and/or Schedules. It loads data acquisition and control instructions into the Advanced Computer Interfaces(s), monitors the status of each system, and processes chromatograms according to the data processing parameters of the ACI Method.

The initial (INIT) conditions in the timed events sub-file of the ACI Method take effect as soon as the Method is loaded into ACI memory. If a gradient program file is loaded to the gradient pump, the program is copied into the pump's run memory. If the initial conditions include an instruction to start the pump motor, the pump begins operating according to the time zero step of the gradient program. Initial conditions remain in effect until the analysis begins, allowing the system time to stabilize.

You can start an analysis via the Start command in the ACI Run program, the RUN button on the ACI front panel, or the RUN input on the ACI rear panel. The ACI timed events clock starts when the analysis starts. Data collection begins when the Start Sampling event occurs.

Raw data from the detectors is stored in ACI memory until retrieved by the computer. The computer uses the data processing parameters set in the ACI Method to process the raw data, store it on disk, and prepare a report of the results.

A Schedule not only allows unattended analysis of multiple samples, but makes it possible to analyze each injection using a different Method and sample name, if desired. When a Schedule is run, only one line at a time is downloaded to the interface. After each line is run, the ACI Run program automatically loads the next line. The raw data used for each sample, as well as a copy of all Method parameters, are stored under the data filename specified in the Schedule.

9.1 Considerations When Using a Gradient Pump

Although you can load gradient programs into the gradient pump while it is in either LOCAL or REMOTE mode, Dionex recommends doing so only in REMOTE. If you load a program while the pump is in LOCAL, the initial control conditions are not executed.

NOTE You must switch to REMOTE before issuing a Start command from the ACI Run program.

The gradient pump operates according to the parameters it used while in LOCAL until you issue the Start command; only then do timed events commands from the interface control the pump. Under these conditions, the INIT step of the Timed Events sub-file must include instructions to start the pump, reset the gradient clock, and hold. One step to hold the gradient clock at initial condition and a second step to run the gradient clock at Time = 0.0 must be included to copy the gradient program into the pump's run memory, where it controls the gradient.

9.2 Starting the ACI Run Program

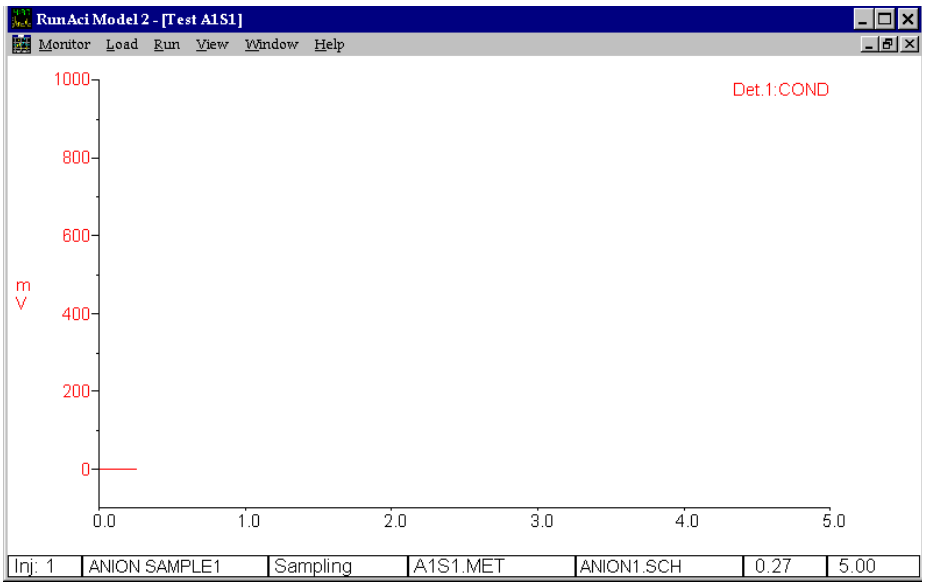
To open the main window of the ACI Run program, click on the RunACI button in the PeakNet MainMenu or double-click on RUNACI.EXE in the directory that holds your PeakNet files.

9.2.1 System Child Windows

The ACI Run program can monitor multiple systems simultaneously. Each active system has a separate child window, with the system name in the title bar. When an ACI starts collecting data, the real-time chromatogram appears in the window and the system status is indicated in the status bar at the bottom of the window. To set the focus to a particular child window, click on the window.

Injection Number indicates which Schedule line or injection is running. If a Schedule is not in use, Inj indicates the number of times the same Method has run since it was last downloaded.

Sample Name displays the name associated with the sample currently running. The sample name can be changed through the Load Method... or Load Schedule... commands on the Load menu.



Injection Number | Sample Run | ACI Status | Method Name | Schedule Name | Elapsed Time | Run Time

ACI Status indicates the status of each system:

MESSAGE	STATUS
NO ACI	No powered-up ACI is connected.
NOT LOADED	The ACI/System is not currently programmed with a Method.
READY	The ACI/System has been programmed with a Method and is ready to begin an analysis.
RUNNING T.E.	The ACI has started executing the timed events in the Method, but is not yet collecting data.
SAMPLING	Data is being collected from the designated system; the partial chromatogram can be uploaded to the computer.
ACQ.DONE	Data collection is finished; the complete chromatogram is stored in ACI memory and is ready for processing and storage by the computer.
ALARM ON	A pressure limit alarm has stopped the pump. After clearing, the alarm status will change to READY. The Method can then be rerun, or a new one downloaded.

ACI FULL	ACI memory is full; no raw data has been uploaded by the computer. The ACI stopped collecting data before the end of the run time specified in the Method.
WRAPPED	ACI memory is full; raw data from the beginning of the chromatogram has been uploaded and the memory used for the early part of the chromatogram is being overwritten.

WARNING If the WRAPPED message appears, do not close the child window; doing so will cause data to be lost.

Method Name indicates the ACI Method in use.

Schedule Name indicates the Schedule in use, if any.

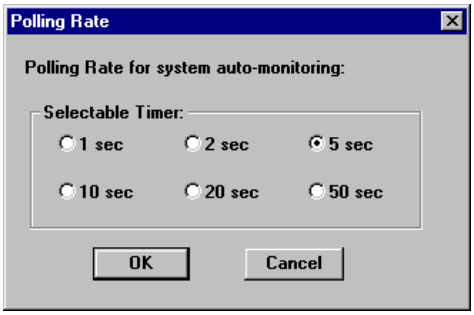
Elapsed Time indicates how much time has elapsed since the beginning of data collection.

ACI Run Time indicates for how long the current ACI Method will collect data. This time is specified by the Run Time parameter in the Method.

9.3 Monitor Menu

9.3.1 Polling Rate...

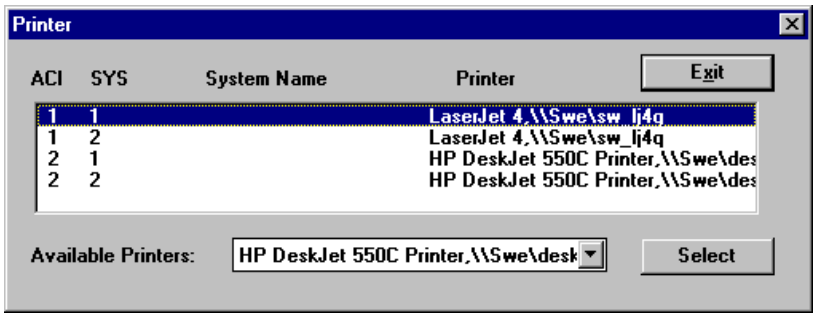
The polling rate determines how often the computer checks the ACI status and retrieves data. The selected polling rate applies to all systems. The polling rate is saved in the AI450.INI file, so the rate last selected will still be in effect the next time ACI Run is started.



For smooth plotting while you are watching real-time plots, select a fast rate (short interval). For minimal delays while using other programs, select a slow rate (long interval).

9.3.2 Printer...

Each system of an ACI can be assigned to a different printer, if more than one printer is installed. The default printer (the printer installed in Windows Control Panel) is listed first in the Available Printers drop-down combo box.



Click on the **ACI/System** name (highlighting it), the desired printer name in the Available Printers drop-down list box, and then on **Select**.

When you finish assigning printers, click on **Exit** to close the dialog box.

9.3.3 Close

Closes the highlighted system window and system. Any plot information on-screen at the time is lost, and polling stops for that system. The interface, however, will continue to run the analysis and collect data.

9.3.4 Exit

Closes the ACI Run program.

9.4 Load Menu

Before selecting a Load menu command, verify that all connections between the chromatograph components and the ACI are complete. Also verify that the ACI is powered-up and is connected to the computer. If you want the initial conditions to control the system during equilibration, set all modules to REMOTE.

NOTE The system status must be either NOT LOADED or READY before a Method or Schedule can be loaded.

9.4.1 Load Method...

Displays a Windows common Open dialog box from which you specify the path and filename of the ACI Method to use for the selected system.

The Method file will be retrieved from disk and loaded into the ACI. If the Method includes a gradient, the gradient program will be loaded into the gradient pump.

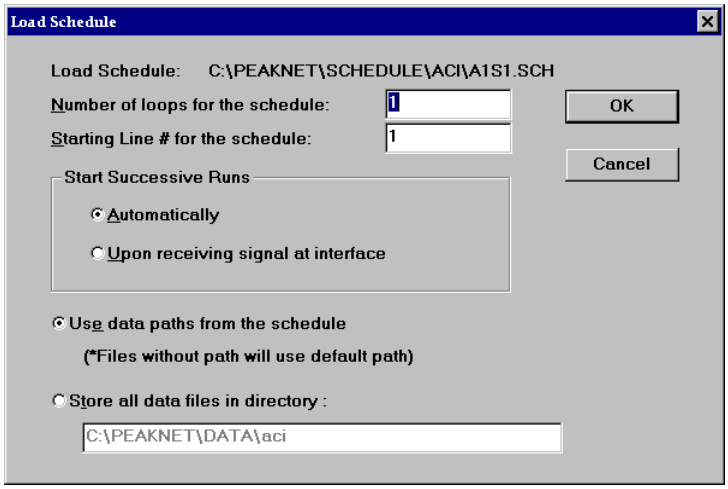
9.4.2 Load Schedule...

Opens a Windows common Open dialog box, from which you select a Schedule to use to analyze a series of samples. There are two types of Schedule files: .SCH files for systems with no autosampler and *.AS3 files for systems on which an AS3500 Autosampler is configured.

Before the Schedule is loaded, another dialog box will prompt you for these Schedule conditions:

Number of loops for the Schedule is the number of times the Schedule is repeated (from 1 to 999). To have the Schedule run continuously, enter -1. (This option is disabled when an AS3500 Autosampler is configured.)

Starting Line # for the Schedule is the Schedule line number at which analyses begin. This option lets you start, or resume with, any line number.



Start Successive Runs determines how the next analysis in the Schedule is started:

Select **Automatically** to have timed events for the next Method in the Schedule automatically start as soon as the data reduction process from the preceding analysis is completed.

Select **Upon receiving signal at interface** to have the ACI delay the start of timed events from the next Method until it receives a signal from the front panel or a remote device. This allows the autosampler to signal the computer that the next sample has been loaded and injected and is ready for analysis.

Select **Use data paths from the Schedule** to automatically store data files in the file path entered previously in the Schedule. To change the data path, or if you did not enter one in the Schedule, select **Store all data files in directory** and type the data path in the space provided.

9.5 Run Menu

9.5.1 Start...

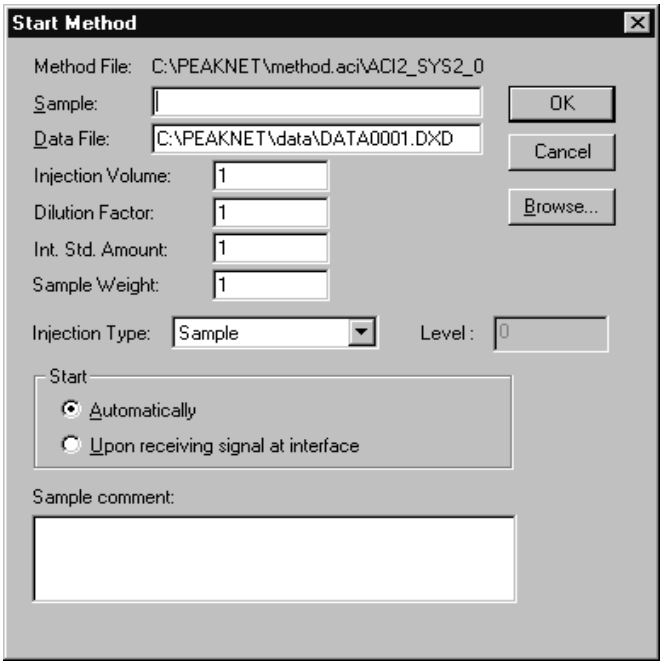
Signals the ACI to begin executing the timed events of the currently loaded ACI Method. As soon as the ACI executes a Start Sampling timed event for a system, the system window displays the real-time plot of data as it is collected.

Timed events can also be started via the RUN button on the ACI front panel, or by receiving a signal at the RUN relay contacts on the ACI rear panel.

Notes

- A Method can be run repeatedly, using the Start... command, without downloading at the end of each run.
- Because of the way raw data is collected and stored by the ACI, both detectors of a dual-detector system must operate at the same data sampling rate.

Selecting Start... opens a dialog box containing the default parameters from the loaded ACI Method file. Use the dialog box controls to modify the default parameters without reloading the Method. Any changes made here will be saved in the raw data file.



Sample lets you enter a name (up to 30 characters) that identifies the sample.

Data File To use a filename other than the one specified in the ACI Method, enter a new name here. PeakNet automatically adds a letter/number identifier code and the extension .DXD, when the data is stored on disk. The filename specified in the Method is not changed.

The following naming scheme is used:

[user assigned name]~xxxyyy.dxd

where:

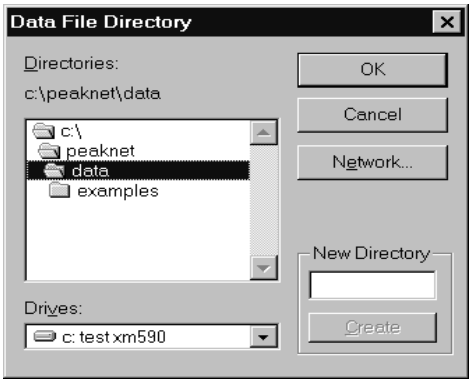
[user assigned name] is the name (including the path) entered into the Data File field.

xxx is a series of letters starting with aaa that increments each time a Method or Schedule is loaded.

yyy is a series of numbers starting with 001 that increments each time the Method is run.

Unless you select a different path name, data will be stored in the default ACI data directory specified on the Options page of the MainMenu program.

To save the file in a different directory, click on the **Browse...** command button and select a directory from the following dialog box. To create a new directory for the file, type the directory name in the New Directory box and click on the **Create** button. The new directory is created under the current directory.



Injection Volume Enter the volume of sample injected (using the same unit as the calibration standards), so that the calculated amount can be corrected for differences in sample volumes. (This parameter is used only in external standard calculations.)

Dilution Factor provides a mathematical correction for dilution effects. For example, for a dilution of 1 to 10, enter 10. If there was no dilution, use the value 1. (This parameter is used by external and internal standards and is ignored by calibration samples.)

Int. Std. Amount Enter the amount of the internal standard (if one is used) so that the calculated amount can be corrected for differences in the internal standard amount. (If you are not using internal standard calibration, this parameter will be ignored.)

Sample Weight specifies the weight of the sample.

Injection Type specifies the type of injection: Sample, Calibration Std., or Check Std. If Calibration Standard is selected, the response values from the analysis are entered automatically into the Method's component table.

Level for Calibration Standard or Check Standard injections, enter the level number of the standard.

Start determines how the next ACI Method is started:

Select **Automatically** if you want timed events for the loaded Method to start immediately.

Select **Upon receiving signal at interface** if you want the ACI to delay the start of timed events until it receives a signal from the front panel or from a remote device. This allows another instrument, such as an autosampler, to signal the ACI that the next sample has been loaded, injected, and is ready for analysis.

9.5.2 End...

Finishes a run early, but retains the data.

End... terminates execution of the Method **and** Schedule for the specified ACI/System. The remaining timed events will be executed immediately, leaving the system operating under the conditions specified in the last step of the Timed Events file.

NOTE Unless the last step of the Timed Events file includes a Reset command, the gradient pump will continue operating according to the last step in the gradient program.

If the Method that was being run so specifies, the result report for the analysis up to the point of interruption will be printed and the raw data will be saved.

Timed events can also be ended via the END button on the ACI front panel or the END contacts on the ACI rear panel.

9.5.3 Abort...

Finishes a run early and discards the data.

Abort... terminates execution of the Method **and** Schedule for the specified ACI/System. The remaining timed events will be executed immediately, leaving the system operating under the conditions specified in the last step of the Timed Events file.

NOTE Unless the last step of the Timed Events file includes a Reset command, the gradient pump will continue operating according to the last step in the gradient program.

Timed events can also be aborted via the ABORT button on the ACI front panel.

NOTE After aborting a run, wait at least 10 seconds before restarting from the front panel. You can restart immediately from the computer screen.

9.6 View Menu

View menu commands control the scaling of the real-time plot. The commands are only active during real-time data acquisition (i.e., when the Status is SAMPLING).

9.6.1 Scale...

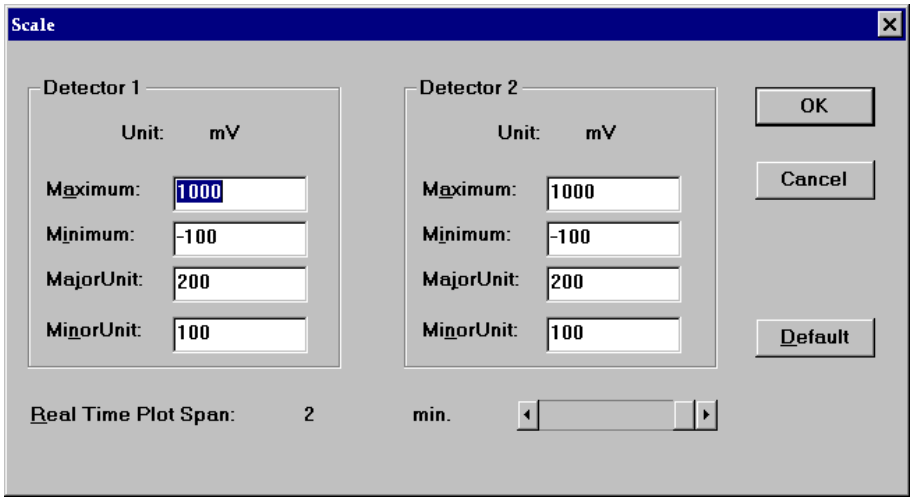
Changes the maximum and minimum points and the major and minor divisions for the Y axis of the real-time plot for each detector. You can also change the length of the time axis for the real-time plot for each detector. This command affects the plotting parameters of the active system only.

Unit indicates the units for the Y axis of the plot specified in the Method.

Maximum Enter the maximum value (in the specified units) for the Y axis of the plot.

Minimum Enter the minimum value (in the specified units) for the Y axis of the plot.

Major Unit Enter the number of units represented by each major division on the Y axis.



Minor Unit Enter the number of units represented by each minor division on the Y axis.

Default sets the Y axis to the values specified in the Method.

Real-Time Plot Span Use the scroll bar to specify, in minutes, the real-time plot span. As the plot reaches the end of the window, the window shifts over automatically.

9.6.2 Superimpose Plots...

NOTE This command is available only for dual-detector systems.

Displays real-time plots in either a superimposed format or as vertically-separated plots on separate axes.

Clicking on this command superimposes one plot over another; clicking on the command again returns the screen to the separated-plot format.

9.6.3 Reverse Background

Selects white or black as the background color of the plot display.

9.6.4 Grid Lines

Superimposes grid lines on the polling window.

9.6.5 MainMenu

Displays the PeakNet MainMenu.

9.7 Window Menu

9.7.1 Tile

Resizes and positions all open windows so that each is fully visible.

9.7.2 Cascade

Arranges windows in an overlapping fashion so that each title bar is visible.

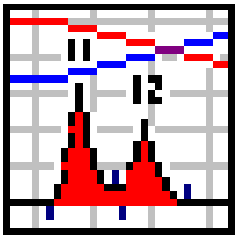
9.7.3 Arrange Icons

Automatically arranges icons neatly on the screen.

9.7.4 Close All

Closes all active windows.

10 • The Optimize Program



The Optimize program has two types of windows for viewing and manipulating chromatograms: Edit Windows let you explore the details of a chromatogram, fine-tune the integration, assign peak names, and update Method files and data files with new parameters. Comparison Windows let you compare multiple data files, and perform mathematical operations on one or two data files and plot the results. From either type of window you can print reports, copy information to the Windows Clipboard, and export data to a database.

Optimize creates and uses the following files:

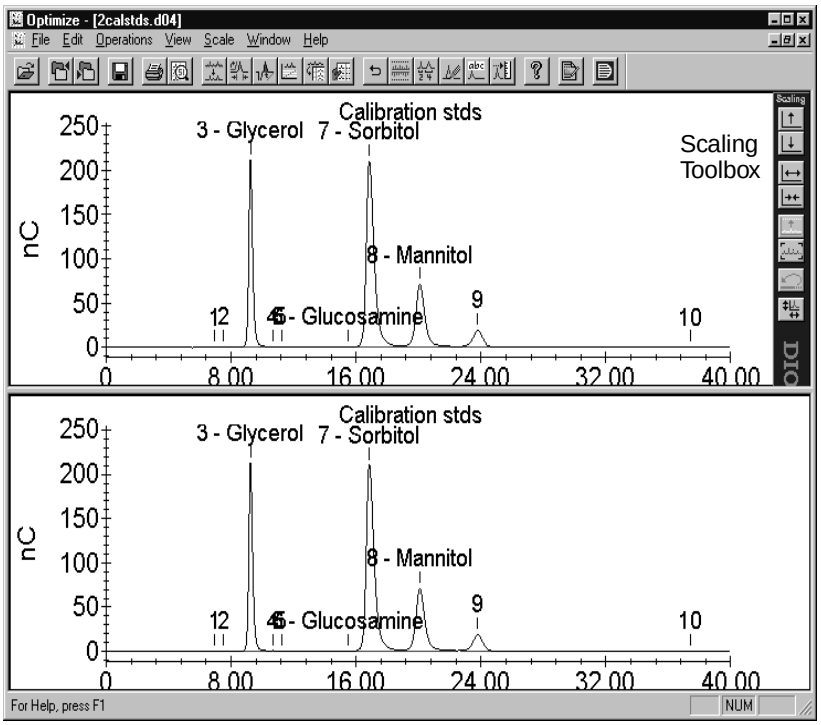
Files Used	Files Saved	Comments
*.MET	*.MET	Methods
*.RPT	*.RPT	Report Format files
*.D??	*.D??	Raw data files
	.TXT	File exported to Lotus 1-2-3 (or other program)

10.1 Starting the Optimize Program

To open the Optimize main window, click on the Optimize button in the PeakNet MainMenu or double-click on OPTIMDX.EXE in the directory that contains the PeakNet program files.

Edit Windows

After an Edit Window has been opened, the Optimize main window resembles the screen shown below:



Scalable Plot

Scaling Toolbox

Reference Plot (Optional)

The **scalable plot** is displayed in the upper window. This plot can be scaled to show any portion of the chromatogram.

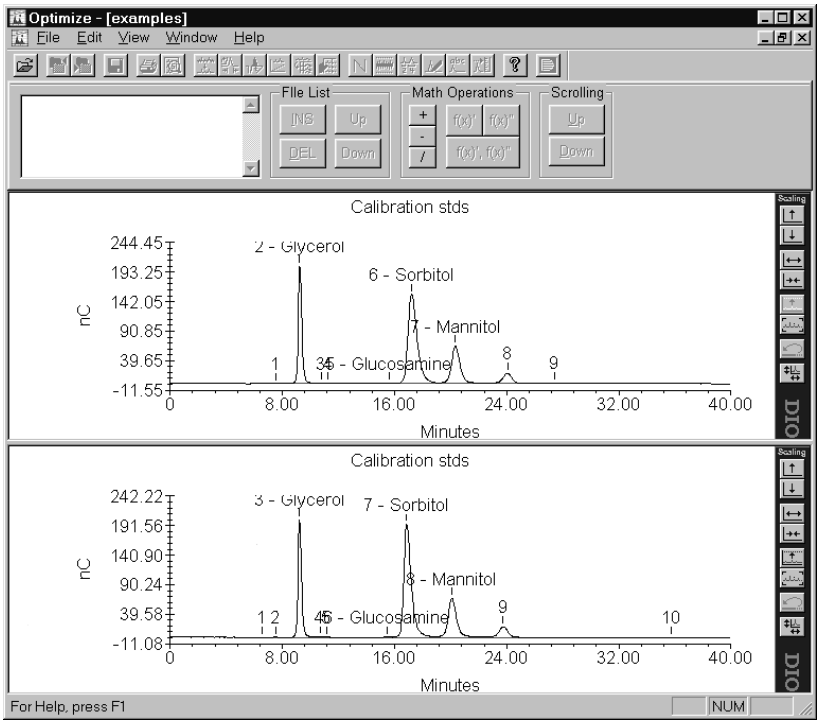
The **reference plot** (optional) shows the complete chromatogram. The box indicates the portion of the plot currently displayed in the scalable plot window. To show or hide the reference plot, select Reference Plot from the View menu.

The **Scaling toolbox** buttons modify the view of the scalable plot by enlarging it, reducing it, zooming in or out, etc.

To show or hide the Scaling toolbox, or change its position in the window, click the right mouse button over an area of the toolbox that does not have a button. Select from the pop-up menu.

Comparison Windows

After a Comparison Window has been opened, the Optimize window resembles the screen shown below:



10.1.1 The Edit Window Toolbar

Click on a toolbar button to quickly implement frequently used Edit Window commands and controls. Click on the buttons for the PeakNet MainMenu and Help to display those programs.

From left to right, the toolbar button functions are:

1. Open Data File
2. Previous File
3. Next File
4. Save Data File
5. Print
6. Print Preview
7. Smoothing
8. Integration
9. Data Events
10. Calibration
11. Component Table
12. Report
13. Normal
14. Auto Threshold
15. Adjust Integration
16. Manual Baselines
17. Name Peaks
18. Calibrate
19. Help
20. Report Designer
21. Switch to MainMenu

10.1.2 The Scaling Toolbox

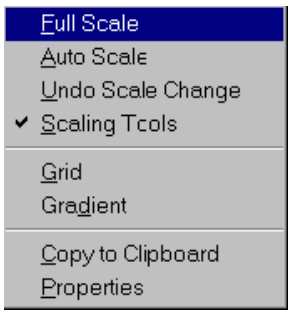
Click on a toolbox button to change the scale of the plot. From top to bottom, the toolbox button functions are:

1. Y Zoom In - View a smaller vertical range at greater magnification
2. Y Zoom Out - View a greater vertical range at lower magnification
3. X Zoom In - View a narrower time span in the Scalable Plot
4. X Zoom Out - View a wider time span in the Scalable Plot
5. Auto Scale - Adjust the vertical scale to show all of the tallest peak and the lowest dip in the Scalable Plot
6. Full Scale - Show the entire chromatogram in the Scalable Plot
7. Undo - Revert to the previous display region. You can undo multiple levels of changes.
8. Scales - Open the Scales tab page of the Plot dialog box

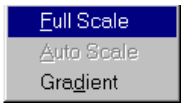
10.1.3 The Pop-Up Menu

If you point to a plot and click the right mouse button, a pop-up menu appears, which varies depending on the type of plot:

Scalable Plot Menu



Reference Plot Menu



The **Full Scale**, **Auto Scale**, and **Undo Scale Change** commands perform the same functions as the equivalent buttons on the Scaling Toolbox.

Grid shows or hides grid lines on the plot. This command is also available from the View menu.

Gradient shows or hides the profiles of the eluent gradients superimposed over the plot. This command is also available from the View menu.

Copy to Clipboard copies the contents of the active Edit Window, or the selected pane of a multi-file Comparison Window, to the Windows clipboard. This command is also available from the Edit menu.

The pop-up menu for the reference plot in an Edit Window is limited to the **Full Scale**, **Auto Scale**, and **Gradient** commands.

10.1.4 Graphics Controls

This section describes other graphics controls used to select viewing options in the Optimize main window.

Enlarge a Selected Area of the Chromatogram

Starting at one corner of the area to be enlarged, drag the mouse cursor diagonally to create a bounding box over the area. When you release the mouse button, everything within the bounding box is enlarged and displayed in the scalable plot window. Although this enlarged view is correctly plotted in reference to the X and Y scales, its aspect ratio may differ from the original.

If you select an area on the reference plot, the scalable plot changes to show the selected region. If you enlarge an area on the scalable plot, the box on the reference plot indicates the area.

Stretch the Chromatogram View Horizontally or Vertically

- Depress the <Shift> key and use the scroll bars.
- Depress the <Shift> key and use the arrow keys.
- Use the Scales menu commands.
- Use the Scaling toolbox buttons.

10.2 File Menu

10.2.1 File Menu Commands for Edit Windows

Open Data File...

Click on the Open Data File toolbar button (or select the menu command) to display the Optimize File Open dialog box and select a data file for display in an Edit Window. You can open up to eight windows.

If the selected data file is from multiple detectors and the File Open dialog box does not list each detector separately, an Optimize Edit window is opened for each detector.

Select the **Process with Method from Disk** check box if you want to have the data file processed with the current version of the Method file on disk, rather than the Method embedded in the data file. This option also reads the current version of the report format file from the disk, rather than the format embedded in the data file.

Previous Data File

Click on the Previous Data File toolbar button (or select the menu command) to open the data file listed above the currently-displayed data file in the File Open dialog box. The file replaces the currently-displayed file in the active window.

Next Data File

Click on the Next Data File toolbar button (or select the menu command) to open the data file listed below the currently-displayed file in the File Open dialog box. The file replaces the currently-displayed file in the the active window.

Open Method File...

Selects a Method to replace in active memory the Method currently being used to interpret open raw data files. The original Method parameters are not replaced permanently in the raw data file unless you save the data file.

Open Dataview...

Select this menu command to display the Open Data Files dialog box and select one or more (up to 12) data files for display in a Comparison Window. Select a data file and click the Add button to move it to the Choose Data Files list. Click Exit when the list contains the desired files.

Save Data File...

Click on the Save toolbar button (or select the menu command) to open the Windows common Save As dialog box and select a name for the currently displayed raw data file. All changes to the integration and component identification will be saved with the file.

Save Data File... is normally used to save a newly optimized file to disk.

Save Method File...

Select this menu command to open the Windows common Save As dialog box and select a file name for the Method parameters. All changes to the integration and component identification will be saved with the file.

Save Method File... is normally used to extract a Method. Since Methods are embedded in raw data files, you can retrieve the original file. This is a convenient way to recover a Method that has been deleted or modified since the data file was generated.

Save Report Format...

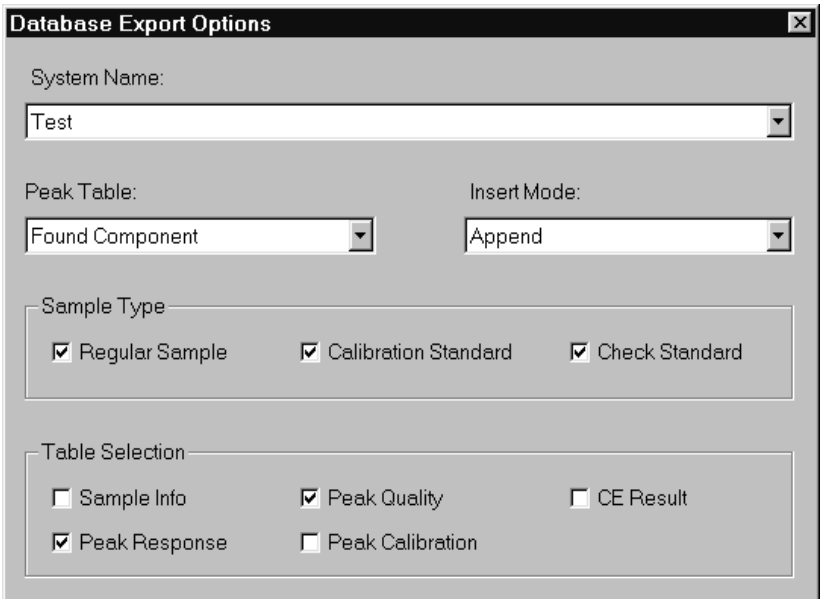
Saves the current report format as a disk file.

Export to Database

Exports a data file’s system and peak information to a database program that supports ODBC.

Database Export Options...

Select options for determining the type of information to export to the PeakNet database.



System Name lists all of the available PeakNet systems (eight) and the available ACI systems (four). Names assigned to systems configured in the Configuration Editor are shown. Default names are shown for unconfigured systems. All other options in the dialog box will apply to the selected system. You can select different options for each system.

Peak Table lists the types of Peak Tables that can be exported.

None no data will be exported to the database. None disables all other options in the dialog box.

All Peaks exports data for all peaks.

All Components exports data for all the components expected to be in the injection

Found Components exports data for components that were matched to peaks detected in the chromatogram.

Insert Mode selects whether to Append or Overwrite the database records.

Append adds the data to the end of the database

Overwrite searches the Injection Table for the most recent record with the same Method start time and replaces the old record with the new.

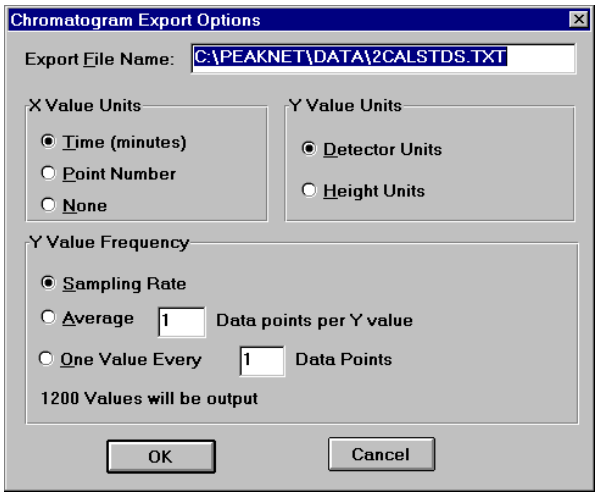
Sample Type selects the types of injection data to export: Sample, Calibration Standard, and Check Standard.

Table Selection selects to which tables data will be exported.

To save the options, select OK. The options selected for all systems are saved.

10.2.2 Export

Exports the current raw data values of a chromatogram in a format compatible with other software programs.



X Value Units exports raw data values as either Time (minutes) or Point Numbers. Select None to omit these values from the file.

Y Value Units exports raw data values in either the units normally used by the detector (for example, AU for an absorbance detector) or the height counts used by the PeakNet integration algorithm.

Y Value Frequency lets you adjust the number of points to suit the capacity of the importing program.

Sampling Rate One data point is exported for each data point in the chromatogram.

Average Each data point exported is the result of averaging the number of data points entered here.

One Value Every One data point is exported per the number of data points entered here. For example, if you enter 10, every tenth data point will be exported.

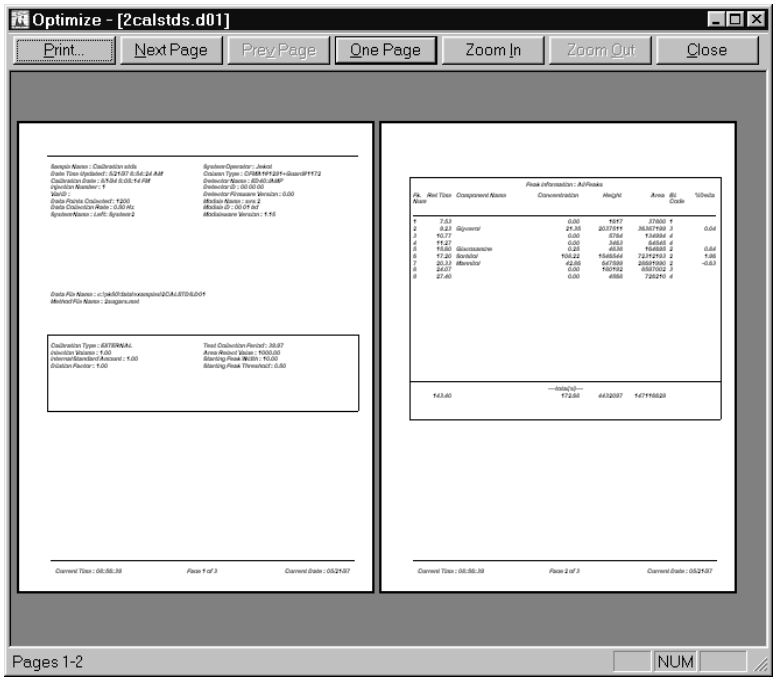
10.2.3 Print...

Opens the Windows common Print dialog box. Use the dialog box controls to select the printing settings. Click OK to print. PeakNet prints the report type that corresponds to the type of sample injection associated with the data file:

- For Sample injections, a Sample Analysis Report is printed.
- For Calibration Standards, a Calibration Update Report is printed.
- For Check Standards, a Check Standard Report is printed.

10.2.4 Print Preview...

Click on the Print Preview toolbar button (or select the menu command) to preview the report before printing. To make changes to the report before printing, click the Report toolbar button or select Report... from the Edit menu and select the type(s) of reports to be printed.



Print... opens the Print dialog box.

Close returns you to the Optimize main window.

10.2.5 Most Recently Used

Open one of the last four data files used by clicking on its name here.

10.3 Edit Menu

10.3.1 Smoothing..., Integration..., Data Events..., Calibration..., Component Table..., Report..., and X-Y Data

NOTE These commands are available only for Edit Windows.

The Smoothing, Integration, Data Events, Calibration, Component Table, Report parameters, and X-Y data of a Method can all be edited directly from Optimize, using the same dialog boxes available from the Method Editor. Click on the toolbar button (or select the menu command) to open the corresponding dialog box. See Chapter 5 for a complete description of these dialog boxes.

10.3.2 Report Format...

Opens the Report Designer and displays the report format for the current data file.

10.3.3 Comment...

Opens a dialog box for adding a comment to the current method.

10.3.4 Copy Graphics

Copies the contents of the active Edit Window, or the selected pane of a multi-file Comparison Window, to the Windows clipboard. The plot is copied exactly as it is shown on the screen. Use the Scaling Toolbox buttons (see Section 10.1.2) and the Plot dialog box (see Section 10.9) to adjust the plot's scale and other properties before copying to the clipboard.

The Copy Graphics command can also be accessed by clicking the right mouse button and selecting the command from the pop-up menu.

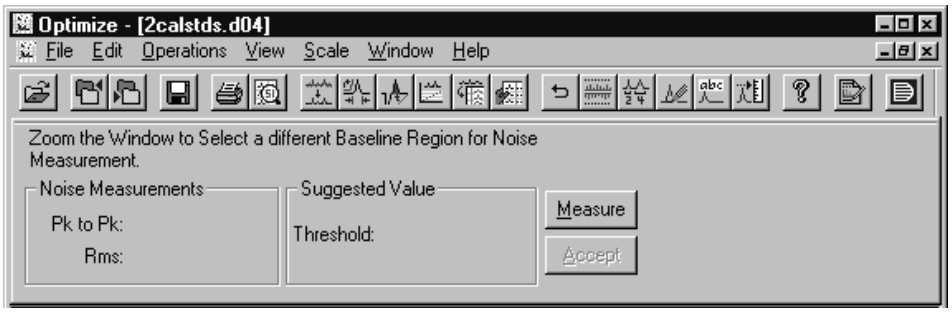
10.4 Operations Menu (Edit Windows Only)

NOTE When you select a command from the Operations menu or click on one of the equivalent toolbar buttons, a set of controls for the type of operation drops down below the toolbar. To remove the drop-down controls, select the Return to Normal Display command or click on the Normal toolbar button.

10.4.1 Auto Threshold...

NOTE Before selecting Auto Threshold, make sure the starting peak width is appropriate, because it will affect the suggested threshold. The starting peak width should be approximately the width of the narrowest peak at half-height.

Click on the Auto Threshold toolbar button (or select the menu command) to open the Automatic Threshold drop-down controls.



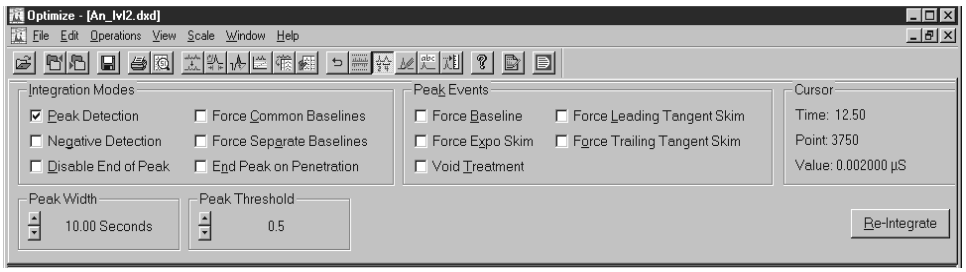
The automatic threshold feature evaluates a section of baseline, displays the average noise for the baseline, suggests a threshold that prevents the baseline from being interpreted as peaks, and, if accepted, updates the current threshold.

1. From the chromatogram in the scalable plot window, locate a peakless segment of baseline that is representative of the entire baseline. Place the mouse cursor at one end of this segment, press and hold the mouse main button while dragging the cursor to the other end of the segment, and release the mouse button. If necessary, click the Auto Scale button on the Scaling toolbox to bring the segment view onto the screen.

2. Click on the Measure command button. Two noise measurements (Peak-to-Peak and Root Mean Squared) and a suggested threshold value are displayed in the dialog box.
3. To repeat the measurements on a different segment of baseline, repeat Steps 1 and 2. Measuring several segments helps you identify the most representative threshold value.
4. Click on the Accept command button to have the chromatogram integrated with the new threshold.

10.4.2 Adjust Integration...

Click on the Adjust Integration toolbar button (or select the menu command) to open the Adjust Integration drop-down controls. Any changes made with these graphics controls can be saved to the Method and applied to other chromatograms.



In general, the first step in optimizing the integration parameters for a data file is to select Data Events... from the Edit menu and delete all unwanted events from the file.

The next step is to evaluate the initial integration parameters and make any necessary changes. To do so, select Integration.. from the Edit menu.

Use the Integration Parameters dialog box controls to make changes that affect an entire chromatogram; for example, change the Peak Width before using other integration features to fine-tune data. The peak width should be approximately equal to the width (in seconds) at half-height of the narrowest peak in the chromatogram. The default Peak Width value is established based on the Method Type.

When you finish editing, click on OK to integrate the data.

Chapter 6 describes the Data Events and Integration Parameters dialog boxes.

Integration Modes

The Integration Modes in the Adjust Integration controls represent six types of data events. The check boxes let you turn data events on or off at selected times in the run. Each time you turn an Integration Modes check box on or off, you are creating a **separate** data event.

To turn an event on (or off), move the hairline Time-Scale cursor to the point at which you want the event turned on (or off), click on the check box for the event, and then click on the Re-Integrate command button. This will modify peak integration throughout the rest of the run, unless you turn the control off (or on) at a later time in the run.

NOTE To adjust the Time-Scale cursor, point to the hairline cursor and drag it to the desired time.

Peak Detection detects peaks on the chromatogram. This control is normally on. Turn it off during a period of void volume column upset or if an apparent peak appears that you do not want reported.

Negative Detection enables detection of negative peaks. Normally, only positive peaks are detected.

Disable End of Peak combines a group of peaks into one new peak. The new peak will be equivalent to the areas of the combined peaks.

Force Common Baselines forces a common baseline below a group of peaks so that areas of fused peaks are determined by drop-line integration.

Force Separate Baselines forces valley-to-valley baselines where drop-line integration was determined by the integration algorithm.

End Peak on Penetration If the integration algorithm causes the baseline to penetrate data on the plot, the End Peak on Penetration control brings the baseline to a logical position relative to the data cluster that was penetrated.

Peak Events

Unlike the Integration Modes, which modify peaks throughout the rest of a run, the Peak Events in the Adjust Integration controls represent data events that modify only one specific peak. Before activating a Peak Event, you need to understand the types of peaks:

Peak Description	Baseline Code Type
Completely resolved	1
Partially resolved	2
Host peak	3
Rider peak	4, 6, or 7

*Type 5 is an internal designation that is reserved for future use.

- **Type 1** peaks are completely resolved. The baseline is a line between the beginning and ending points of the peak. The separation between the end of the first peak and the start of the second peak must be at least 20% of the width of the first peak.
- **Type 2** peaks are partially resolved peaks. The peaks are separated by a drop-line extending from the valley between the peaks to a common baseline.
- **Type 3** peaks are host peaks fused with rider peaks (type 4, 6, or 7) that have 20% or less of the height of the host peak.
- **Type 4** peaks are closely following rider peaks that are separated from the host peak by an exponential projection of the backside of the host peak. The area under the exponential line is added to the host peak, not the rider.
- **Type 6** peaks are closely following rider peaks that are separated by a tangential line from the host peak to the outer edge of the rider peak. The area under the tangential line is added to the host peak, not the rider.
- **Type 7** peaks are closely leading rider peaks that are separated by a tangential line from the host peak to the outer edge of the rider peak. The area under the tangential line is added to the host peak, not the rider.

Force Baseline forces a separate baseline between two Type 2 peaks where no baseline is evident. To activate the event, move the Time-Scale cursor onto the peak to the right of the area where you want to force a baseline, then click first on the Force Baseline check box and then on the Re-Integrate command button.

Force Exponential Skim If you separate a host peak (Type 3) from a closely following rider peak (Type 4) by dropping a vertical line between them, some of the area allotted to the rider peak is actually part of the tailing slope of the host peak. The Force Expo Skim control extrapolates the exponential decay rate of the tailing slope of the host peak, and then adjusts the areas of the host and rider peaks accordingly. Exponential skim is automatic when all of the following conditions occur:

- The height of the rider peak is 20% or less of the height of the host peak.
- The height of the valley between the host and rider peaks is 33% or more of the height of the rider peak.
- The height of the valley between the host and rider peaks is 10% or more of the height of the host peak.

To activate the event, move the Time-Scale cursor to a point within the host and rider peaks to be modified, then click first on the Force Expo Skim check box and then on the Re-Integrate command button.

Force Leading Tangent Skim forces a host peak (Type 3) to be separated from a closely leading rider peak (Type 7) using a tangential-skim treatment.

Force Trailing Tangent Skim forces a host peak (Type 3) to be separated from a closely following rider peak (Type 6) using a tangential-skim treatment.

Tangential-skim treatment is automatically applied to rider peaks if all of the following conditions are met:

- The height of the rider peak is 20% or less of the height of the host peak.
- The height of the valley between the host and rider peak is 33% or more of the height of the rider peak.

- The height of the valley between the host and rider peak is less than 10% of the height of the host peak.

Void Treatment When the upward slope of a peak starts at a negative data point, Void Treatment looks back along the baseline and starts the slope at the first non-negative data point encountered. This control is used chiefly to correct for water dips and void volume upsets.

To activate the control, move the Time-Scale cursor to a point immediately before the negative dip, and then click first on the Void Treatment check box and then on the Re- Integrate command button.

Peak Width

The Peak Width in the Adjust Integration controls determines how many data points are combined into each data bunch. Increasing the peak width increases the number of data points per bunch, while decreasing the peak width lowers the number of data points per bunch.

Peak width requirements are directly interrelated with slope requirements, as explained later in the **Peak Threshold** section. Narrow peaks require small data bunch sizes, to allow enough bunches across narrow peaks to permit peak detection. Wide peaks require large data bunches so that small changes in amplitude can be detected over long time intervals. If the peak width is narrow enough, the peak tick appears at the apex of the peak.

The Peak Width control is typically used to re-integrate a lengthy chromatogram in which narrow peaks increase to wide peaks as the run progresses. If this occurs, the chromatogram may be badly integrated, with the baselines of wider peaks ending too soon because the integration program had difficulty finding the true ends of the peaks. One solution is to increase the Peak Width setting before the first wide peak. This can also occur if the Threshold is set too high; refer to the **Peak Threshold** section for more information.

If a peak's tick mark is not at the peak apex, the Peak Width setting is probably too wide and you should select a narrower width. The best way to optimize integration is by on-screen experimentation.

Move the Time-Scale cursor to a point immediately before the area where you want to change the peak width, click the cursor on Wider or Narrower, and then click on the Re-Integrate command button.

Peak Threshold

The threshold is a value derived from the averaged slopes of data bunches sampled along a baseline sector. It is applied as a limiting slope to determine peaks. The integration algorithm measures the slope between every two data bunches in the entire chromatogram. It marks the potential start of a peak when two consecutive data bunches have a slope higher than the peak threshold value; if a third data bunch exceeds the threshold value, the algorithm marks the start of a peak.

The algorithm continues to view data and look for the top of the peak. It determines the top of a peak when the slope of the sampled data drops below the positive threshold value. The end of a peak is determined when data bunches reach and maintain the threshold value, or when the beginning of another peak is found.

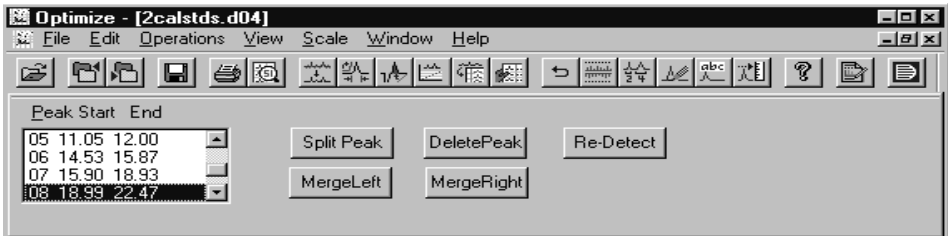
The threshold value normally changes very little from the value provided by the Auto Threshold control, but you may occasionally find it necessary to make minor changes to balance modifications to peak width or to compensate for increased noise levels. To do so, move the Time-Scale cursor to a point immediately before the area where you want to change the threshold value, click the up or down arrow to select the new value. The up arrow doubles, and the down arrow halves, the current value. Click on the Re-Integrate command button to have the chromatogram integrated with the new threshold.

Cursor Move the Time-Scale cursor by positioning the mouse cursor on either the right or left arrow of the scroll bar and then pressing the mouse main button. The number of data points and value for the selected time will automatically be displayed.

10.4.3 Set Baselines Manually...

NOTE Unlike other controls, Manual Baseline Editing can adjust the baseline only for the file you are working on.

Click on the Manual Baselines toolbar button (or select the menu command) to open the Manual Baseline drop-down controls.



The **Peak Start End** list box indicates the number, starting time, and ending time for each peak in the file. There are three ways to select a peak whose baseline you want to modify:

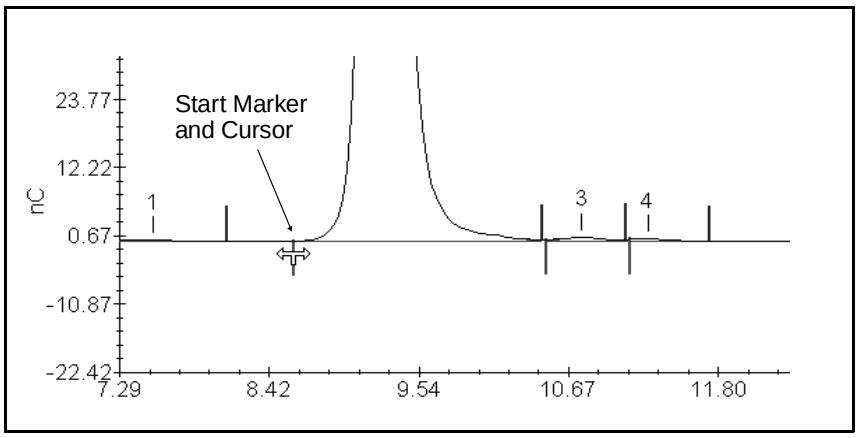
- Click on the peak number in the Peak Selection list box.
- Point to the hairline Time-Scale cursor and drag it to the desired peak.
- Click the left or right arrow on the keyboard to move the cursor between peaks.

Changing a Peak's Start or Stop Time

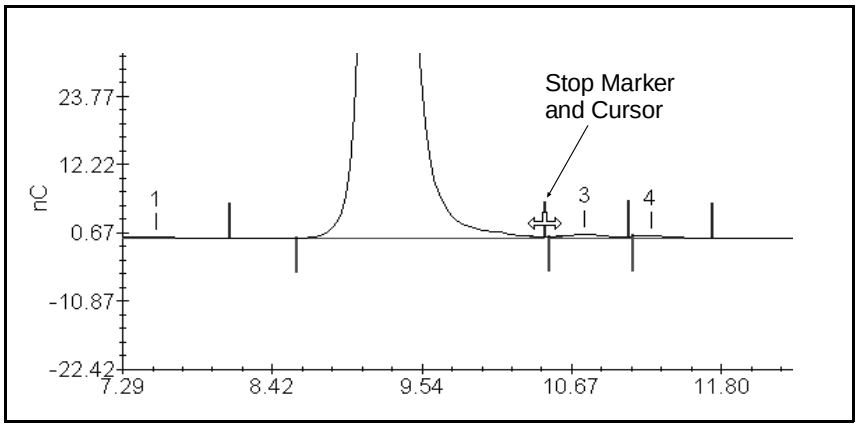
Start and stop markers (short vertical lines on the baseline) indicate the beginning and end of a peak. If they are not currently visible, select Start/Start Markers from the View menu. By default, start markers are green and stop markers are red.

- **To change the start time of a peak,** point to the peak's start marker. The cursor changes to a double-ended arrow with a tail that points down (see the following figure). Drag the marker to the point on the time-scale where you want the peak to start, and release the mouse button. The new time will be updated in the Peak Start End list box.

NOTE If two adjacent peaks are not fully resolved, dragging the start marker of one of the peaks, also drags the stop marker of the other peak, and vice versa.



- **To change the end time of a peak,** point to the peak's stop marker. The cursor changes to a double-ended arrow with a tail that points up (see the figure below). Drag the marker to the point on the time-scale where you want the peak to end, and release the mouse button.



Split Peak adds a new peak by splitting an existing peak into two. Position the Time-Scale cursor at the point you want the peak split and select the Split Peak command.

Delete Peak deletes a selected peak from the Peak Table and from integration results.

Merge Peak Right combines the areas of the selected peak and the peak adjoining it to its right on the time-scale. The combined right peak loses its separate identity as a peak.

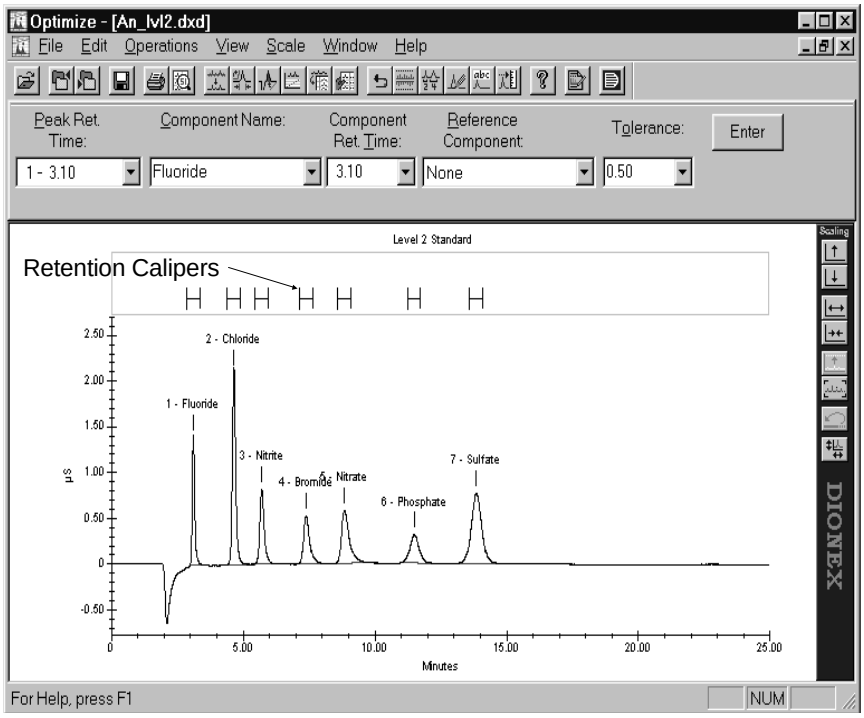
Merge Peak Left combines the areas of the selected peak and the peak adjoining it to its left on the time-scale. The combined left peak loses its separate identity as a peak.

Re-Detect Peaks deletes the results of all baseline changes made to a chromatogram during editing and returns the chromatogram to its previous configuration.

10.4.4 Name Peaks...

Click on the Name Peaks toolbar button (or select the menu command) to open the Name Peaks drop down controls and do the following:

- Create a new component table by entering names for the peaks of a chromatogram, or add components to an existing component table
- Match unidentified or misidentified peaks to the correct components
- Adjust retention time tolerances and component references graphically to ensure proper peak identification



Selecting a Peak

Click the peak's retention time in the Peak Ret. Time drop-down list. If the selected peak is already identified as a component, the component name and other component information is filled in.

Selecting a Component

There are two ways to select a component:

- Click the cursor on the Retention Caliper above the desired component.
- Use the arrow to the right of the Component Name drop-down list box to display the available component names. Click the cursor on the desired component name.

Naming Unidentified Peaks

After selecting the peak of interest, open the drop-down list box under Component Name. If the corresponding component is already

listed, select it to display current component information. Update the component time, using one of these methods:

- Select the new time from the Component Time drop-down list.
- Use the mouse to move the Retention Caliper over the correct peak.
- Type the new component time in the Peak Ret. Time edit box.

If the component name is not listed, type the name in the Component Name box and press <Tab> to enter the peak time as the Component Time.

Edit the Reference Component and Tolerance, if desired, then press <Enter>. To enter a window size as a percentage, enter a percent sign with the number; a value without a percent sign is interpreted as an absolute window (expressed in minutes). The new component assignment is entered in the component table and should appear in the scalable plot. If the new component assignment does not appear, the reference component has probably shifted too much. Refer to **Renaming Misidentified Peaks** for a corrective procedure.

Renaming Misidentified Peaks

Peaks can be misidentified for several reasons: a problem with the Reference Component, an excessively wide Tolerance, or a mismatch between the expected and actual retention time.

When the Name Peaks controls are displayed, Retention Calipers appear over peaks that have been identified as components. When you select a component's Retention Caliper the other calipers move up, allowing you to drag the selected caliper to a new position.

The caliper is black when positioned over a peak and red if there is no peak. If you drag a component's Retention Caliper over a peak and press Enter, the peak will be identified as that component.

If a component has a reference component, when you select its Retention Caliper, a dashed line connects to the reference component's caliper.

To rename peaks:

1. Select the peak of interest.
2. Check the Reference Component, if any.

   If a reference component is listed, make sure that the reference component's Retention Caliper is centered over the reference component peak. If it is not, the Tolerance of the current component has been adjusted, possibly enough to miss the peak. To correct this, follow one of these procedures:

   Change the reference component to None.

   No adjustment will be made to the component's Tolerance.

   or

   Re-align the Retention Caliper of the Reference Component.

   Drag the reference component's Retention Caliper until it is centered over the reference peak.

   Repeat the above for all reference components before proceeding.
3. Eliminate any Tolerance overlaps.

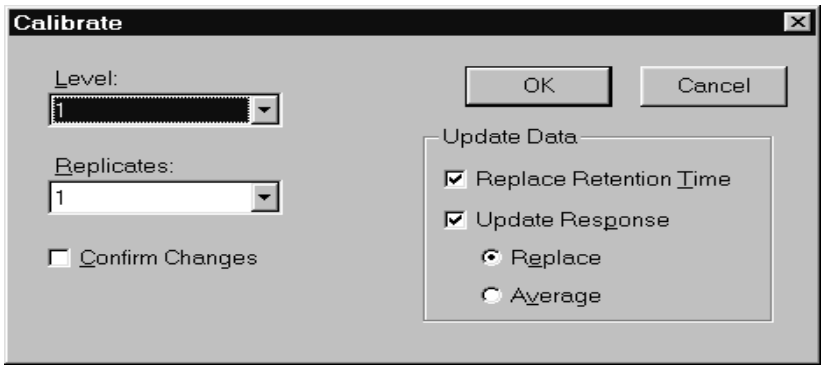
   If any Retention Calipers overlap, reduce their widths by selecting or typing in a narrower Tolerance, and selecting Enter. Include "%" if you want the Tolerance determined as a percentage (±) of the retention time; otherwise the Tolerance will be in minutes (±).
4. Center the Retention Calipers.

   Select the first component from the Component Name list, then center the Retention Caliper over the proper peak. If appropriate, re-adjust the Tolerance. Repeat for all other components.

10.4.5 Calibrate...

Click on the Calibrate toolbar button (or select the menu command) to calibrate the Method with the current data file and update the height, area, and retention time values for each peak, or just the retention times.

Calibrate is normally selected only after all other adjustments to the Method have been completed.



Level lets you choose the calibration level you want updated. Select the calibration level (1 to 10) from the drop-down list box.

Replicates lets you choose which replicate values you want updated.

Update Data

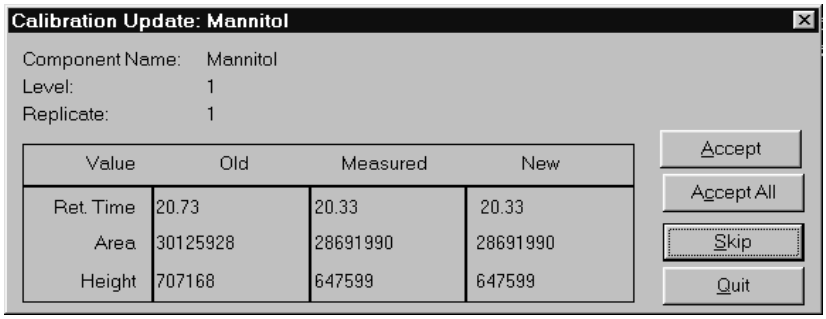
Replace Retention Time updates the Method by replacing the retention time values currently stored in the Component Table with the values determined by the current integration of the current data file.

Update Response updates the Method by replacing the response values currently stored in the Component Table with the values determined by the current integration of the current data file.

Replace updates the Method b replacing the existing values with the new. Replace is only available when replicates is greater than one.

Average updates the Method with values obtained by averaging the values currently in it with values in your data file.

Confirm Changes, if checked, the following dialog box appears when you click **OK**, which allows you to accept or skip changes to values for each component as you calibrate:



Accept accepts the new values for a component.

Accept All accepts new values for all components, including those not displayed.

Skip skips this component without accepting a new value.

Quit abandons the procedure, although changes already accepted remain in effect.

10.5 View Menu

10.5.1 Overlay Plots

NOTE This command is available for Comparison Windows only.

Displays the plots on a single set of axes. When plots are overlaid, you can use the Plot dialog box - Data tab page to change the overlaid display. See Section 10.9 for details.

10.5.2 Reference Plot, Baselines, Dynamic Threshold, Start/Stop Markers, Peak Fills, Peak Labels

NOTE These commands are available for Edit Windows only.

Selecting (or deselecting) one of these commands displays (or removes) the corresponding graphics feature from the chromatogram.

10.5.3 Toolbar

Shows or hides the toolbar.

10.5.4 Status Bar

Shows or hides the status bar.

10.5.5 MainMenu

Click on the MainMenu toolbar (or select the menu command) to display the PeakNet MainMenu.

10.6 Scale Menu

Notes

- The commands on the Scale menu are also available from the Scaling toolbox, or from the pop-up menu displayed by clicking the right mouse button on the plot.
- The Scale menu is not available if a Comparison Window is active.

10.6.1 Undo Scale Change

Revert to the previous display region selected in the Scalable Plot.

10.6.2 Scales...

Displays the Plot dialog box - Scales tab page.

10.6.3 Full Scale

Show the entire chromatogram in the Scalable Plot.

10.6.4 AutoScale

Adjust the vertical scale to show all of the tallest peak and the lowest dip in the Scalable Plot.

10.6.5 Zoom

Zoom In Vertically

View a smaller vertical range at greater magnification in the Scalable Plot.

Zoom Out Vertically

View a greater vertical range at lower magnification in the Scalable Plot.

Zoom In Horizontally

View a narrower time span in the Scalable Plot.

Zoom Out Horizontally

View a wider time span in the Scalable Plot.

10.6.6 Scaling Tools

Shows or hides the Scaling toolbox.

10.7 Window Menu

10.7.1 Cascade

Arrange all windows in a diagonally descending pattern (overlapped) so that the title bar of each is visible.

10.7.2 Tile Horizontally

Arrange all windows horizontally (one above another), non-overlapped.

10.7.3 Tile Vertically

Arrange all windows vertically (side-by-side), non-overlapped.

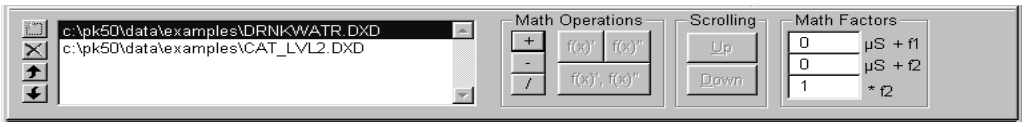
10.7.4 Arrange Icons

Arrange all window icons at the bottom of the main window.

10.7.5 Open Windows List

Make an open window active by choosing its name from this list. All open system windows are listed, including those that have been reduced to icons.

10.8 Math Operations



The Optimize program can calculate and plot the mathematical sum, difference, or ratio of any two raw data files. It can also calculate and plot the first and second derivatives of a stored raw data file. The results can be stored as a new data file and used to improve plot quantitation.

For example, a baseline data file can be stored and subsequently subtracted from each sample data file. The resulting data file can then be reintegrated, to improve quantitation of detected peaks.

To perform a mathematical sum, difference, or ratio:

1. Open a Comparison Window that contains only the two data files of interest.
2. Select the desired math operation button: +, -, or /.

   The Comparison Window will display a third plot showing the result of the operation.

To calculate and plot the first and second derivatives of a data file:

1. Open a Comparison Window that contains only the data file of interest.
2. Select the desired math operation button: f(x)′, f(x)″ or f(x)′, f(x)″ button.

   The Comparison Window will display a third plot showing the result of the operation.

Offsets and Normalization

When the selected operation is a mathematical operation involving two data files, the Math Factors controls appear. These controls enable offsets and normalization to be applied to the operation formula.

***unit* + f1** and ***unit* + f2** is the data offset value that is required to compensate for incompatible vertical offsets in the two data files for subtraction, ratio, and addition operations. These values are then subtracted from every data point in the designated plot. This is a useful technique when the baseline of one plot is higher above the zero baseline than the other. If the two baselines are at about the same level, use zero offset (the default value)

***f2** is the normalization factor for file #2. The normalization factor compensates for differences in sample preparation, response factor, or background signal level. It is used as a multiplier for the divisor (in a ratio calculation) or the subtrahend (in a subtraction calculation). A value of one is used when there are no differences; one is the default.

Floating-point entries are permitted.

For example, to determine the ratio of plot A to plot B (A/B) using a normalization factor of 1.5, the actual ratio of every data point is calculated as:

$$\frac{plot\,A}{1.5 \times plot\,B}$$

Similarly, in order to subtract plot B from plot A (A-B) using a normalization factor of 2.3, the actual difference is calculated as:

$$(plot\,A) - (2.3 \times plot\,B)$$

10.9 Plot Properties

The Plot Properties dialog box lets you change the scale, fonts, line colors, and other properties of plots displayed in PeakNet programs. The dialog box is available from the Run, Run ACI, Optimize, and Report Designer programs.

To open the Plot dialog box:

- Point anywhere over the displayed plot and press the right mouse button. Select Properties from the pop-up menu.

  or

- Double-click anywhere on the displayed plot.

NOTE If you double-click over a particular area of the plot, the Plot dialog box opens to the tab page appropriate for the area you clicked.

When you make changes to a plot's display properties, the changes are saved as follows:

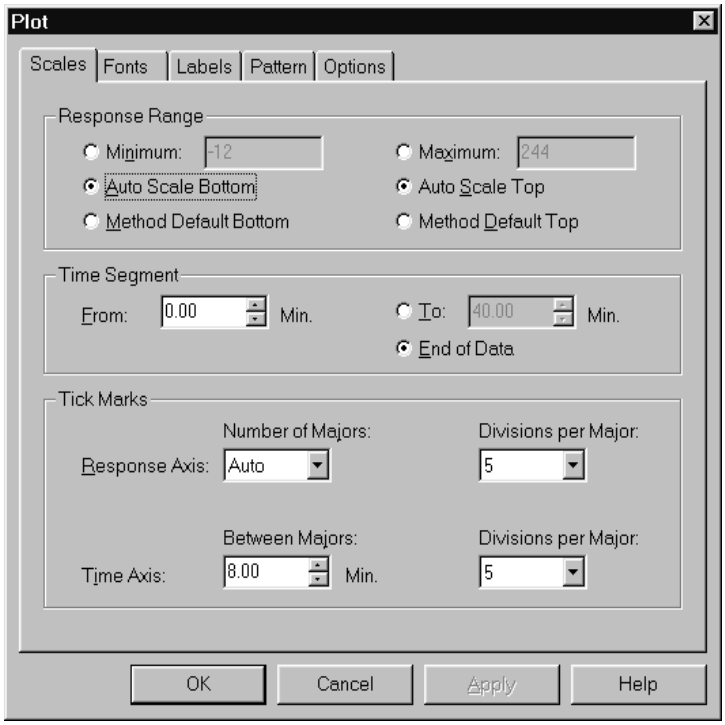
- From the Run program, plot properties are saved when the system window is closed, or when you exit the program.
- From Report Designer, plot properties are saved with the report format.

The Plot dialog box consists of six tab pages:

- Use the **Scales** tab page to set the scales for the plot axes, and to select the number of major and minor tick marks on each axis.
- Use the **Fonts** tab page to change the typeface, size, style, and color of fonts on the plot.
- Use the **Labels** tab page to change how items are labeled on the plot.
- Use the **Pattern** tab page to change the color, style, and weight of lines on the plot, and the color of plot regions.
- Use the **Options** tab page to show or hide plot features, such as the gradient overlay, baselines, start/stop markers, the grid, etc.
- Use the **Data** tab page to change the way overlaid plots are displayed.

  NOTE The Data tab page is only available when plots are overlaid in a Comparison Window.

10.9.1 Scales Tab Page



Response Range specifies the scale for the response axis.

Minimum lets you set the low limit of the response axis to an exact value.

Auto Scale Bottom adjusts the scale to show the bottom of the lowest dip in the plot.

Method Default Bottom uses the Minimum setting from the Plot Scales section of the Method Editor window.

Maximum lets you set the high limit of the response axis to an exact value.

Auto Scale Top adjusts the scale to show the top of the highest peak in the plot.

Method Default Top uses the Maximum setting from the Plot Scales section of the Method Editor window.

Time Segment specifies the scale for the time axis.

From specifies the beginning time.

To lets you specify an exact time at which to end the plot.

End of Data extends the plot to include the last data point.

Tick Marks

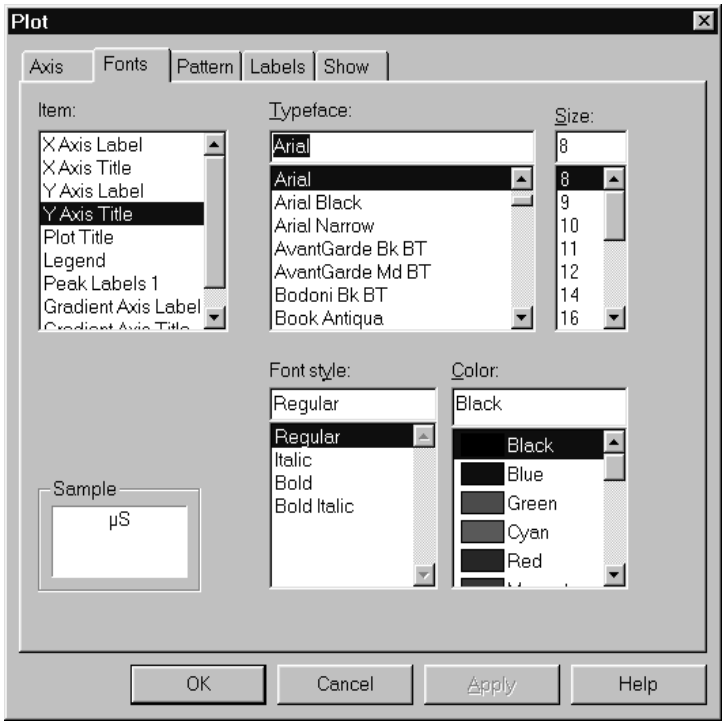
Response Axis: Number of Majors determines the total number of major tick marks to include on the axis. The **Auto** option selects the tick mark spacing, based on the current plot scale. When you zoom in or out on the plot, the tick marks and the Y-intercept are adjusted.

Time Axis: Divisions per Major is the number of minor tick marks to display between each major tick mark.

Time Axis: Between Majors lets you specify the time interval between each major tick mark.

Time Axis: Divisions per Major is the number of minor tick marks to display between each major tick mark.

10.9.2 Fonts Tab Page



Item lists the various text items shown on the plot. Select an item and then select the desired typeface, size, font style, and color.

Sample shows the current font for the selected item.

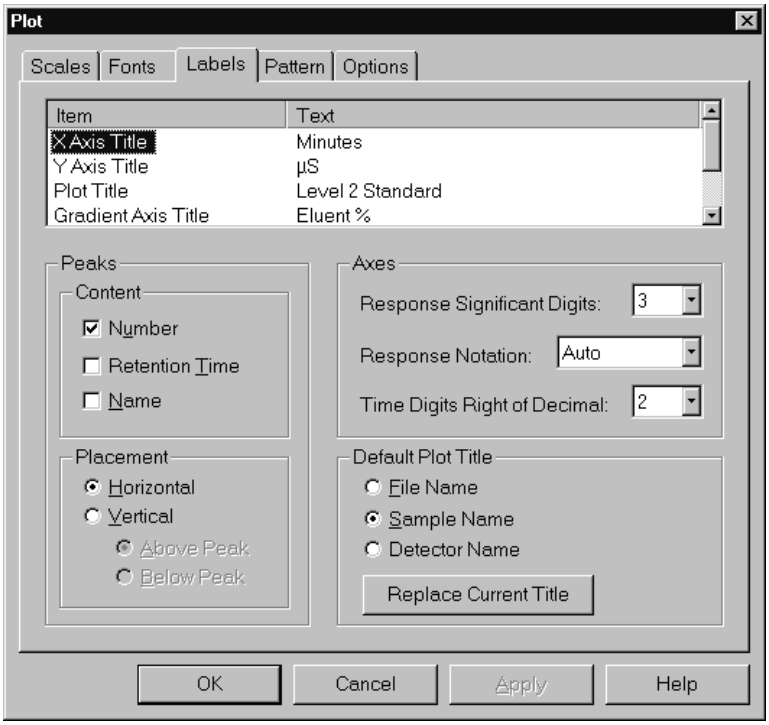
Typeface selects the typeface for the item.

Size selects the font size for the item.

Font Style selects the font style for the item.

Color selects the text color for the item.

10.9.3 Labels Tab Page



Item lists the items that can be labeled on the plot

Text lists the current text used for the item labels. To change a label, click the text and type the new title.

Peaks

Content selects the content of the peak labels (Number, Retention Time, and/or Name).

Placement selects whether the peak labels are printed horizontally or vertically.

Axes

Response Significant Digits selects the number of significant digits for the response axis labels.

Response Notation selects the notation (Auto, Decimal, or Scientific) used for the response axis labels. If Auto is selected, the type of notation is determined as follows:

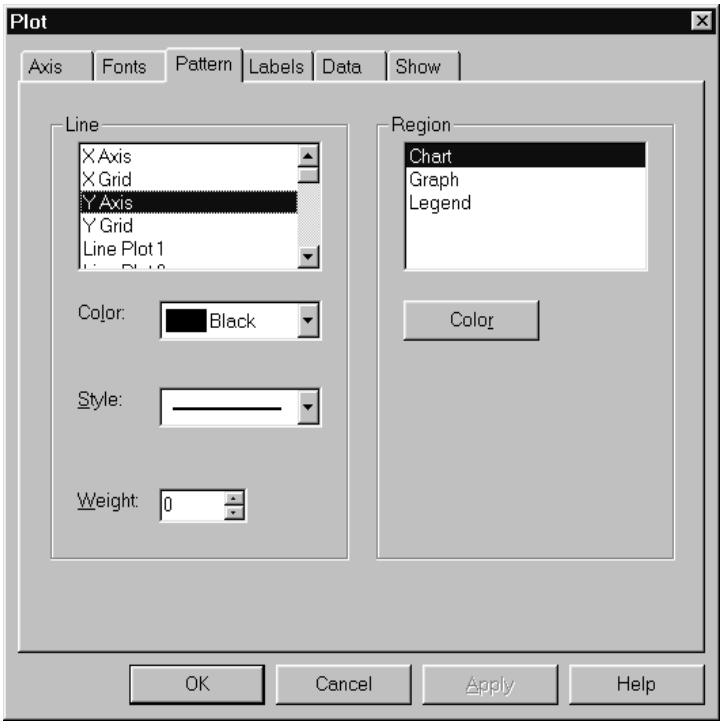
- If either the upper or lower response limit value is less than 0.1, scientific notation is used for all labels.
- If either limit has more digits left of the decimal than the selected Response Significant Digits, scientific notation is used for all labels.
- Decimal notation is used in all other situations.

Time Digits Right of Decimal selects the number of decimal places for the time axis labels.

Default Plot Title (available only when an Edit Window is active) selects whether to use the File Name, Sample Name, or Detector Name for the default title. Click the **Replace Current Title** button to enter a new default in the Plot Title's Text field in the list box above.

Default Legend (available only when a Comparison Window is active and displaying overlaid plots) selects whether the plot legend will display the overlaid plots File Names, Sample Names, or Detector Names.

10.9.4 Pattern Tab Page



Line List box shows the type of lines that can be displayed.

Color shows the color of the line selected in the list, and allows you to select a new color.

Style shows the style of the line selected in the list and allows you to select a new style.

Weight shows the weight of the line selected in the list and allows you to select a new weight.

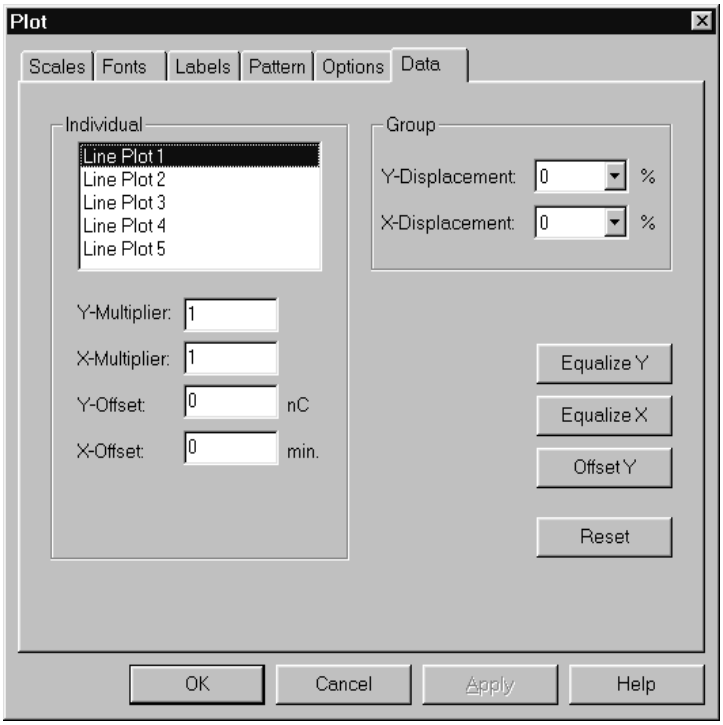
Region lists the areas of the plot. Chart is the area outside of the plot axes. Graph is the area defined by the plot axes.

Color (button) opens the Color dialog box to allow you to select a new color for the selected region.

NOTE The settings in the Pattern tab page do not determine which lines or regions are shown on the plot. Check boxes in the Options tab page are used to show or hide lines and regions.

10.9.5 Data Tab Page

NOTE The Data tab page is only available, when plots are overlaid in a Comparison Window in the Optimize program.



Individual lists the line plots currently shown in the overlaid plot and allows you to select a line plot to change.

Y-Multiplier applies a multiplier factor to the Y-axis of the selected line plot.

X-Multiplier applies a multiplier factor to the X-axis of the selected line plot.

Y-Offset offsets the Y-axis of the selected line plot by the specified amount.

X-Offset offsets the X-axis of the selected line plot by the specified amount.

Group

Y-Displacement, starting with Line Plot 2, the Y-axis of each line plot in the overlaid plot is offset from the previous plot axis by the specified percentage.

X-Displacement, starting with Line Plot 2, the X-axis of each line plot in the overlaid plot is offset from the previous plot axis by the specified percentage.

Equalize Y changes the Y-Multiplier value of each plot so that the distance between all of the plot baselines and their highest peaks is equal. Other peaks in each plot are adjusted by the new multipliers.

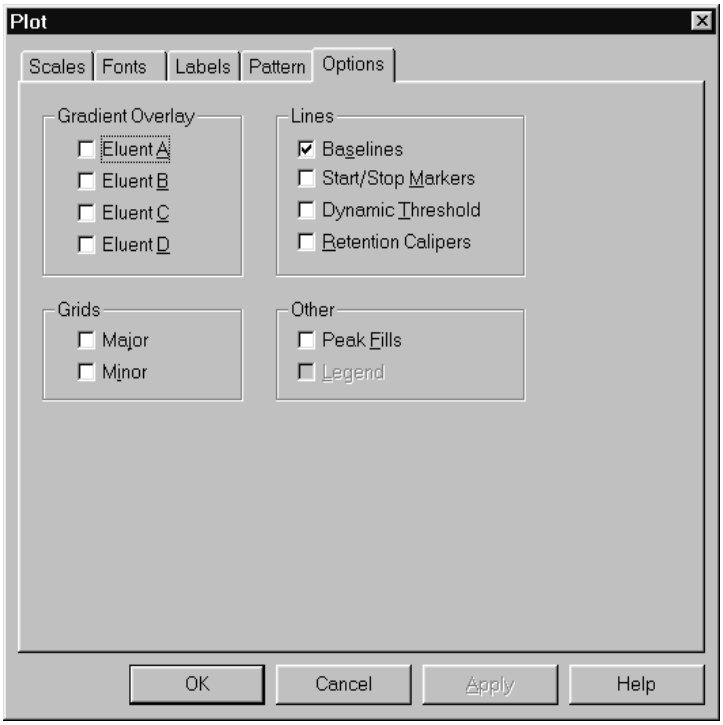
Equalize X changes the X-Multiplier value of each plot to make the plot run times equal. The multiplier is normalized to the longest run time.

For example, if Plot 1 has a run time of 40 minutes and Plot 2 has a run time of 20 minutes, and their current X-Multiplier values are both 1, clicking Equalize X, changes the X-Multiplier of Plot 2 to 2. Plot 2 will be "stretched" to a run time of 40 minutes.

Offset Y adjusts the Y-offset of each plot so that the plots start at the same point on the Y-axis.

Reset sets all X- Y- parameters to their default values.

10.9.6 Options Tab Page



Gradient Overlay selects which pump gradient lines to show overlaid on the plot.

Lines selects which lines to show on the plot.

> **NOTE The Lines options are disabled for plots displayed in the Run or Run ACI programs.**

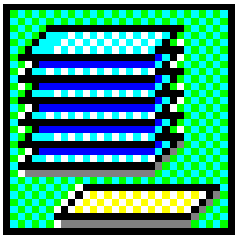
Grids selects which grid lines to show on the plot.

Other

Peak Fills selects whether to show or hide peak fills on non-overlaid plots. Peak fills cannot be turned on for plots in the overlaid view in a Comparison Window.

Legend selects whether to show or hide the Legend on overlaid plots.

11 • The Batch Program



The Batch program is used to reprocess groups of data files. To do so, Batch requires a Schedule that lists all the data files and Methods to be used. This may be the same Schedule used when the data was acquired during automated sample analysis, or you may create a new Schedule from within Batch.

When reprocessing is complete, Batch can perform the following tasks:

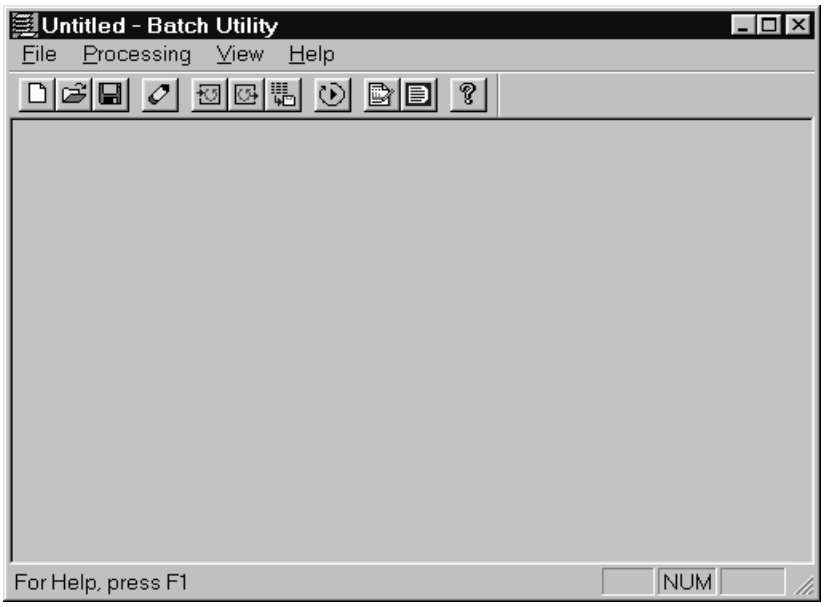
- Store the reprocessed data
- Print reports
- Update the Method(s)
- Export results to spreadsheet and database programs

Batch uses and saves the following files:

Files Used	Files Saved	Comment
*.ME?	*.ME?	Methods
*.SCH	*.SCH	Schedules
*.D??	*.D??	Raw data files
*.BCH	*.BCH	Batch Settings File
	*.CSV	File exported to Microsoft Excel

11.1 Starting the Batch Program

To open the Batch main window, click on the Batch button in the PeakNet MainMenu or double-click on BATCHDX.EXE in the directory that contains the PeakNet program files.



11.1.1 The Toolbar

Click on a toolbar button to quickly implement frequently used Batch menu commands and controls. Click on the buttons for the PeakNet MainMenu and Help to display those programs.

From left to right, the toolbar button functions are:

1. New
2. Open Settings
3. Save Settings
4. Clear
5. Input Options
6. Output Options
7. Export Options
8. Start
9. Switch to Report Designer
10. Switch to MainMenu
11. Help

11.2 File Menu

11.2.1 New

Click on the New toolbar button (or select the menu command) to reset Batch to the settings specified in the DEFAULT.BCH file (if it exists) or the program defaults. This clears all of the options you selected while working on a file.

See Save..., below, for more information about DEFAULT.BCH.

11.2.2 Open...

Click on the Open toolbar button (or select the menu command) to open the Open and select a batch settings file.

A batch settings file is a convenient way to save specifications (Schedule name, reprocessing options, export options, etc.) for a particular batch reprocessing job. If you expect to frequently reprocess using similar options, using a batch settings file will simplify setting up the job.

11.2.3 Save...

Click on the Save toolbar button (or select the menu command) to save all current reprocessing specifications (input options, output options, and export options) to the currently open batch settings file. If a batch settings file is not currently open, the Save As dialog box appears.

11.2.4 Save As...

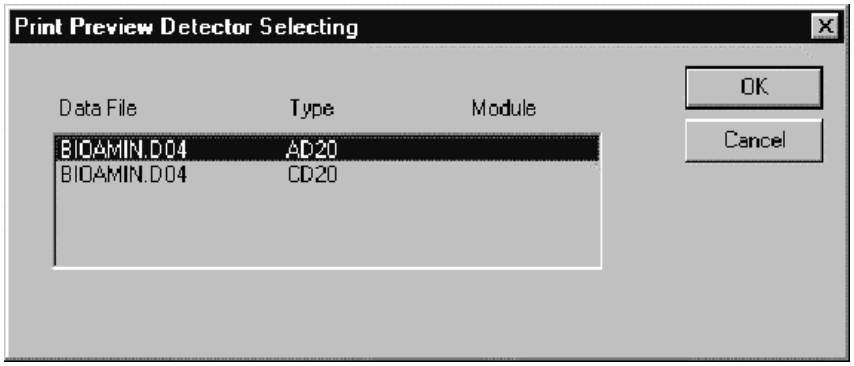
Select Save As to save all current reprocessing specifications (input options, output options, and export options) to a new batch settings file. This file can then be used with other reprocessing jobs.

Type in a filename of one to eight characters (no punctuation or spaces) in the Save As dialog box. The extension ".BCH" will automatically be added to identify the file as a batch settings file. The file will be stored in the ...\SCHEDULE directory specified in the PEAKNET.INI file, unless you specify otherwise.

NOTE If you assign the name DEFAULT.BCH to a file, the settings in the file are used as the program defaults when Batch is opened or whenever the New command is selected.

11.2.5 Print Preview

Select Print Preview to open the Batch Summary Report in the Print Preview window. A Schedule must be selected in order for this command to be available (see Section 11.3.1). If the selected Schedule contains multiple detector signals, a dialog box appears, which asks you to choose the detector to process.



The list box displays the name of the data file, the type of each detector used to collect the data, and the module name assigned in the system configuration.

Select the desired detector from the list and click OK. The data from the selected detector will then be displayed in the Print Preview dialog box.

11.2.6 Exit

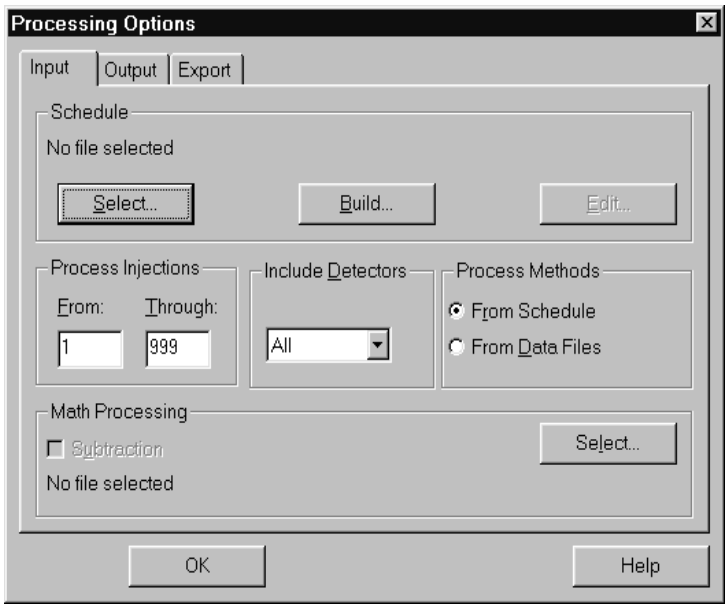
Closes the Batch program.

11.3 Processing Menu

Processing options specify which files are to be reprocessed, the type and content of any printed reports, and what occurs to raw data after reprocessing. The Processing Options dialog box contains a separate tab page for each of the three types of options: Input, Output, and Export.

11.3.1 Input...

Click on the Input Options toolbar button (or select this menu command) to display the Input tab page. If another page of the Processing Options dialog box is currently displayed, click on the Input tab to view this page.

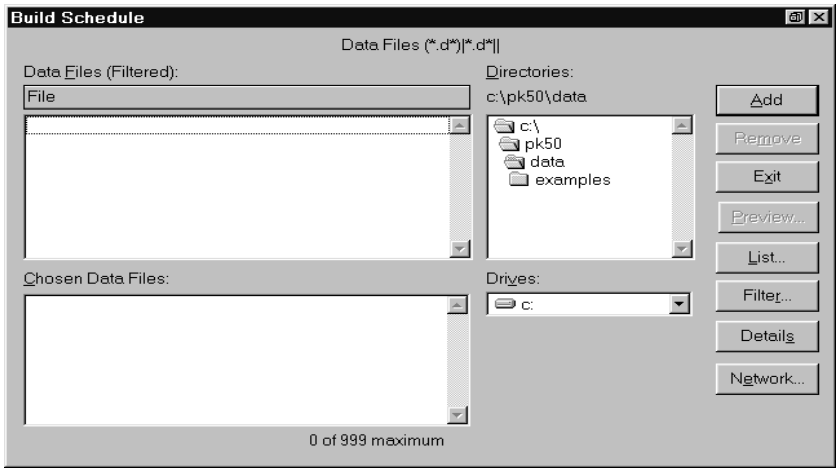


Schedule specifies the Schedule containing the data files and Methods to be used for the reprocessing.

Select... lets you select an existing Schedule to reprocess.

Build.. lets you create a new Schedule from a list of raw data files. Use Build when the Schedule previously used to collect data is no longer available, or needs to be modified.

Selecting Build... displays the Build Schedule dialog box.



From the Data Files list box, begin selecting raw data files (up to 999 per processing job) for inclusion in the new Schedule. Double-click a filename to add it to the Chosen Data Files list. When you finish, click on the **Exit** command button.

This closes the dialog box and opens the Save As dialog box. Specify a name for the new Schedule.

Edit... opens the Schedule Editor, where you can edit the selected Schedule. When you have finished editing, save the Schedule and return to the Batch program. To use the modified Schedule, click the Select... button and re-open the modified Schedule.

Process Injections From X Through X specifies the first and last injections to be reprocessed. The range automatically adjusts to the Schedule size when you select or build a new Schedule. A Schedule can include a maximum of 999 injections; each row of the Schedule spreadsheet represents one injection. Enter the desired row numbers in these edit boxes.

Include Detectors specifies from which detector(s) data is processed. Select All, 1, 2, 3, or 4 from the drop-down list box.

Process Methods

From Schedule uses the parameters of the Methods specified in the Schedule (the Methods that are saved on disk). Select this option if you want to reprocess the data files with an updated

Method file, for example, if you have optimized the Method and now want to reprocess the data files with the optimized Method parameters.

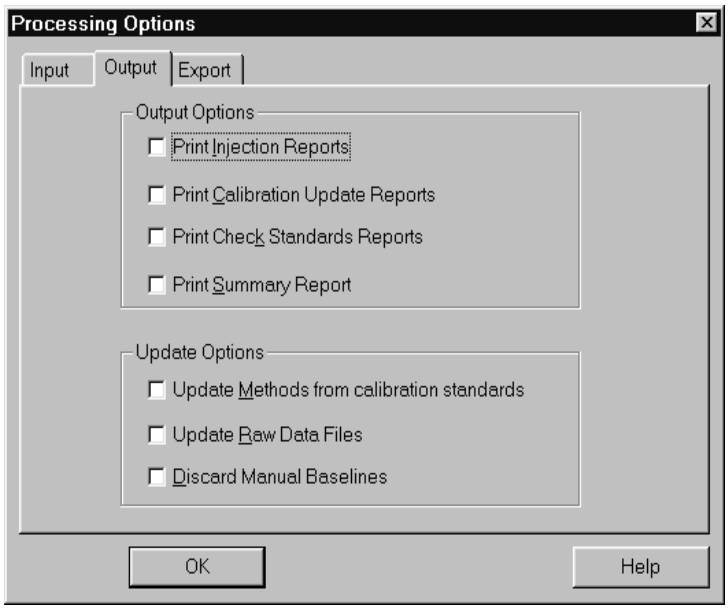
From Data Files uses the parameters of the Methods that are embedded in data files. Select this option if calibrations have changed or if baselines have been drawn manually since the Schedule was last run and you do not want to overwrite the changes.

Math Processing

To have a data file subtracted from other files in the Schedule, click on the **Select...** command button. When the file selection dialog box appears, select the data file to be subtracted and click on **OK**. The **Math Processing Subtraction** check box is now selected.

11.3.2 Output...

Click on the Output Options toolbar button (or select this menu command) to display the Output tab page. If the Processing Options dialog box is currently displayed, click on the Output tab to view this page.



Output Options specify the report types to be printed at the end of the Batch processing. Check one or more type.

Update Options determine how disk files are updated.

Update Methods from calibration standards updates the Component Table of each Method used to reprocess the data whenever a data file with the sample type Calibration Standard (or with the sample name AUTOCAL) is processed. This update provides revised peak heights and areas for each component.

Update Raw Data Files stores reprocessed data files on disk. The original data points and current Method parameters are stored under the same filename as the original data. **When you select this option, the original data points and instrument control timed events remain unaltered.** However, sample names, Method names, Method data reduction parameters, volume, dilution factor, and the Internal Standard amount in

each raw data file will be replaced by those values in the Schedule.

Discard Manual Baselines causes Batch to ignore any baselines established manually in the Optimize Program, and reintegrate the chromatogram according to the Integration Parameters and Data Events of the current Method.

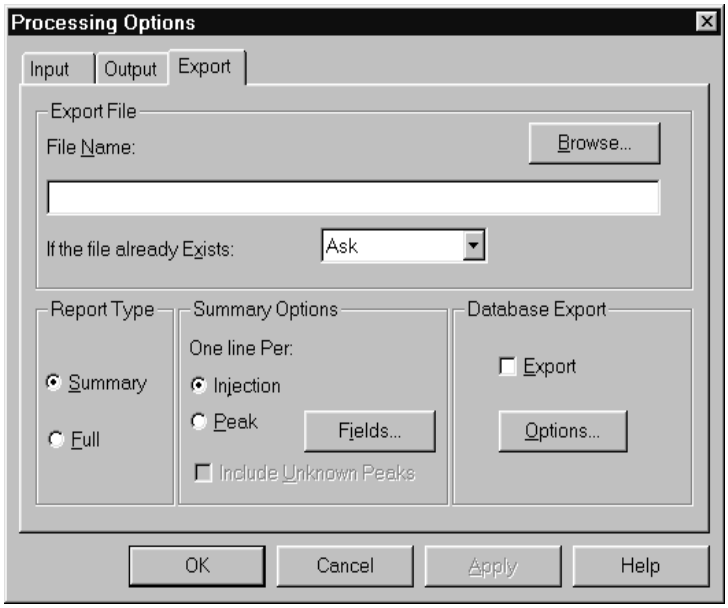
11.3.3 Export...

Export options provides two ways to export report information from a group of data files to other programs:

- Create an ASCII file that can be imported directly into Microsoft Excel
- Export data to a database that supports the ODBC (Open Database Connectivity) standard

NOTE: For details about data file export, refer to the Peaknet Help.

Click on the Export Options toolbar button (or select this menu command) to display the Export tab page. If the Processing Options dialog box is currently displayed, click on the Export tab to view this page.



Export File

File Name Enter a filename and path for the file to be exported, or click the Browse... button to open an Open dialog box, from which you can select an existing file. Add a .CSV extension to the file name to allow it to be imported into Microsoft Excel.

If you do not include a path, the default data path from the PeakNet MainMenu Options tab page will be added.

Browse... opens the Open dialog box, from which you can select a path, and filename.

If the file already exists, controls the action taken by the Batch program if the export file is found to be already present:

Ask asks you for a decision each time, if the report file already exists.

Append automatically adds the updated report to the end of the existing export file.

Overwrite automatically writes over the contents of the existing export file.

Report Type

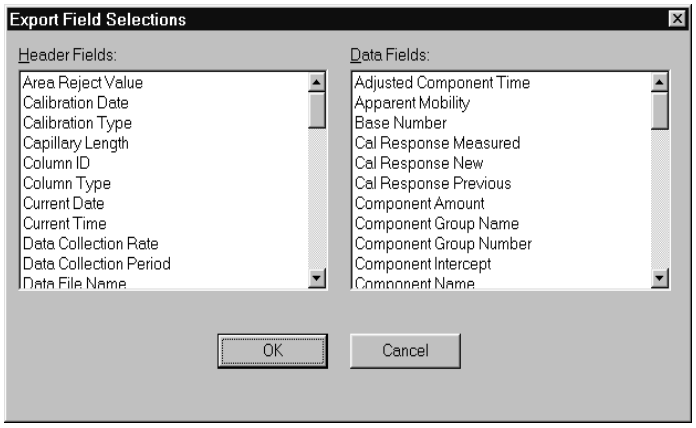
Summary contains only the variables selected in the Summary Options (see below).

Full includes all selected Peak Table and Title Table options.

Summary Options

When Summary Report Type is selected, these options determine the type and format of information to include in the report.

Fields... opens the Export Fields Selections dialog box, from which you can select the Header and Data fields to include in a Summary report. Click the desired items from each list.



One Line Per Injection generates one set of Header fields for each injection and repeats the Data fields N times, where N is the number of components in the first detector Method processed. The component name is included with each Data field.

This format is useful for summarizing data where the Method contains component names and the same components are identified in all of the injections.

One Line Per Peak generates one line in the report for each peak and/or component in the sample and Method. The first line contains the column labels for each selected Header and Data field. The Data fields are output once only and the component name is not included with the fields. When One Line Per Peak is selected, you should include Data fields to identify the data for each peak, for example, Peak Number, Peak Name, and/or Peak Retention Time.

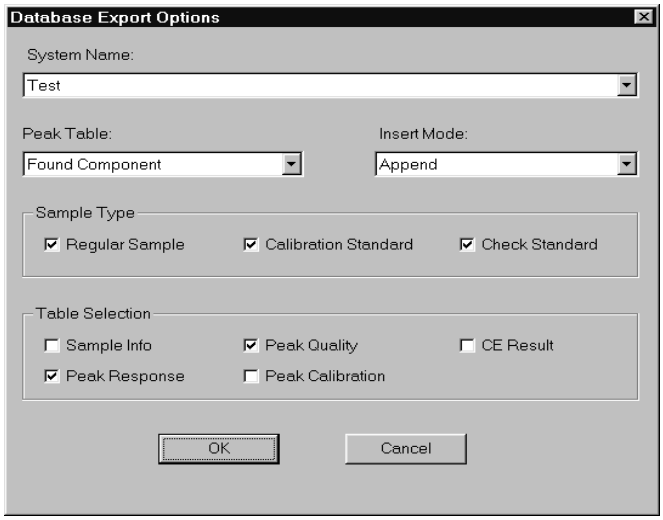
This format is useful for summarizing data from multiple detectors or different Methods, or when including unidentified peaks.

Include Unknown Peaks includes both identified and unidentified peaks in the report.

Database Export

Export enables exporting to the database using the options specified in the Database Export Options dialog box.

Options... opens the Database Export Options dialog box, from which you select the type of information to be exported to the database.



System Name lists all of the available PeakNet systems (eight) and the available ACI systems (four). Names assigned to systems configured in the Configuration Editor are shown. Default names are shown for unconfigured systems. All other options in the dialog box will apply to the selected system. You can select different options for each system.

Peak Table selects the type of Peak Tables to be exported.

None No data will be exported to the database. Selecting None disables all other options in the dialog box.

All Peaks exports data for all peaks.

All Components exports data for all the components expected to be in the injection.

Found Components exports data for components that were matched to peaks detected in the chromatogram.

Insert Mode selects whether to Append or Overwrite the database records.

Append adds the data to the end of the database

Overwrite searches the Injection Table for the most recent record with the same Method start time and replaces the old record with the new.

Sample Type selects the types of injection data to export: Sample, Calibration Standard, and Check Standard.

Table Selection selects to which tables in the database records will be exported.

OK saves the options. The options selected for all systems are saved.

11.3.4 Start

Begins the Batch processing job.

11.4 View Menu

11.4.1 Clear

Removes the messages from the Batch window. This option does not clear the selected processing options.

11.4.2 Toolbar

Shows or hides the toolbar.

11.4.3 Status Bar

Shows or hides the status bar.

11.4.4 Report Format

Opens the Report Designer program. If a Batch settings file is currently selected, the Summary Report format associated with the settings file is displayed.

11.4.5 MainMenu

Click on the MainMenu toolbar button (or select the menu command) to display the PeakNet MainMenu.

11.5 Importing Files into Microsoft Excel

1. Start the Excel program.
2. Select the Open... command from the Excel File menu.
3. In the List Files of Type box, change the file specification to "Text Files."

NOTE If you have an international version of Excel, substitute the local-language equivalent extension for a comma-separated variable file. You may also need to change the List Separator to a comma in the International section of the Windows Control Panel.

4. Select the directory that contains the file being exported from Batch, and then select (or type) in the filename.
5. Click on the OK button. Excel will then load the export data file into a spreadsheet.

11.6 Command Line Instructions

You can load a batch settings file, select Schedule and export files, and begin processing automatically by issuing instructions from the command line in Windows.

If a batch job is currently in progress, a new instance of Batch will be started so that the current job can continue without interruption.

1. In Windows, click the Start button on the Taskbar and select Run from the options menu.

2. Type the batch job parameters into the edit box. The items in brackets are optional, but you must observe this syntax:

   BATCH [SETTINGS FILE] [SCHEDULE FILE] [EXPORT FILE] [/A] [/O]

   Settings File specifies the full path and file name of a batch settings file. When present, this parameter must appear first on the command line.

   Schedule File specifies the full path and file name of a Schedule to use for batch processing. This overrides the Schedule file name in the settings file.

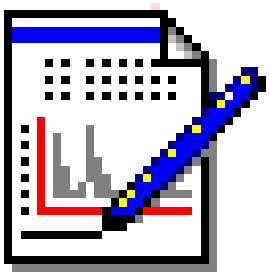
   Export File specifies the full path and file name of an export file. The file must end with a .CSV to be recognized as an export file. This overrides the export file name in the settings file.

   /A automatically starts batch processing and closes the program when the job is complete.

   /O overwrites existing export files.

3. Select <OK> or press <Enter>.

12 • The Report Designer Program



The Report Designer program creates and edits formats for single-injection and multiple-injection reports. Single-injection reports are generated by the Run, Run ACI, Optimize, and Batch programs. Multi-injection reports are generated by the Batch program.

There are three types of single-injection reports for three types of samples:

- A Sample Analysis Report is generated for a sample of unknown composition.
- A Calibration Update Report is generated for a Calibration Standard.
- A Check Standard Report is generated for a Check Standard.

All three types of report formats are included in a report format file (*.RPT), which Report Designer creates and saves to disk. Each Method has a report format file assigned to it. When a data file is created, the Method's report format is embedded into the data file.

There is one type of multi-injection report, called a Summary Report. Summary Reports are generated by the Batch Program from processing multiple injections. The Summary Report format is embedded into the batch settings file; it is not saved as a separate file.

PeakNet provides a default format for each type of report.

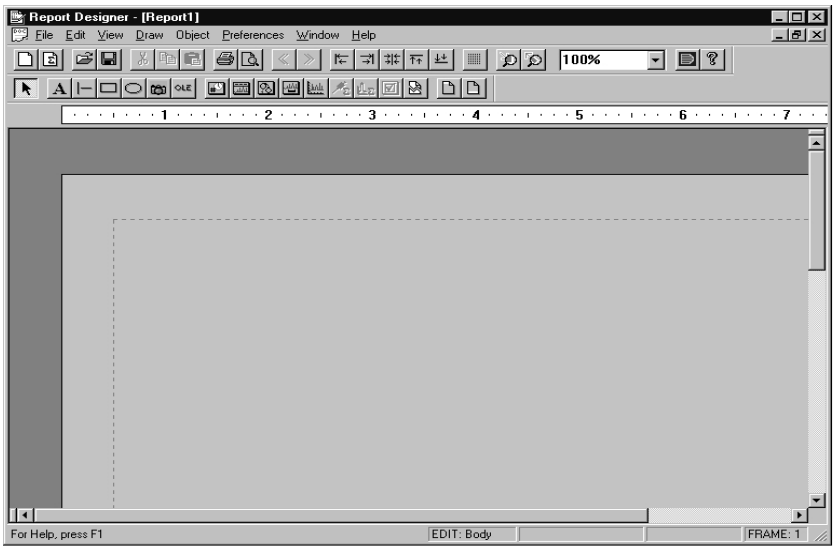
The Report Designer creates and uses the following files:

Files Used	Files Saved	Comments
*.RPT	*.RPT	Single-injection report formats saved on disk
*.BCH	*.BCH	Batch settings file with embedded Summary Report format
*.PRF	*.RPT	Form Editor files (before Release 5.0)

12.1 Starting the Report Designer Program

The Report Designer can be started from the PeakNet MainMenu or launched from the Method Editor, Optimize, or Batch programs.

To start the Report Designer from the MainMenu, click the Accessories tab and then the Report Designer button. You can also double-click on REPORTDX.EXE in the directory that contains the PeakNet program files.



To start the Report Designer from the Method Editor or Optimize program:

1. In the Method Editor, open a Method and select the detector in the Module list. In the Optimize program, open a data file and select a detector if prompted.
2. Click on the Report Options icon in the Method Editor or the Report Options button on the Optimize program toolbar. The Report Options dialog box opens.
3. Click on the button for the type of report you want to edit. The Report Designer opens and displays the report format for the selected detector and report type.

To start the Report Designer from the Batch program, click the Report Designer button on the toolbar. The Report Designer opens and displays the Summary Report format for the selected batch settings file.

12.1.1 The Toolbar

Click on a toolbar button to quickly implement frequently used Report Designer menu commands and controls. Click on the buttons for the PeakNet MainMenu and Help to display those programs.

From left to right the toolbar button functions are:

1. New Format File
2. New Summary File
3. Open
4. Save
5. Cut
6. Copy
7. Paste
8. Print
9. Print Preview
10. Previous Frame
11. Next Frame
12. Align left
13. Align right
14. Center
15. Align top
16. Align bottom
17. Toggle Grid
18. Zoom In
19. Zoom Out
20. Zoom control
21. Switch to MainMenu
22. Help

12.1.2 The Drawing Toolbox

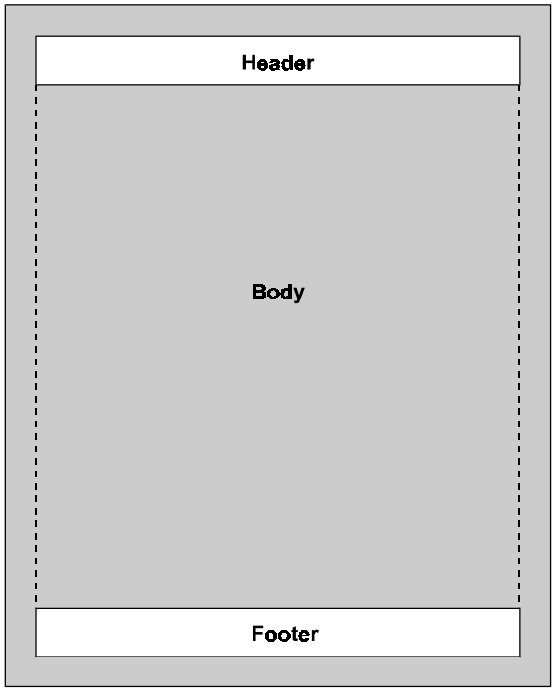
Click on a Drawing Toolbox button to quickly access the commands available from the Draw menu. The available tools depend on whether a single-injection or a Summary Report is being created or edited.

From left to right, the toolbox button functions are:

1. Select
2. Text
3. Line
4. Rectangle
5. Ellipse
6. Bitmap
7. New Object
8. Title Table
9. Peak Table
10. Method Table
11. Group Table
12. Chromatogram
13. Concise Summary Table
14. Peak Detail Summary Table
15. System Suitability Table
16. Page Break
17. Show/Hide Header
18. Show/Hide Footer

12.2 Overview of the Report Page Layout

A report page consists of three regions: a header, a footer, and a page body.



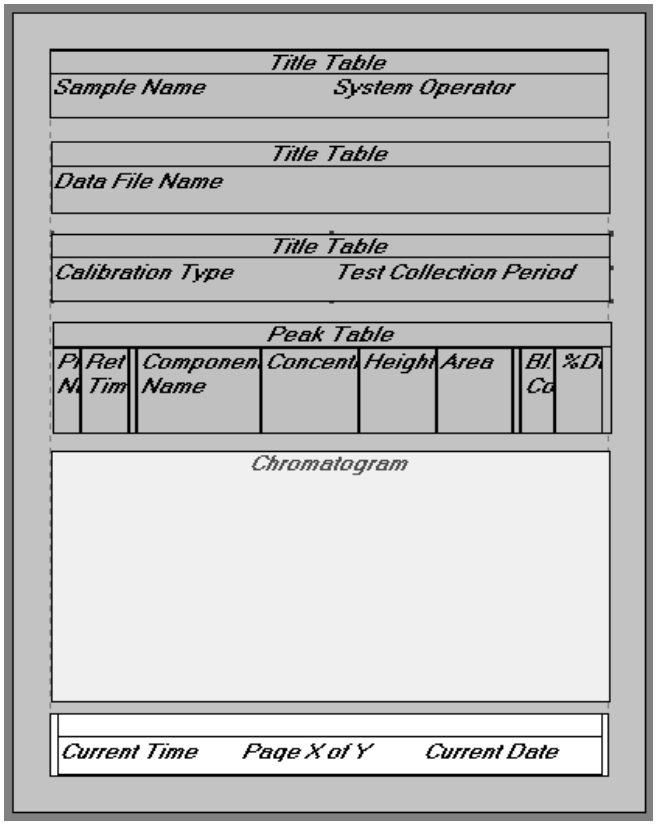
To design the report, you place a combination of the objects from the Drawing Toolbox on the report page. Objects placed in the header and footer regions will print on every page of the report.

Tables allow you to choose the type of information to include in a report:

- Title Tables provide system, injection, or general report information.
- Peak Tables (for single-injection reports only) provide information about the peaks found in the injection.
- Group Tables (for single-injection reports only) provide information about component groups.
- Method Tables provide information about the Method's parameters.
- Concise Summary and Peak Detail Summary Tables (for Summary Reports only) let you summarize information about the peaks from multiple injections.

- System Suitability Tables (for Summary Reports only) report the results of suitability tests for a set of injections.

A typical page layout for a Sample Analysis Report is shown below.



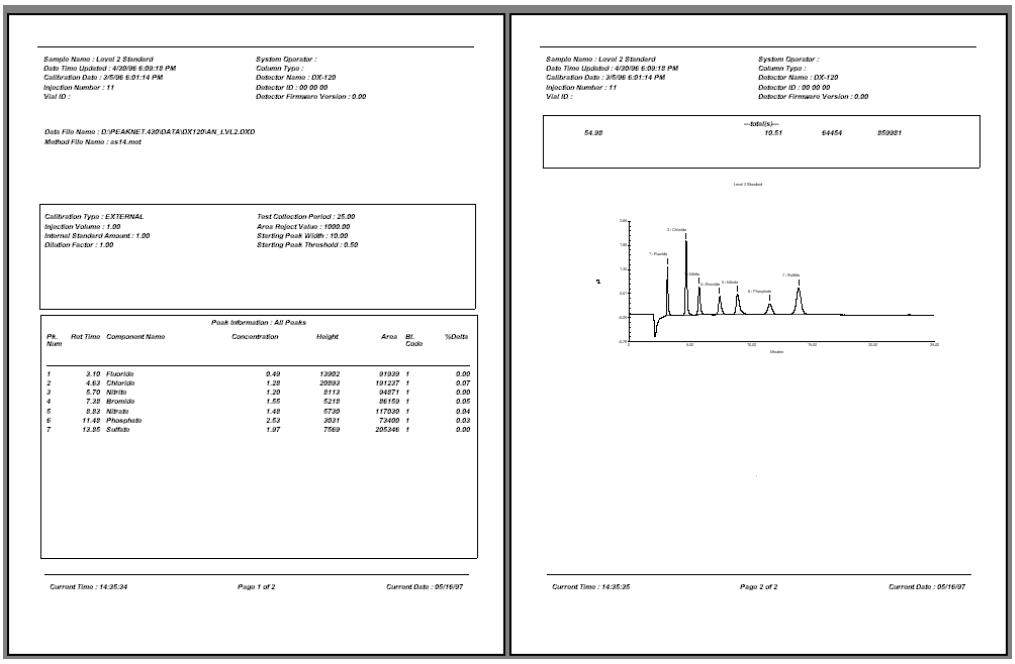
To add an object to a report, click on the object's tool in the Drawing Toolbox and draw the object at the desired location on the page.

To edit a report object, double-click inside the object. A dialog box appears, which allows you to edit the object's properties (add or remove items from a table, change fonts, change line widths, and so on.)

To see an example of how the report will look when printed:

1. Assign data to the report:
   - For single-injection reports, select Assign Data from the File menu and select an existing data file.
   - For Summary Reports, select Assign Schedule from the File menu and select an existing Schedule file.
2. Click the Print Preview button on the toolbar.

When the example Sample Analysis Report is printed, it will resemble the following example:



Sample Name : Level 2 Standard
Data Time Updated : 4/30/96 6:09:19 PM
Calibration Date : 3/5/96 6:01:14 PM
Injection Number : 11
Vial ID :

System Operator :
Column Type :
Detector Name : DX-120
Detector ID : 00 00 00
Detector Firmware Version : 0.00

Data File Name : D:\PEAKNET-430\DATA\DX120\AN_LVL2.DXD
Method File Name : as14.mat

Calibration Type : EXTERNAL
Injection Volume : 1.00
Internal Standard Amount : 1.00
Dilution Factor : 1.00

Test Collection Period : 25.00
Area Reject Value : 1000.00
Starting Peak Width : 10.00
Starting Peak Threshold : 0.50

Peak Information : All Peaks

Pk. Num	Ret Time	Component Name	Concentration	Height	Area	Bl. Code	%Dotts
1	3.10	Fluoride	0.49	13982	91939	1	0.00
2	4.63	Chloride	1.28	28893	191237	1	0.07
3	5.70	Nitrite	1.20	9113	94871	1	0.00
4	7.38	Bromide	1.55	5218	96159	1	0.05
5	8.93	Nitrate	1.48	5736	117030	1	0.04
6	11.48	Phosphate	2.52	3031	73400	1	0.03
7	13.95	Sulfate	1.97	7569	205346	1	0.00

Current Time : 14:35:34 Page 1 of 2 Current Date : 05/16/97

Sample Name : Level 2 Standard
Data Time Updated : 4/30/96 6:09:19 PM
Calibration Date : 3/5/96 6:01:14 PM
Injection Number : 11
Vial ID :

System Operator :
Column Type :
Detector Name : DX-120
Detector ID : 00 00 00
Detector Firmware Version : 0.00

	--totals--		
54.38	10.51	64454	859981

Current Time : 14:35:35 Page 2 of 2 Current Date : 05/16/97

Notice that, although the report format was a single page in the Report Designer window, the report printed out on two pages. This is because the tables and the chromatogram are sized dynamically when the report is generated, depending on the amount of data to be reported.

12.3 File Menu

12.3.1 New Format File

Opens a new blank single-injection report file.

12.3.2 New Summary File

Opens a new batch file.

12.3.3 Open...

Click on the Open toolbar button (or select the menu command) to display the Open dialog box and select an existing report format. Select the type of format to open from the Files of type list.

12.3.4 Close

Closes the active report format.

12.3.5 Save

Click on the Save toolbar button (or select the menu command) to save the current report format to disk. If the format was not previously saved, the Save As dialog box opens for you to assign a name.

12.3.6 Save As...

Opens the Save As dialog box for saving the active format to a new name.

12.3.7 Assign Data...

Opens the Open dialog box. Select an existing data file to be used for displaying example data in a single-injection report format.

12.3.8 Assign Schedule...

Opens the Open dialog box. Select an existing Schedule to be used for displaying example data in a Summary Report format.

12.3.9 Print...

Prints the assigned data in the active report format.

12.3.10 Print Preview

Opens the Print Preview window, which displays the current report format with the assigned data, as it will look when printed.

12.3.11 Page Setup...

Changes the Paper, Orientation, and Margin settings of the active report format.

12.4 Edit Menu

12.4.1 Cut

Click on the Cut toolbar button (or select the menu command) to cut the current selection before pasting it to another location. Use the Select tool on the Drawing Toolbox to select one or more objects on the Report Designer frame.

NOTE Report objects are any of the items added to the report using the Drawing Toolbox tools, including text, tables, and graphics. The frame is the area in the Report Designer window in which you place the report objects.

12.4.2 Copy

Click on the Copy toolbar button (or select the menu command) to copy the current selection before pasting it to another location.

12.4.3 Paste

Click on the Paste toolbar button to insert the previously cut or copied object(s).

12.4.4 Select All

Selects all objects on the Report Designer frame.

12.4.5 Add Frame

Add a new frame to the active report format.

NOTE Because the tables placed on a frame are sized dynamically when the report is printed (depending on the amount of data to be reported), objects placed on one frame may print out on several pages of the report.

12.4.6 Remove Frame

Remove the current frame from the active report format.

12.4.7 Next Frame

Click on the Next Frame toolbar button (or select the menu command) to show the next frame.

12.4.8 Previous Frame

Click on the Previous Frame toolbar button (or select the menu command) to show the previous frame.

12.5 View Menu

12.5.1 Sample Analysis Report

Displays the Sample Analysis Report format of the current Method.

12.5.2 Calibration Update Report

Displays the Calibration Update Report format of the current Method.

12.5.3 Check Standard Report

Displays the Check Standard Report format of the current Method.

12.5.4 Summary Report

This menu command will be selected automatically when a batch settings file is opened.

12.5.5 Header

Click on the Header toolbar button (or select the menu command) to show or hide the header region on the report frame.

12.5.6 Footer

Click on the Footer toolbar button (or select the menu command) to show or hide the footer region on the report frame.

12.5.7 Ruler

Show or hide the ruler.

12.5.8 Zoom>

Use the Zoom controls on the toolbar (or select from the Zoom cascade menu on the View menu) to select a pre-set page magnification.

12.5.9 Grid Lines

Click on the Toggle Grid toolbar button (or select the menu command) to show or hide the drawing grid.

12.5.10 Drawing Toolbox

Show or hide the Drawing Toolbox.

12.5.11 Toolbar

Show or hide the toolbar.

12.5.12 Status Bar

Show or hide the status bar.

12.5.13 MainMenu

Display the PeakNet MainMenu.

12.6 Draw Menu

12.6.1 Select

Click on the Select button on the Drawing Toolbox (or select the menu command), to select one or more report objects.

12.6.2 Text

Click on the Text button on the Drawing Toolbox (or select the menu command), to add text to the report format.

1. Position the text pointer where you want the text to appear.
2. Drag to create a rectangle for the text.
3. Click inside the rectangle and type the text.
4. Click outside the rectangle to complete the text entry.

12.6.3 Line

Click on the Line button on the Drawing Toolbox (or select the menu command), to draw a horizontal or vertical line on the report format.

1. Point to where you want to start the line and drag either horizontally or vertically to draw the line.
2. Release the mouse button.

NOTE The line will snap to a straight horizontal or vertical position. The Report Designer does not allow diagonal lines.

12.6.4 Rectangle

Click on the Rectangle button on the Drawing Toolbox (or select the menu command), to draw a rectangle or square on the report format.

1. Point to where you want to start the rectangle or circle and drag.
2. Release the mouse when the rectangle is the desired size.

NOTE To draw a square, check the SIZE column on the Status Bar after you release the mouse. If the two numbers are not equal, point to one of the rectangular resize handles in the center of the rectangle (not one on a corner) and drag to adjust the size until the numbers are the same.

12.6.5 Ellipse

Click on the Ellipse button on the Drawing Toolbox (or select the menu command), to draw an ellipse or circle on the report format.

1. Point to where you want to start the ellipse or circle and drag.
2. Release the mouse when the ellipse is the desired size.

NOTE To draw a circle, check the SIZE column on the Status Bar after you release the mouse. If the two numbers are not equal, point to one of the rectangular resize handles on the circle and drag to adjust the size until the numbers are the same.

12.6.6 Bitmap

Click on the Bitmap button on the Drawing Toolbox (or select the menu command), to insert a picture from a graphic file into the report format.

1. Point to where you want the picture to be inserted and drag to create a rectangle.
2. Release the mouse button,

   The Open dialog box appears.

4. Select the picture to be inserted. You can open either a BMP (Windows Bitmap) or DIB (Device-Independent Bitmap) file.
5. After you close the dialog box, if the size of the picture is different from the rectangle you drew, the Report Designer asks whether you want the rectangle fitted.
    - If you click yes, the Report Designer resizes the rectangle to fit the picture.
    - If you click no, the Report Designer fits the picture into the drawn rectangle. This may distort the picture if the rectangle does not have the same aspect ratio as the original picture.

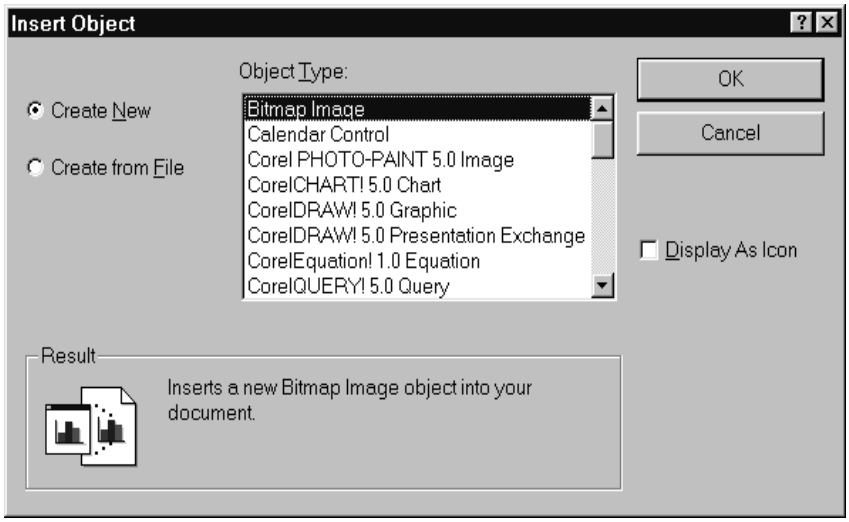
NOTE

- You can move, resize, or delete the picture.
- You cannot edit a picture that has been inserted using the Picture tool. To edit pictures from within the Report Designer, insert them as OLE objects.

12.6.7 OLE Object

Click on the OLE Object button on the Drawing Toolbox (or select the menu command) to insert a linked or embedded object into the report format.

The Insert Object dialog box appears.



NOTES

- An OLE object is information that is created by an application that supports OLE (Object Linking and Embedding) and that can be inserted (linked or embedded) into the report. The other application must be installed on your computer. Examples of OLE objects include chemical structures, word processing files, and spreadsheet files.
- You can insert new or existing OLE objects into a PeakNet report.
- When new OLE objects are embedded into the report, they become part of the report format and are not saved as separate files.
- Objects created previously can be either embedded or linked. When linked, the object retains a connection to the original file; any changes made to the original are reflected in the object in the report, and vice versa.

Create New is used to insert a new object into the report format. The object will be the type selected in the the Object Type list.

Object Type lists the installed applications that support OLE linking and embedding.

Create from File is used to insert an existing object into the report format. When this button is selected the dialog box displays a field for entering the name of the file to insert. Click the **Browse...** button to select the file from a Browse dialog box.

Link inserts a copy of the existing object into the report. Linked objects appear outlined with a dashed line on the Report Designer frame.

Display As Icon inserts the new or existing object in the report as an icon.

OK closes the dialog box and inserts the object into the report.

- If you inserted a new object (not as an icon), the Report Designer application window switches to the menus, toolbars, and other controls for the type of object you inserted. After you create the new object, press the Esc key to return to the Report Designer menus and toolbars.
- If you inserted a new object as an icon, the application for the type of object being created opens. After you create the new object, select Exit from the File menu. The new object appears as an icon on the report page.

You can move, re-size, and align OLE objects just as you do other objects in the report. In addition, you can edit the contents of the OLE object directly from the Report Designer.

To edit the OLE object, double-click anywhere inside the object or, if it was inserted as an icon, double-click the icon.

12.6.8 Title Table

Click on the Title Table button on the Drawing Toolbox (or select the menu command) to add a Title Table to the report format. Title Tables provide system, injection, or general report information such as dates, detector information, operator name, sample information, etc. Title Tables can be added to the header and footer, and to the body of any type of report. See Section 12.10 for details about creating tables.

12.6.9 Peak Table

Click on the Peak Table button on the Drawing Toolbox (or select the menu command) to add a Peak Table to the report format. Available for single-injection report formats only. See Section 12.10 for details about creating tables.

12.6.10 Group Table

Click on the Group Table button on the Drawing Toolbox (or select the menu command) to add a Group Table to the report format. Available for single-injection report formats only. See Section 12.10 for details about creating tables.

12.6.11 Chromatogram

Click on the Chromatogram button on the Drawing Toolbox (or select the menu command) to add a Chromatogram to the report format. Available for single-injection report formats only. See Section 12.11 for details about adding chromatograms to a report format.

12.6.12 Method Table

Click on the Method Table button on the Drawing Toolbox (or select the menu command) to add a Method Table to the report format. See Section 12.10 for details about creating tables.

12.6.13 Concise Summary Table

Click on the Concise Summary Table on the Drawing Toolbox button (or select the menu command) to add a Concise Summary

Table to the report format. Available for Summary Report formats only. See Section 12.10 for details about creating tables.

12.6.14 Peak Detail Summary Tables

Click on the Peak Detail Summary Tables button on the Drawing Toolbox (or select the menu command) to add Peak Detail Summary Tables to the report format. Available for Summary Report formats only. See Section 12.10 for details about creating tables.

12.6.15 System Suitability Table

Click on the System Suitability Table button on the Drawing Toolbox (or select the menu command) to add a System Suitability Table table to the report format. Available for Summary Report formats only. See Section 12.10 for details about creating tables.

12.6.16 Page Break

Click on the Page Break button on the Drawing Toolbox (or select the menu command), and then click the location on the report frame where you want a new page to start when the report is printed.

12.7 Object Menu

12.7.1 Properties...

Opens the Properties dialog box for the selected report object.

12.7.2 Move>

Forward moves the selected report object forward one layer.

Back moves the selected object back one layer.

To Front moves the selected object to the top layer.

To Back moves the selected object to the bottom layer.

12.7.3 Align>

Center, centers the objects horizontally on the page.

Left aligns the left edges of the selected objects with the highlighted object.

Right aligns the right edges of the objects with the right edge of the last selected object.

Top aligns the top edges of the objects with the top edge of the last selected object.

Bottom aligns the bottom edges of the objects with the bottom edge of the last selected object.

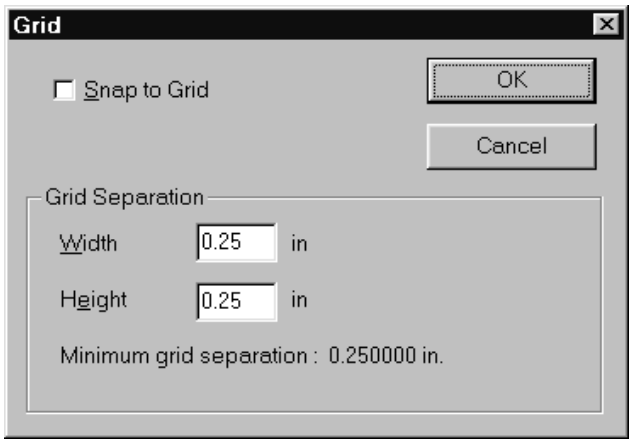
12.7.4 Links...

Opens the Links dialog box, for changing parameters relating to the OLE objects linked to the report format.

12.8 Preferences Menu

12.8.1 Grid

Opens the Grid dialog box, for changing parameters relating to the drawing grid. The grid is a network of horizontal and vertical lines that helps you align objects on the report page.



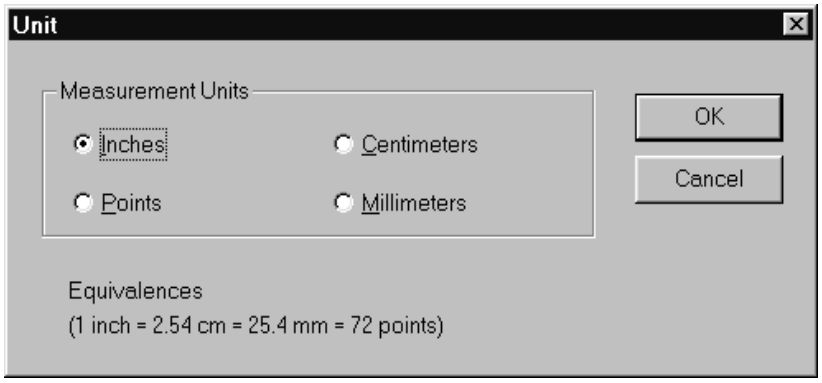
Snap to Grid makes objects that you add or move align at the nearest grid intersections. The "snap" occurs when you release the mouse button.

Grid Separation

Width/Height specifies the space between vertical grid lines (width) and the space between horizontal grid lines (height). The width and height spacing does not have to be the same.

12.8.2 Unit

Opens the Unit dialog box, for changing the ruler and grid units of measure. When the units are changed, the existing grid size is converted to the new units. For example, if the grid size was originally 0.25 inches and the units are changed to centimeters, the grid size will be converted to 0.635 centimeters. When you switch units, you will probably also want to select a new grid size that is more useful for the selected units.



12.8.3 Default Font

Opens the Font dialog box, for changing the default font used for text in tables and text that you add with the Text tool.

12.8.4 Page Color

Opens the Color dialog box, for changing the background color of the report page (for display purposes only).

12.9 Window Menu

12.9.1 New Window

Creates a new view of the currently selected report format. Changes you make in one window will be updated in all views of that report format; scrolling one of the views does not scroll the others.

12.9.2 Cascade

Arranges all windows in a diagonally descending pattern (overlapped) so that the title bar of each is visible.

12.9.3 Tile

Arranges all windows in a non-overlapped pattern.

12.9.4 Arrange Icons

Arranges all window icons at the bottom of the main Report Designer window.

12.9.5 Open Windows List

Make an open window active by choosing its name from this list.

12.10 Report Tables

To add a table to a report format:

1. On the Drawing Toolbox, click the button for the type of table to be added.

   The pointer changes to a small table with a pencil.

2. Position the pencil pointer where you want the table to begin, and drag to create the table.

Notes

- You can change the width and length of the table and move it to a different position on the page.
- The final length of the table depends on the amount of data to be printed. If the space allocated in the report format is smaller than the amount of data, the table expands to include all of the information. Other tables or report objects are shifted down. (The table does not reduce in length, however, if more space is allocated in the report format than is needed.)
- In the same way, the table's final page position depends on whether there are other variable length tables positioned before it, which shift it down the page.
- Use the line numbers in the table format to estimate what the vertical length of a table will be when it is printed. For example, if you are creating a Peak Table that will include information about eight peaks, adjust the vertical length of the table until eight numbered lines are visible.

12.10.1 Table Properties

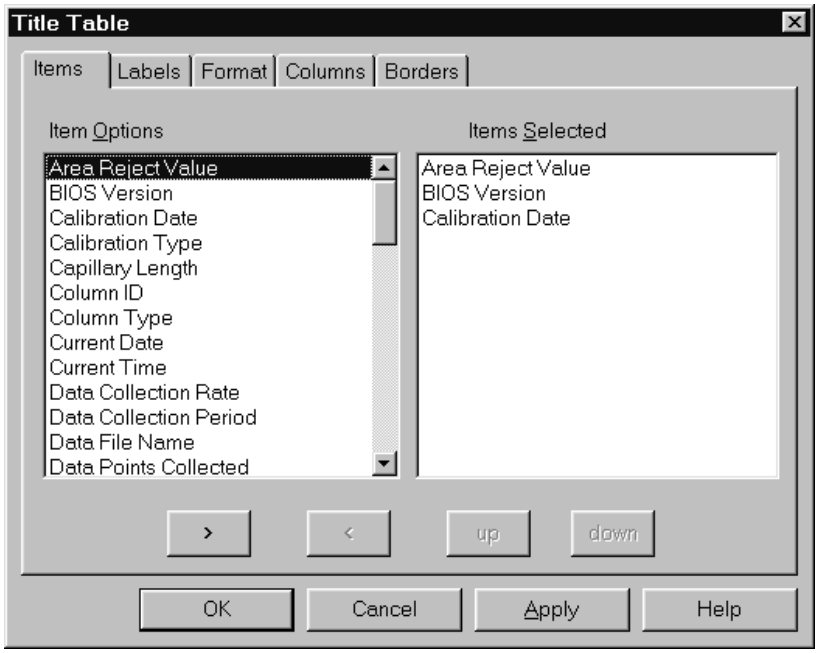
To edit a table's properties (add or delete items, change the format, change the item labels, etc.), double-click inside the table or select the table and select Properties... from the Object menu. The table's properties dialog box appears.

The tab pages and controls included in the properties dialog box will vary, depending on the type of table being edited.

The following sections describe table properties tab pages that are common to all table types. Following that are descriptions of unique features for each type of table.

NOTE When editing a table's properties, if you make a change and then click another tab to move to a different tab page, the current settings are "remembered" and applied when the dialog box is closed.

Items Tab Page



Item Options contains all the items that can be included in the table. Double-click an item to include it in the table, or select it and click the right arrow (>) button.

Items Selected contains the items to be included in the table. The items will appear in the table in the order in which they appear in this list. To move an item back to the Item Options list, double-click it, or select it and click the left arrow (<) button.

Except for Title Tables, each item added to the Selected Items list will create a new column in the table.

Title Table items are included in the table in a vertical list. The list can be divided into columns if desired using the controls in the Columns tab page.

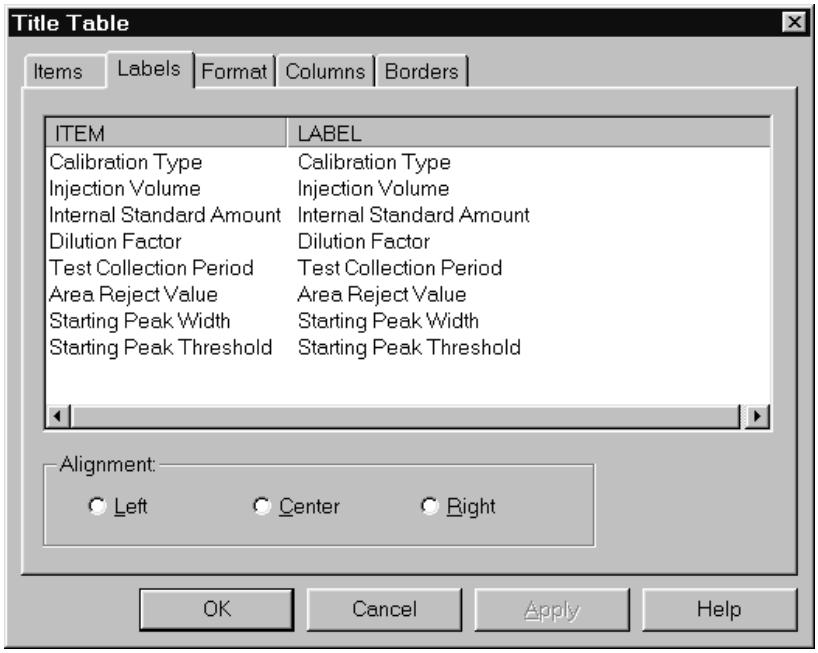
> moves a selected item to the Items Selected list.

> removes a selected item from the Items Selected list.

up moves a selected item up the Items Selected list.

down moves a selected item down the Items Selected list.

Labels Tab Page



ITEM shows the items to be included in the table.

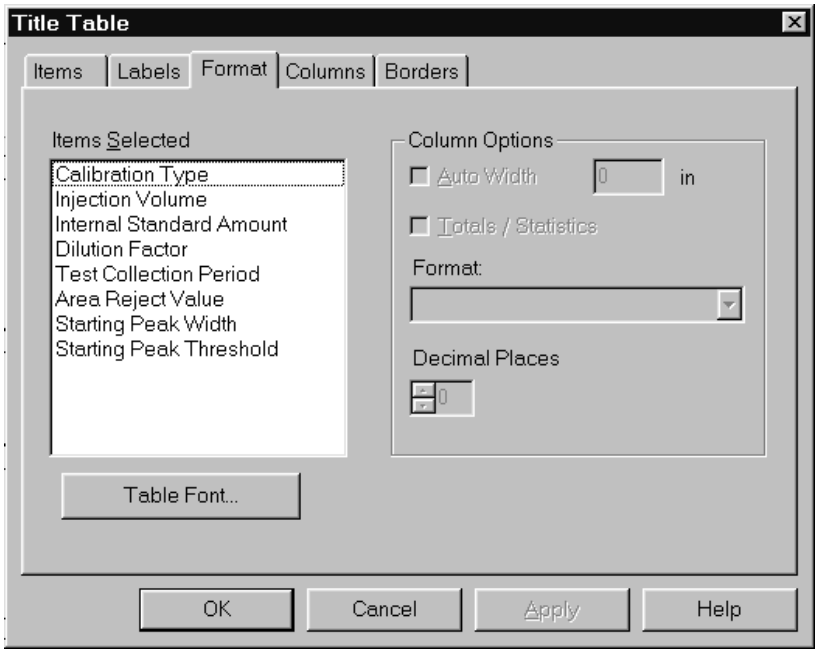
LABEL shows the column label for each item. **To change a label,** click with the right mouse button on the item label and type the new label.

Alignment determines how the items are aligned within a column. The default is left-aligned. To change the alignment, select an item in the ITEM list and click Left, Center, or Right.

Item Type (Peak Detail Summary Tables only)

> **Injection Variables** when selected, the ITEM list shows the Injection Variables to be included in the table. An Injection Variable has a single, unique value that can be different for each injection, but not for each peak
>
> **Peak Variables** when selected, the ITEM list shows the Peak Variables to be included in the table. Peak Variables can have a different value for each peak in a chromatogram

Format Tab Page



Items Selected shows the list of items selected in the Items tab page.

Item Type (Peak Detail Summary Tables only) selects which list of items (Injection Variables or Peak Variables) will appear in the Items Selected box.

Column Options

Auto Width when checked, an item's default column width is used. To manually set an item's column width, click the item in the list. Then, clear the Auto Width check box and enter a value in the edit box. This parameter is not available in Title Tables.

Totals/Statistics when checked for an item in a Peak Table, the total of the item's values is displayed at the bottom of the table. When checked for an item in an Concise Summary or Peak Detail Summary Table, the item's statistics are displayed. This parameter is not available for all items or in Title Tables.

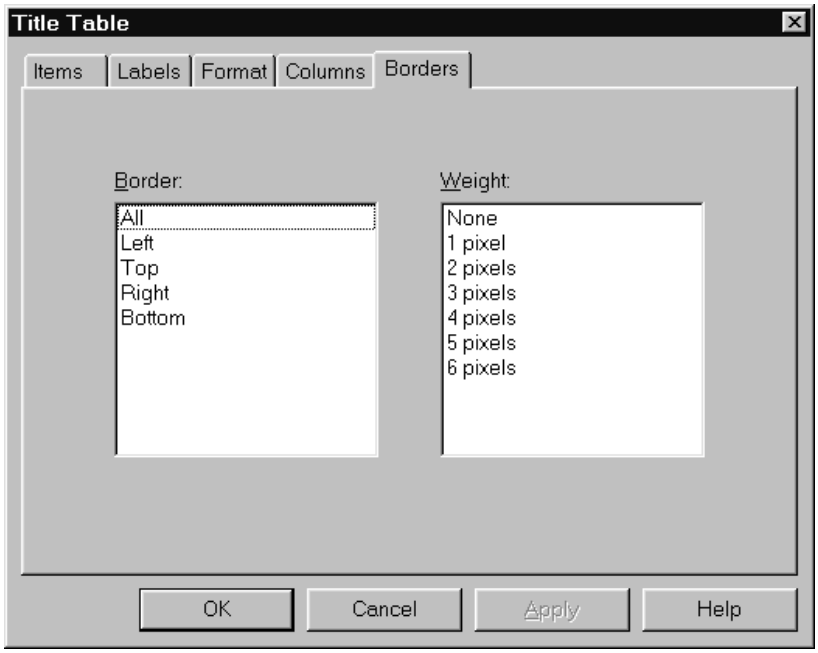
Format: Standard/Scientific selects a format for table items that contain decimal places. Standard shows decimal places; Scientific shows exponential notation.

Decimal Places selects the number of decimal places to display for items with more than integer precision.

Table Font... opens the Font dialog box to select a font for the table items.

Borders Tab Page

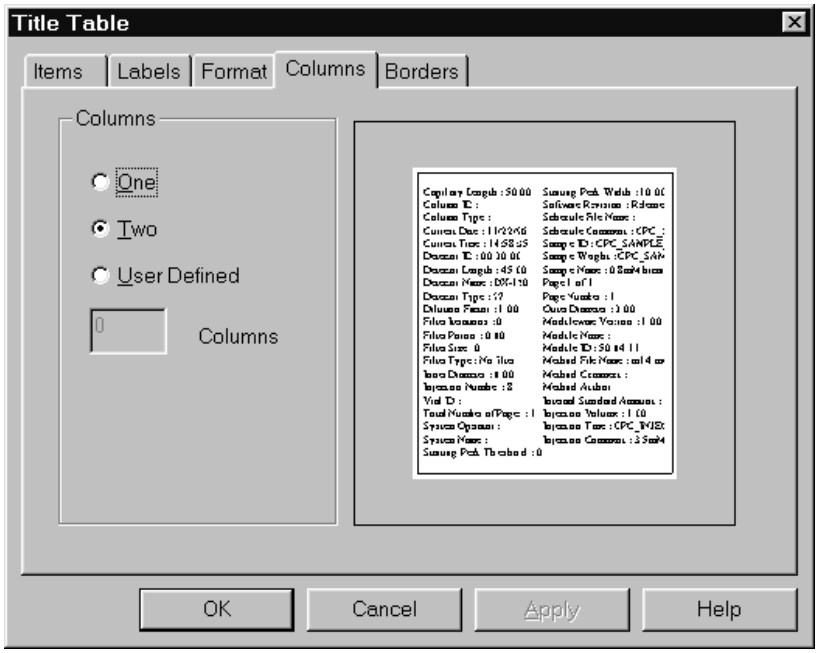
The Borders tab page lets you select a line weight for borders around the outside edges of the table.



Border selects the border whose line weight is to be changed.

Weight selects the desired line weight for the border. The default is None.

Title Table - Columns Tab Page

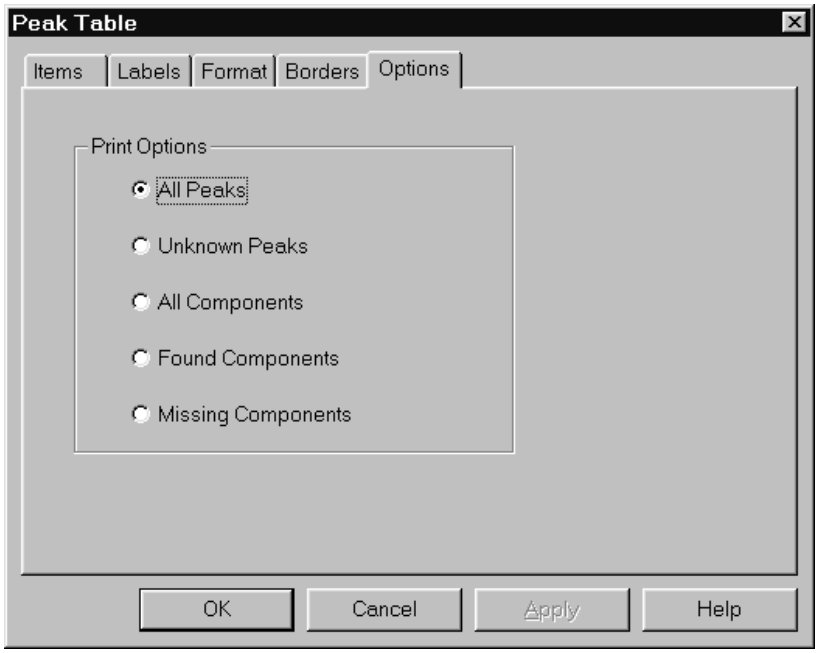


Columns determines the number of columns in which the items in the Title Table will be distributed. For more than two columns, select User Defined and enter the desired number of columns.

Items from the Selected Items list are distributed into the columns according to the following rules:

- The Report Designer determines how many items will be in each column and then places them sequentially. For example, if there are going to be two items in each column, the first two items are placed in the first column, the next two in the second column, and so on.
- If there is an uneven number of items per column, the column(s) on the left will contain the additional item(s).

Peak Table - Options Tab Page



All Peaks prints all the peaks with areas greater than the Area Reject setting of the Integration Parameters dialog box.

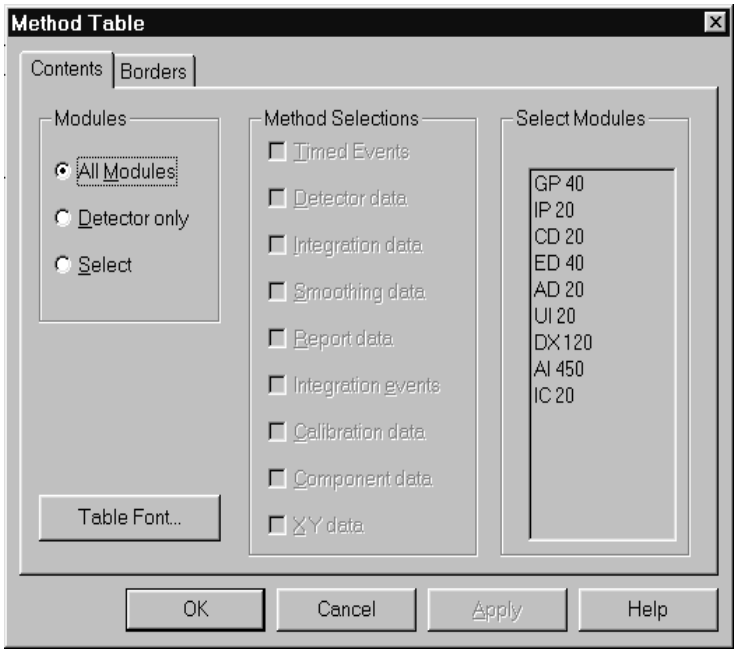
Unknown Peaks prints the peaks with areas greater than the Area Reject setting of the Integration Parameters that were not matched to expected components. Unknown peaks are numbered independently from the identified peaks, according to their retention times, that is, Unknown 1 has the shortest retention time of the unknowns, Unknown 2 has the next shortest retention time, and so on.

All Components prints all the components listed in the Component Table of the Method, whether they were found or not.

Found Components prints only the components that were matched to peaks detected in the chromatogram.

Missing Components prints only the expected components that were not matched to peaks detected in the chromatogram.

Method Table - Contents Tab Page



Modules

All Modules, when selected, Method information for all modules configured in the system will be included.

Detector only, when selected, Method information for the detector only will be included.

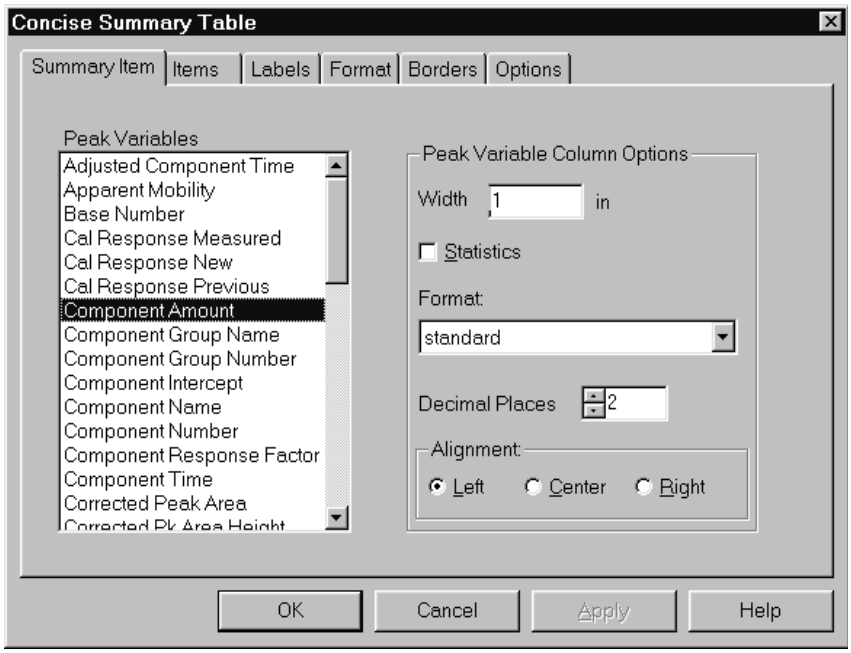
Select lets you select the modules and the type of Method information to include in the table.

Method Selections (available if the Select option is chosen) select one or more types of Method data to include in the table.

Select Modules (available if the Select option is chosen) select the modules whose Method data should be included in the table.

Table Font... opens the Font dialog box to select a font for the table items.

Concise Summary Table - Summary Item Tab Page



Peak Variables lists the items that can be summarized. Only one Summary Item can be selected. For each peak in the schedule, the table will contain a column showing the values for the selected item.

Peak Column Options

The Peak Column Options fill in automatically with default settings for the selected item. These settings can be customized if desired:

Width selects the width of the table columns.

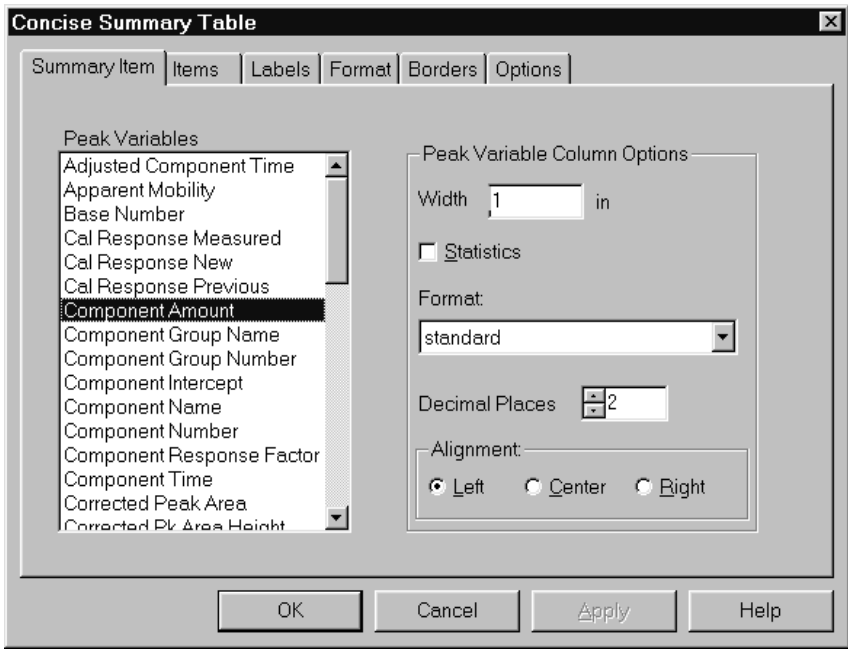
Totals/Statistics, when checked, the total and the %RSD (percent relative standard deviation) is printed below the item's column.

Format selects the format for non-integer numeric items. Standard shows decimal places; Scientific shows exponential notation.

Decimal Places selects the number of decimal places to display for items with more than integer precision.

Alignment selects the alignment of the item in the columns.

Concise Summary Table - Options Tab Page



All Peaks prints all the peaks with areas greater than the Area Reject setting of the Integration Parameters dialog box.

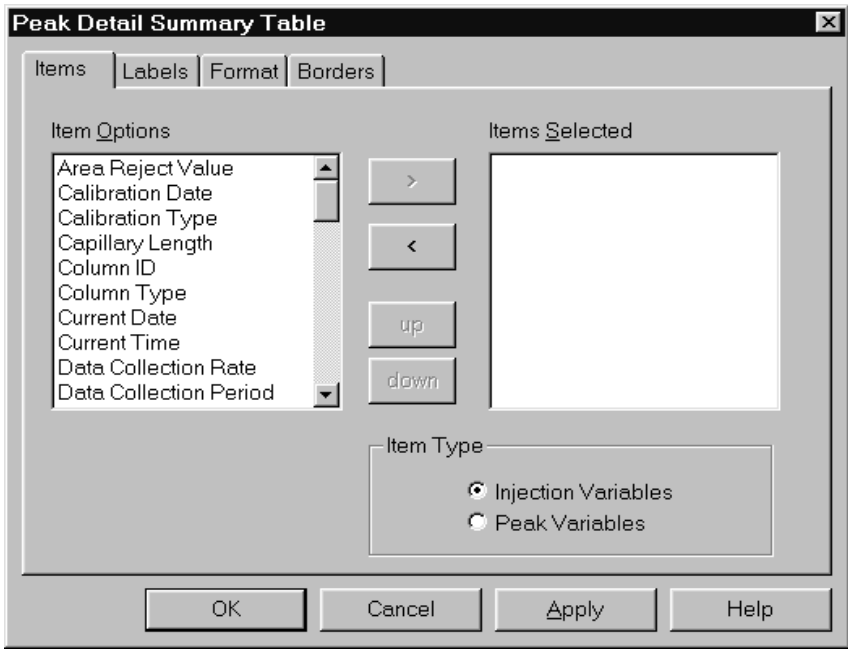
Unknown Peaks prints the peaks with areas greater than the Area Reject setting of the Integration Parameters that were not matched to expected components. Unknown peaks are numbered independently from the identified peaks, according to their retention times, that is, Unknown 1 has the shortest retention time of the unknowns, Unknown 2 has the next shortest retention time, and so on.

All Components prints all the components listed in the Component Table of the Method, whether they were found or not.

Found Components prints only the components that were matched to peaks detected in the chromatogram.

Missing Components prints only the expected components that were not matched to peaks detected in the chromatogram.

Peak Detail Summary Tables - Items Tab Page



Item Options lists items that can be added to the Peak Detail Summary Tables. Each selected item creates a new column in the table. The list changes depending on whether Injection Variables or Peak Variables is selected in the Item Type options (see below). The total number of items that can appear in one table is limited by how many columns will fit on the width of the page.

To include an item in the table, double-click it, or select it and click the right arrow (>) button.

Items Selected lists the items to be included in the table. The items are included in the order in which they appear in this list. To move an item back to the Item Options list, double-click it, or select it and click the left arrow (<) button.

Item Type determines which items are shown in the Item Options list. When **Injection Variables** is selected, the Items Options list shows the Injection Variables. When **Peak Variables** is selected, the Items Options list shows the Peak Variables. Peak Detail Summary Tables can contain both types of items.

System Suitability Table - Format Tab Page

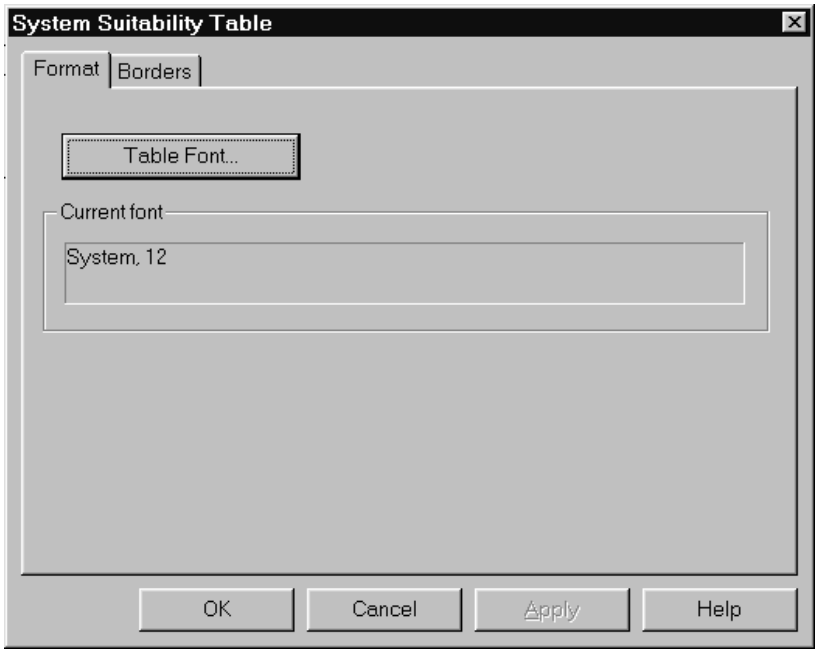


Table Font... opens the Font dialog box to select a font for the table text.

12.11 Chromatograms

Chromatograms can be included in single-injection reports (Sample Analysis, Calibration Update, and Check Standard).

To insert a chromatogram into the report:

1. On the Drawing Toolbox, click the Chromatogram tool, or select Chromatogram from the Draw menu.

   The pointer changes to a small chromatogram with a pencil.

2. Position the pencil pointer where you want to insert the chromatogram and drag to create a box.

   When the report is printed, the chromatogram will be inserted into the position indicated by the box.

Notes

- The chromatogram's final position in the report depends on whether there are variable-length tables before it. The data in the tables above may shift the chromatogram down the page or onto a new page.
- The chromatogram's characteristics (labels, plot colors, peak fills, etc.) are determined by the settings in the Plot dialog box. To open the dialog box, double-click inside the chromatogram (or click the right mouse button and select Properties from the menu). The dialog box is also available from the Optimize and Run programs. The options that you set in the Plot dialog box, are saved with the chromatogram and printed in the report. See Chapter 10 for a description of the Plot dialog box.

13 • The Qualification Programs

PeakNet provides three qualification programs for verifying that PeakNet is installed and operating correctly:

- Installation Qualification (see Section 13.1).
- Operational Qualification (see Section 13.2).
- Gradient Pump Qualification (see Section 13.3).

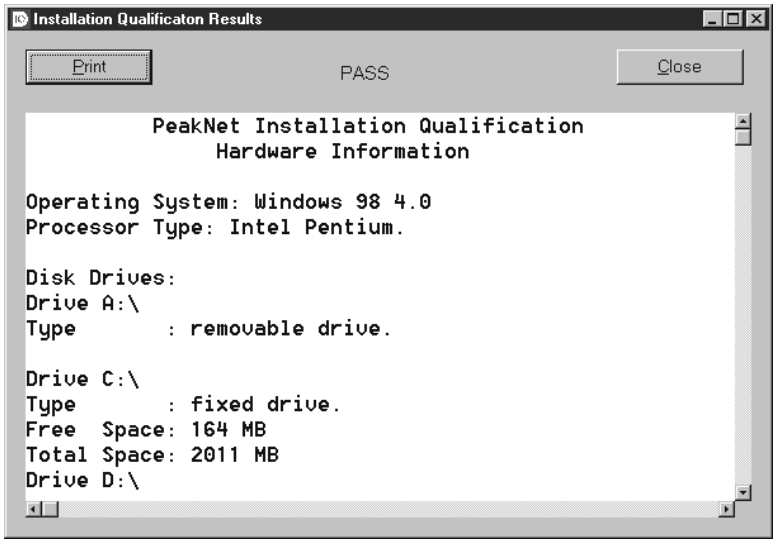
13.1 Installation Qualification

The Installation Qualification program uses an error detecting technique called Cyclic Redundancy Check (CRC) to verify that all files are installed correctly during PeakNet setup. The Installation Qualification determines a CRC value for PeakNet program files and for Windows system files that are installed with PeakNet. These calculated CRC values are compared with expected CRC values for each checked file. For the installation to qualify, all files must be present and their CRC values must match the expected CRC values.

NOTE The Installation Qualification does not check the following Operational Qualification files: CORE.BCH and CORE.SCH, because these files can be edited in the Batch program. After editing, their CRC values would not match the expected values, which would cause the CRC to fail.

The Installation Qualification runs automatically after PeakNet setup is complete. A report of the results is printed to the default Windows printer.

Once PeakNet is installed, the Installation Qualification can be started from the PeakNet MainMenu by selecting the Installation Qualification icon on the Accessories tab. Results are displayed in a Results window.



The overall status of the CRC is listed first:

- PASS indicates that all files were present and their CRC values match the expected CRC values.
- FAIL indicates that one or more PeakNet program files failed the check (either was not present or the CRC value did not match the expected value).
- WARNING indicates that one or more system files failed the check (and no PeakNet files failed).

Details about the qualification are listed in the lower portion of the window, in two parts:

- Hardware information

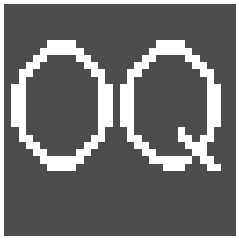
  Displays information about the computer on which PeakNet was installed, including the operating system, microprocessor type, local and network drive space, and amount of memory installed.

- CRC results

  Pass, fail, warning, and file missing results for the individual files are listed after the hardware information.

  All fail, warning, or file missing results are also logged in the PEAKNET.LOG file.

13.2 Operational Qualification



The Operational Qualification (OQ) program checks PeakNet operation by generating reports and exported values from reference data files. The exported values are then compared with reference exported values.

The OQ program uses or creates the following files when performing the qualification check:

Files Used	Description
CORE.BCH	Batch settings file
CORE.SCH	Schedule file
CORE.DXD	Write-protected reference raw data file
_CORE.CSV	Write-protected per-peak summary file (contains the reference exported values)
CORE.CSV	Per-peak summary file exported by the OQ program

To start the OQ program, select the Accessories tab on the PeakNet MainMenu and click on the Operational Qualification icon.

When the OQ program starts, it opens the Batch program and executes the CORE.BCH batch settings file. This processes the CORE.DXD raw data file and creates two reports: a per-peak summary report and a sample analysis report. The OQ program then compares the per-peak summary report with the reference per-peak summary report and generates a pass/fail report.

NOTE **If PeakNet was not installed in the default location (C:\PEAKNET), the OQ stops immediately after the Batch program opens and an error message appears in the Batch program window: "Error: Could not open export file c:\PeakNet\data\core.csv." To correct this, see Changing the OQ Default File Name Path.**

13.2.1 Operational Qualification Pass/Fail Report

The pass/fail report displays in the Results window. Click the Print button to print the results to the default Windows printer.

To pass, all test values in the exported file (CORE.CSV) must exactly match the values in the reference file (_CORE.CSV). If the qualification failed, exported test values that did not match their reference values are listed. These errors are also logged in the PEAKNET.LOG file.

Reference values from the _CORE.CSV file are listed below:

Sample Name	Component Name	Peak Area	Peak Height	Peak Retention Time
Diabetic Candy	Unknown 1	10542.000000000	1052.333333333	6.433333333
Diabetic Candy	Unknown 2	397150.000000000	14570.851063830	7.566666667
Diabetic Candy	Glycerol	181460.000000000	7943.589743590	9.233333333
Diabetic Candy	Unknown 3	681538.181546200	28175.306930693	10.666666667
Diabetic Candy	Unknown 4	203771.600817347	7347.336633663	11.900000000
Diabetic Candy	Unknown 5	49462.594961584	778.035821274	12.666666667
Diabetic Candy	Glucosamine	27396755.831814647	873466.670588235	15.533333333
Diabetic Candy	Sorbitol	236121772.352941190	6377945.988235294	16.800000000
Diabetic Candy	Mannitol	16771377.411764706	371843.929411765	20.133333333
Diabetic Candy	Unknown 6	179321.985127958	3370.577981651	26.200000000
Diabetic Candy	Unknown 7	326322.201834862	5161.366972477	26.866666667
Diabetic Candy	Unknown 8	566042.000000000	7192.400000000	29.800000000
Diabetic Candy	Unknown 9	215502.000000000	1293.021978022	34.533333333

13.2.2 Operation Qualification Sample Analysis Report

The sample analysis report is printed automatically to the default Windows printer. It includes a chromatogram and a peak table showing retention times, peak areas, and peak heights. The printed report can be compared to the example report shown on the next page.

Sample Analysis Report

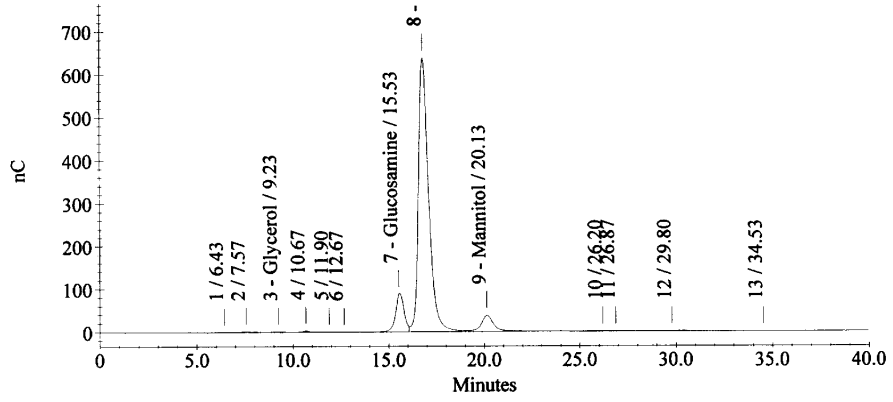
Sample Name : Diabetic Candy Sample
Data File Name : C:\PEAKNET\DATA\CORE.DXD

Method File Name : C:\PeakNet\method\2sugars.met
Date Time Collected : 7/7/94 10:29:28 PM
System Operator : Jekot

Peak Information : All Peaks

Component Name	Retention Time	Peak Area	Peak Height
Unknown 1	6.43	10542	1052
Unknown 2	7.57	397150	14571
Glycerol	9.23	181460	7944
Unknown 3	10.67	681538	28175
Unknown 4	11.90	203772	7347
Unknown 5	12.67	49463	778
Glucosamine	15.53	27396756	873467
Sorbitol	16.80	236121772	6377946
Mannitol	20.13	16771377	371844
Unknown 6	26.20	179322	3371
Unknown 7	26.87	326322	5161
Unknown 8	29.80	566042	7192
Unknown 9	34.53	215502	1293

Diabetic Candy Sample



13.2.3 Changing the OQ Default File Name Path

If PeakNet was not installed in the default location (C:\PEAKNET), the Operational Qualification cannot proceed because PeakNet looks in the default program file location for certain files used in the OQ. The following error message appears: "Error: Could not open export file c:\PeakNet\data\core.csv."

To correct this, you can change the file name paths to reference the actual PeakNet installation location.

1. If necessary, start the Batch program and then open the CORE.BCH Batch settings file. (The Batch program and CORE.BCH file will already be opened if you tried to run the OQ and it failed.)
2. Click the Export Options button on the toolbar.

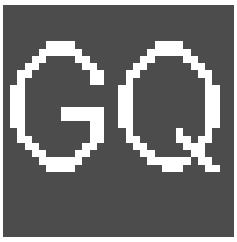
   The Export tab page of the Processing Options dialog box appears.
3. The file name C:\PEAKNET\DATA\CORE.CSV is shown in the Export File Name box. Change the path for the CORE.CSV file to the location where PeakNet was installed. For example, if PeakNet was installed in D:\PEAKNET, change the drive letter to D.
4. Click the Input tab and click the Select button. Select the CORE.SCH file and click Open.
5. Click the Edit button to open the file in the Schedule Editor.
6. Double-click the CORE.DXD file name in the Data File column. Navigate to find the new location for the CORE.DXD file (in the Data folder where PeakNet was installed). Select the file and click Open.
7. Save the Schedule file. When asked about the missing Method file, click Yes to proceed.
8. Exit the Schedule Editor.

9. In the Batch program, click OK to close the Processing Options dialog box. Save the edited CORE.BCH file and exit the program.

10. The Results dialog box from the failed OQ will then appear. Click the Close button to close this dialog box.

To re-run the Operational Qualification, return to the PeakNet MainMenu, select the Accessories tab and click the Operation Qualification icon. The OQ should now proceed correctly.

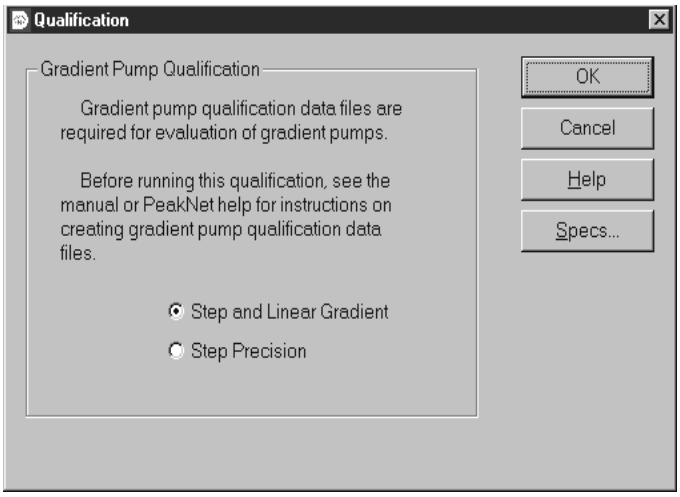
13.3 Gradient Pump Qualification



The Gradient Pump Qualification program tests for the correct operation of Dionex gradient pumps. The program analyzes gradient profile raw data files, created using example Methods supplied by Dionex, and performs a series of tests to determine whether the pump is operating within specified performance limits. The tests include baseline noise and drift, gradient step deviation and noise, linear gradient deviation, and step deviation precision.

To start the Gradient Pump Qualification program, select the Accessories tab on the PeakNet MainMenu and click on the Gradient Pump Qualification icon.

The Qualification dialog box appears.



There are two types of gradient pump qualifications:

Step and Linear The qualification tests are performed on a single gradient profile data file.

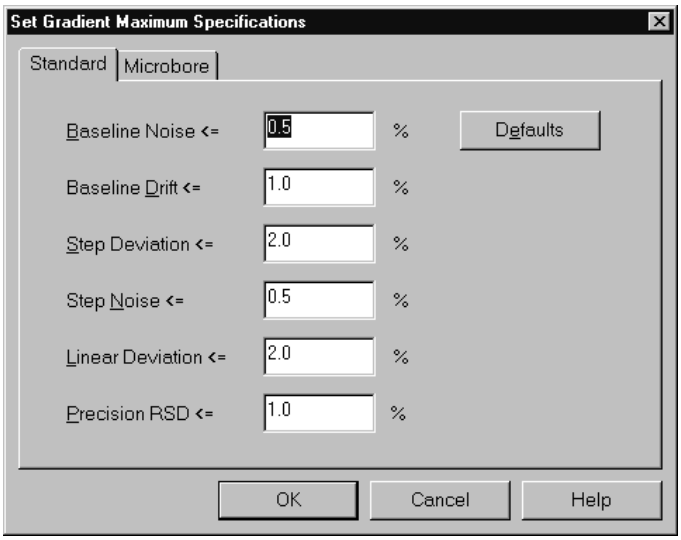
Step Precision The qualification tests are performed on three gradient profile data files and the pump's precision is calculated based on the step deviation values obtained from the three files.

Click on the **OK** button to close the Qualification dialog box.

A File Open dialog box appears in which you select the gradient profile data file(s).

- For the Step and Linear test, select one gradient profile data file.
- For the Step Precision test, select three gradient profile data files. The three files must be the same type of profile files (i.e., created with the same gradient profile Method). See Section 13.3.2 for details.

Click on the **Specs...** button to open the Set Gradient Maximum Specifications dialog box.



This dialog box lets you enter limits for Gradient Pump Qualification tests. To pass a particular test, the value obtained during the test must be less than or equal to the value set in this dialog box. Separate tab pages are provided for the standard bore and microbore pumps. See Section 13.3.1 for a description of each test.

Click on the **Default** button to restore default values for the current tab page's specifications. Except for Step Noise%, default values are identical for standard bore and microbore pumps.

Test	Default Maximum Specifications
Maximum Baseline Noise	0.5%
Maximum Baseline Drift	1%
Maximum Step Deviation	2%
Maximum Step Noise	0.2% (Standard bore); 1% (Microbore)
Maximum Linear Deviation	2%
Maximum Precision RSD	1%

13.3.1 Gradient Pump Qualification Tests

The Results window displays the results of the qualification tests. The overall results of the qualification (PASS or FAIL) are displayed at the top of the window. Detailed results are displayed in the lower part of the window.

Press the Print button to print the result report to the default Windows printer.

Basic Values

Before running the Gradient Pump Qualification tests, PeakNet determines the following values and then uses them to calculate various test results.

Maximum Data Value = the maximum amplitude of the gradient chromatogram

Baseline Data Value = the minimum amplitude of the gradient chromatogram

Full Scale = (Maximum Data Value - Baseline Data Value)

1% Maximum Data Value = Full Scale/100

System Tests

Gradient Delay is the difference between the time a step gradient was observed and the time it was programmed to occur. The maximum delay allowed is 1 min. If the gradient delay is over 1 min, an error message occurs and the qualification is stopped. The

Gradient Delay value is used to adjust expected times for all gradient ramps and isocratic segments.

Dwell Volume is the volume in mL of the gradient delay: Gradient Delay Time (min) x Flow Rate (mL/min).

Measured Baseline Noise % is the measured baseline noise divided by the 1% Maximum Data Value. The baseline noise measurement is taken from a 0.5 to 2.5 min time interval. The test fails if the Measured Baseline Noise % is more than the Baseline Noise % limit set in the Set Gradient Maximum Specifications dialog box.

Measured Baseline Drift % is the absolute value of the difference between the average baseline values at the beginning of the chromatogram and the average baseline values at the end of the chromatogram, divided by the 1% Maximum Data Value. The test fails if the Measured Baseline Drift % is more than the Baseline Drift % limit set in the Set Gradient Maximum Specifications dialog box.

Step Gradient Tests

The Step Gradient Tests are performed for every change of proportion programmed in the Method. The 50% to 90% time interval of the step duration is determined. Within this interval, Deviation and Noise are calculated.

Step Deviation % is the difference between the actual proportion achieved and the proportion programmed in the Method. The test fails if the Step Deviation % is more than the Step Deviation % limit set in the Set Gradient Maximum Specifications dialog box.

Step Noise % is the measured baseline noise divided by the 1% Maximum Data Value. The test fails if the Step Noise % is more than the Step Noise % limit set in the Set Gradient Maximum Specifications dialog box.

Linear Gradient Test

The Linear Gradient Test is performed only if a step and linear type gradient profile raw data file is selected for the Gradient Pump Qualification (see Section 13.3.2 for details). The Linear Gradient Test calculates a deviation % for every point within the 5% to 95%

time interval of the linear ramp for both the progression and the regression parts of the linear step.

Linear Deviation (%) is the maximum deviation divided by the 1% Maximum Data Value. The maximum deviation is the largest deviation calculated for any point in the 5% to 95% time interval of the linear ramp. The test fails if the full-scale percentage of the standard deviation of the linear ramp data set is more than Maximum Linear Deviation % of the theoretical gradient slope. The Maximum Linear Deviation % limit is specified in the Set Gradient Maximum Specifications dialog box.

Step Deviation Precision Test

The Step Deviation Precision Test is performed on three gradient data files of the same profile type. Before the precision test is performed, each file is first qualified using the Step Gradient Test and the Linear Gradient Test (if required). The result of the precision test (pass or fail) is independent from the results of the individual qualification tests. The test produces four reports: three gradient pump qualification reports (one for each data file) and one precision report. For the precision test, a %RSD is calculated for each step in the gradient profile.

%RSD is the %RSD of (n step deviation file A, n step deviation file B, n step deviation file C).

Where n is the deviation of the particular step (20%, 50%, 80%, or 100%).

The test fails if the %RSD is more than the Precision RSD % limit set in the Set Gradient Maximum Specifications dialog box.

13.3.2 Creating Gradient Profile Data Files

Two types of gradient profile raw data files can be created, depending on the type of gradient qualification tests to be performed.

- The step precision gradient profile consists of step gradients at 20%, 80%, and 100% for valve pairs A,B and C,D.
- The step and linear gradient profile maintains compatibility with the Performance Validation Kit. It consists of step gradients at 20%, 80%, and 100% and a linear ramp gradient for valve pairs A,B and C,D.

Methods for both types of gradient profiles are supplied with PeakNet. See Section 13.3.3 for details.

In addition to the gradient pump, either a UV or a conductivity detector is required. The procedure for creating the gradient profile data files depends on the type of detector used. See "Creating a Gradient Profile Data File Using a UV Detector" on page 13-15 or "Creating a Gradient Profile Data File Using a Conductivity Detector" on page 13-17.

Creating a Gradient Profile Data File Using a UV Detector

Preparing the System

Notes

- Use only ASTM Type 1, 18 MΩ or better, filtered, deionized water to prepare eluents
- Eluents must be degassed and pressurized with helium.

1. Connect the gradient pump transducer outlet tubing to the absorbance cell inlet port using about 25 cm (10 in) of yellow 0.076-mm ID (0.003-in) backpressure tubing (P/N 049715). Backpressure must be over 7 MPa (1000 psi).
2. Connect the absorbance cell outlet to waste using a 75 psi backpressure regulator (PEEK regulator, P/N 046480; stainless steel regulator, P/N 039670) or enough 0.25-mm (0.010-in) backpressure tubing to create 0.5 MPa (75 psi).
3. Set the UV detector wavelength to 254 nm.
4. Prepare the following eluent: 0.3% v/v acetone / 99.7 % deionized water.
5. Insert eluent lines A and C into one bottle containing the eluent prepared in Step 4.
6. Insert eluent lines B and D into one bottle containing deionized water.
7. Prime each of the four eluent lines. Then, select 100% eluent B and a flow rate of 3 mL/min (for standard bore) or 0.75 mL/min (for microbore).
8. Allow the system to stabilize for at least 10 min.

Creating and Running the Method

1. Open the Configuration Editor and double-click on the pump to be qualified. Enter the pump's serial number (shown on the rear panel of the pump). Save the configuration and exit.
2. In the Method Editor, open the example Method that corresponds to the type of gradient profile to be used and to the type of pump and detector configured in your system. For example, if you want to use a Step Precision profile and your system consists of a standard bore GP50 pump and an AD20 detector, open GP50SBAD20PRECISION.met from the \Method\Gradient Precision folder.
3. Select Configuration from the Edit menu. Select the system configuration that includes the gradient pump and UV detector. Add the pump and detector to the Method configuration and then exit the Configuration dialog box.
4. Save the Method.
5. In the Run program, load the Method and start the run.

   When the run is complete, the data file created during the run can be used for gradient pump qualification.

Creating a Gradient Profile Data File Using a Conductivity Detector

Preparing the System

Notes

- Use only ASTM Type 1, 18 MΩ or better, filtered, deionized water to prepare eluents
- Eluents must be degassed and pressurized with helium.

1. Connect the gradient pump transducer outlet tubing to the absorbance cell inlet port using about 25 cm (10 in) of yellow 0.076-mm ID (0.003-in) backpressure tubing (P/N 049715). Backpressure must be over 7 MPa (1000 psi).
2. Connect the conductivity cell outlet to waste.
3. Prepare 1 mM KCL eluent as follows:

   Prepare 1 liter of 10 mM KCl by dissolving 0.746 grams of KCl in 1 liter of deionized water. Then, dilute the 10 mM KCl 1:10 with deionized water.
4. Insert eluent lines A and C into one bottle containing the 1 mM KCl eluent prepared in Step 1.
5. Insert eluent lines B and D into one bottle containing deionized water.
6. Prime each of the four eluent lines. Then, select 100% eluent B and a flow rate of 3 mL/min (for standard bore) or 0.75 mL/min (for microbore).
7. Allow the system to stabilize for at least 10 min.

Creating and Running the Method

1. Open the Configuration Editor and double-click on the pump to be qualified. Enter the pump's serial number (shown on the rear panel of the pump). Save the configuration and exit.
2. In the Method Editor, open the example Method that corresponds to the type of gradient profile to be used and to the type of pump and detector configured in your system. For example, if you want to use a Step Precision profile and your system consists of a standard bore GP50 pump and a CD20 detector, open GP50SBCD20PRECISION.met from the \Method\Gradient Precision folder.
3. Select Configuration from the Edit menu. Select the system configuration that includes the gradient pump and conductivity detector. Add the pump and detector to the Method configuration and then exit the Configuration dialog box.
4. Save the Method.
5. In the Run program, load the new Method and start the run.

   When the run is complete, the data file created during the run can be used for gradient pump qualification.

13.3.3 Gradient Profile Methods

PeakNet includes two example gradient profile Methods for use in creating the data files required for gradient pump qualification.

- The step precision Method includes timed events for creating a gradient profile consisting of step gradients at 20%, 80%, and 100% for valve pairs A,B and C,D.
- The step and linear gradient Method includes timed events for creating a gradient profile consisting of step gradients at 20%, 80%, and 100% and a linear ramp gradient, both for valve pairs A,B and C,D.

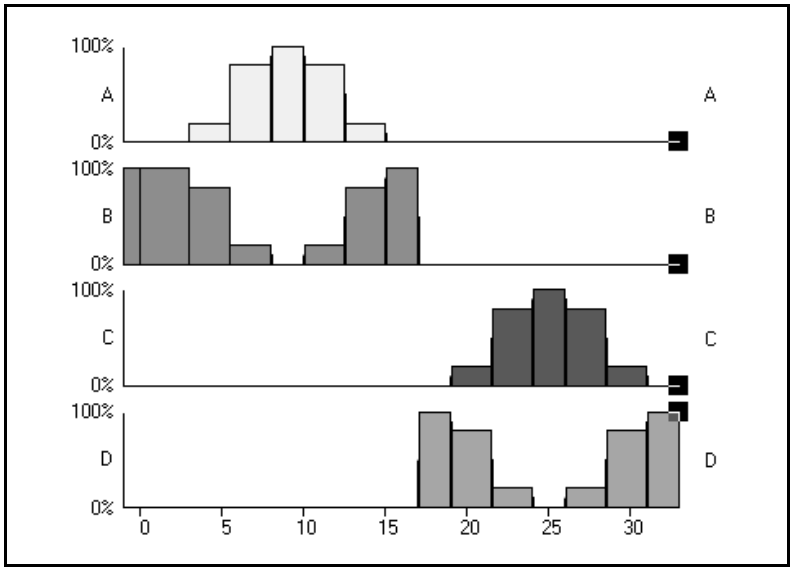
Timed events and gradient profiles for the step precision and step and linear gradient Methods follow.

Step Precision Gradient Method Timed Events

The standard bore flow rate is shown. The flow rate for microbore is 0.75 mL/min.

Time	Flow	%A	%B	%C	%D	Curve
Init	3.00	0.00	100.00	0.00	0.00	5
0.00	3.00	0.00	100.00	0.00	0.00	5
3.00	3.00	0.00	100.00	0.00	0.00	5
3.10	3.00	20.00	80.00	0.00	0.00	5
5.50	3.00	20.00	80.00	0.00	0.00	5
5.60	3.00	80.00	20.00	0.00	0.00	5
8.00	3.00	80.00	20.00	0.00	0.00	5
8.10	3.00	100.00	0.00	0.00	0.00	5
10.00	3.00	100.00	0.00	0.00	0.00	5
10.10	3.00	80.00	20.00	0.00	0.00	5
12.50	3.00	80.00	20.00	0.00	0.00	5
12.60	3.00	20.00	80.00	0.00	0.00	5
15.00	3.00	20.00	80.00	0.00	0.00	5
15.10	3.00	0.00	100.00	0.00	0.00	5
17.00	3.00	0.00	100.00	0.00	0.00	5
17.10	3.00	0.00	0.00	0.00	100.00	5
19.00	3.00	0.00	0.00	0.00	100.00	5
19.10	3.00	0.00	0.00	20.00	80.00	5
21.50	3.00	0.00	0.00	20.00	80.00	5
21.60	3.00	0.00	0.00	80.00	20.00	5
24.00	3.00	0.00	0.00	80.00	20.00	5
24.10	3.00	0.00	0.00	100.00	0.00	5
26.00	3.00	0.00	0.00	100.00	0.00	5
26.10	3.00	0.00	0.00	80.00	20.00	5
28.50	3.00	0.00	0.00	80.00	20.00	5
28.60	3.00	0.00	0.00	20.00	80.00	5
31.00	3.00	0.00	0.00	20.00	80.00	5
31.10	3.00	0.00	0.00	0.00	100.00	5
33.00	3.00	0.00	0.00	0.00	100.00	5

The gradient profile for the step precision Method is shown below.

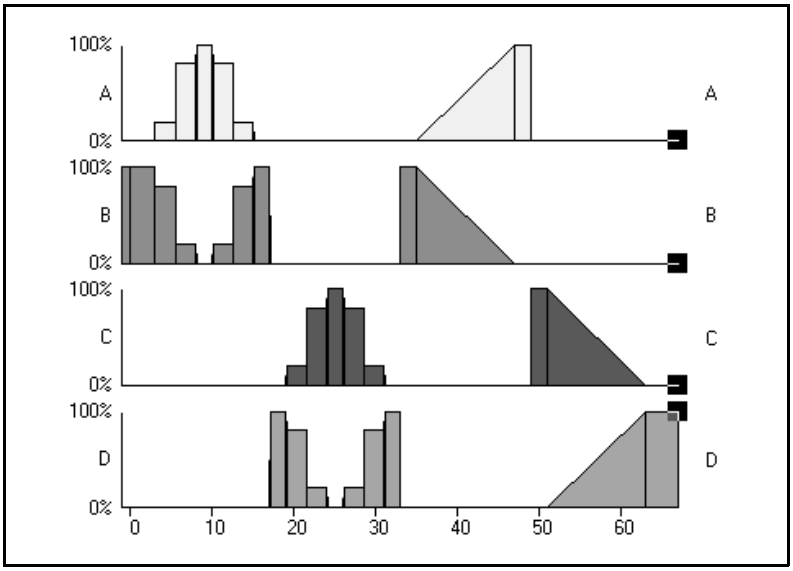


Step and Linear Gradient Method Timed Events

The standard bore flow rate is shown. The flow rate for microbore is 0.75 mL/min.

Time	Flow	%A	%B	%C	%D	Curve
Init	3.00	0.00	100.00	0.00	0.00	5
0.00	3.00	0.00	100.00	0.00	0.00	5
3.00	3.00	0.00	100.00	0.00	0.00	5
3.10	3.00	20.00	80.00	0.00	0.00	5
5.50	3.00	20.00	80.00	0.00	0.00	5
5.60	3.00	80.00	20.00	0.00	0.00	5
8.00	3.00	80.00	20.00	0.00	0.00	5
8.10	3.00	100.00	0.00	0.00	0.00	5
10.00	3.00	100.00	0.00	0.00	0.00	5
10.10	3.00	80.00	20.00	0.00	0.00	5
12.50	3.00	80.00	20.00	0.00	0.00	5
12.60	3.00	20.00	80.00	0.00	0.00	5
15.00	3.00	20.00	80.00	0.00	0.00	5
15.10	3.00	0.00	100.00	0.00	0.00	5
17.00	3.00	0.00	100.00	0.00	0.00	5
17.10	3.00	0.00	0.00	0.00	100.00	5
19.00	3.00	0.00	0.00	0.00	100.00	5
19.10	3.00	0.00	0.00	20.00	80.00	5
21.50	3.00	0.00	0.00	20.00	80.00	5
21.60	3.00	0.00	0.00	80.00	20.00	5
24.00	3.00	0.00	0.00	80.00	20.00	5
24.10	3.00	0.00	0.00	100.00	0.00	5
26.00	3.00	0.00	0.00	100.00	0.00	5
26.10	3.00	0.00	0.00	80.00	20.00	5
28.50	3.00	0.00	0.00	80.00	20.00	5
28.60	3.00	0.00	0.00	20.00	80.00	5
31.00	3.00	0.00	0.00	20.00	80.00	5
31.10	3.00	0.00	0.00	0.00	100.00	5
33.00	3.00	0.00	0.00	0.00	100.00	5
33.10	3.00	0.00	100.00	0.00	0.00	5
35.00	3.00	0.00	100.00	0.00	0.00	5
47.00	3.00	100.00	0.00	0.00	0.00	5
49.00	3.00	100.00	0.00	0.00	0.00	5
49.10	3.00	0.00	0.00	100.00	0.00	5
51.00	3.00	0.00	0.00	100.00	0.00	5
63.00	3.00	0.00	0.00	0.00	100.00	5
67.00	3.00	0.00	0.00	0.00	100.00	5

The gradient profile for the step and linear Method is shown below.



A • Principles of Peak Integration (Standard Algorithm)

A.1 Data Points

Chromatographic detectors generate a voltage signal which varies with changes in the composition of the materials passing through the detector cell. The analog signal is then digitized in the circuitry of either the DX-LAN based detector or the Advanced Computer Interface (ACI) to produce a voltage/time integral called a *data point*.

A.1.1 Data Collection Rate

The *data collection rate* determines how many data points per second are collected and stored in detector or ACI memory. Increasing the data collection rate (that is, selecting a larger number of samples per second) increases the accuracy of detecting and integrating very fast peaks by increasing the number of data points collected in each data collection period.

The data collection rate also affects the amount of data that can be stored in detector or ACI memory. Increasing the collection rate decreases the length of time that data can be stored before it must be retrieved by the computer. Faster collection rates also consume more disk space and slow down reprocessing of stored data. It is usually best to choose a rate that defines the narrowest peak with 20-30 data points.

The data collection rate for a DX-LAN detector depends on the type of detector and, in the case of the ED40 Electrochemical Detector, on the detection mode. The default rate, 1 Hz, is usually adequate. Each detector has 512K of memory and can hold about 7 hours of raw data at 5 samples/second.

The table below shows for how long DX-LAN detectors can collect data while off-line from PeakNet.

Peak Width (Seconds)	Data Collection Rate (Hz)	Detector Capacity (Hours)
> 10.0	1	35
2.0 - 5.0	5	7
1.0 - 2.0	10	3.5

The Advanced Computer Interface (ACI) simultaneously digitizes data from two detectors. The ACI data collection rate can be set to 1, 2, 5, 10, 20, or 50 samples per second (Hz).

In an ACI-based system, the amount of data that can be stored depends on the amount of ACI memory and on the noise level of the signal. (Noisy signals use more memory than quiet ones.) Approximate capacities are shown below.

For a system with only one detector, an ACI with 256K of memory per system will hold about 6 hours of raw data at 5 samples/second; at 50 samples/second, it will hold about 34 minutes. Adding a second detector to the system reduces these times by approximately half.

NOTE For ACIs with 64K (shipped before June 1, 1992), all capacities are lower by a factor of 4.

		ACI Capacity with One Detector (Minutes)		
Peak Width (Seconds)	Sampling Rate (Hz)	Minimum	Typical	Maximum
> 10.0	1	840	1680	4200
5.0 - 10.0	2	840	420	2100
2.0 - 5.0	5	168	336	840
1.0 - 2.0	10	84	168	420
0.5 - 1.0	20	46	84	210
< 0.5	50	16.8	33.6	84

A.1.2 Peak Width and Data Bunching

PeakNet stores raw, digitized data. Smoothing is done between the time raw data is read and the time it is integrated. Raw, digitized data is collected and transmitted to the computer, the software sums groups of data points into ***data bunches***. By adjusting the number of data points in a bunch (the ***bunching factor***), the resulting filtering can be tailored to the requirements for peak detection in an individual chromatogram.

The bunching factor is calculated from the minimum peak width and "time per sample" (the inverse of the data collection rate) selected in the Method. If the bunching factor is 1, no values are averaged, and the software considers every raw data point in its evaluation of peaks and areas. If the bunching factor is 5, the software averages every 5 consecutive raw data points to form a bunched data point.

The optimal bunching factor can be determined by measuring the baseline width, in seconds, of the narrowest peak in the chromatogram. This peak width parameter is specified in the Method and, along with the data collection rate, establishes the initial bunching factor. Using a higher factor screens out more noise. However, too high a bunching factor may cause small peaks to be missed in the analysis.

In general, very narrow peaks require a very small bunching factor to prevent them from being treated as noise. Conversely, very broad peaks must have a relatively large number of data points per bunch to prevent them from being treated as baseline drift.

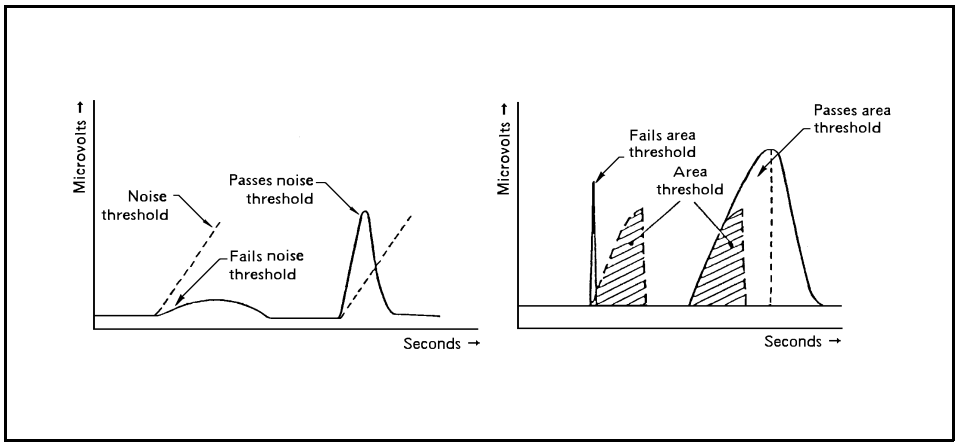
Late-eluting peaks in a chromatogram are typically broader than peaks that elute earlier, but if there is a significant difference you may need to increase the bunching factor during the run so that the broadest peaks are detected as peaks and not as baseline drift. This can be done by including one or more Data Events in the Method to change the bunching factor.

A.1.3 Peak Threshold and Peak Detection

PeakNet software uses slope, or rate of change in signal level, to detect peaks. A slope is calculated between each pair of data bunches. Thus, the peak width parameter in the Method also determines how frequently the slope is calculated. Narrow peaks require small bunches so that the slope is calculated frequently enough to detect and confirm a peak. Wide peaks, on the other hand, require larger bunches so that a more gradual change in the signal level is detected as a peak.

The Peak Threshold specified in the Integration Parameters dialog box is a measure of how much the leading edge of the peak must rise before it is recognized as a peak. The larger the number (slope), the sharper the peak must be. When the data exhibits a slope greater than this threshold, the first data point is marked as the potential beginning of a peak. A peak is confirmed if the slope continues positively until the accumulated area is 100 times the peak threshold.

After confirming the beginning of a peak, the software begins searching for the peak crest. The crest is indicated when the signal reaches a maximum and then steadily declines from that maximum until the accumulated area is 100 times the peak threshold value. Finally, the software searches for the end of the peak; this is detected when the slope fails to decline by the peak threshold value for three consecutive data bunches.



A.1.4 Peak Integration

After completing peak detection, PeakNet software classifies each peak as one of the following types:

Peak Description	Baseline Code Type
Completely resolved	1
Partially resolved	2
Host peak	3
Rider peak	4, 6, or 7

*Type 5 is an internal designation that is reserved for future use.

- **Type 1** peaks are completely resolved. The baseline is a line between the beginning and ending points of the peak. The separation between the end of the first peak and the start of the second peak must be at least 20% of the width of the first peak.
- **Type 2** peaks are partially resolved peaks. The peaks are separated by a drop-line extending from the valley between the peaks to a common baseline.
- **Type 3** peaks are host peaks fused with rider peaks (type 4, 6, or 7) that have 20% or less of the height of the host peak.
- **Type 4** peaks are closely following rider peaks that are separated from the host peak by an exponential projection of the backside of the host peak. The area under the exponential line is added to the host peak, not the rider.
- **Type 6** peaks are closely following rider peaks that are separated by a tangential line from the host peak to the outer edge of the rider peak. The area under the tangential line is added to the host peak, not the rider.
- **Type 7** peaks are closely leading rider peaks that are separated by a tangential line from the host peak to the outer edge of the rider peak. The area under the tangential line is added to the host peak, not the rider.

Drop-line treatment is automatically applied if the second peak starts within 20% of the width of the first peak and either of the following conditions is also true:

- The height of the second peak is greater than 20% of the height of the first peak.
- The height of the valley between the peaks is 33% or more of the height of the second peak.

Exponential skim treatment is automatically applied to rider peaks if all of the following conditions are met:

- The height of the rider peak is 20% or less of the height of the host peak.
- The height of the valley between the host and rider peaks is 33% or more of the height of the rider peak.
- The height of the valley between the host and rider peaks is 10% or more of the height of the host peak.

Tangential-skim treatment is automatically applied to rider peaks if all of the following conditions are met:

- The height of the rider peak is 20% or less of the height of the host peak.
- The height of the valley between the host and rider peak is 33% or more of the height of the rider peak.
- The height of the valley between the host and rider peak is less than 10% of the height of the host peak.

Initially, PeakNet groups peaks into clusters that share a common baseline. To be classified as a cluster, the start of each peak in the cluster must begin within 20% of the width of the previous peak. If the separation between two peaks is greater than 20% of the width of the previous peak, then the cluster ends and a new cluster begins. Each peak in a cluster is initially classified as a type 2 (partially resolved) peak. PeakNet then scans the valleys between the peaks for baseline penetration; if the valley between two peaks extends below the cluster's baseline, the cluster is separated at that point. If separation leaves a single peak at one or both ends of the cluster, the peak(s) is reclassified as type 1.

PeakNet then determines whether to separate clustered peaks by drop-lines, exponential skimming, or tangential skimming. With the baseline established, the software then integrates the data bunches under the peak to determine the area. The peak areas or heights are then used to calculate amounts. See Appendix B for an explanation of PeakNet quantitation techniques.

B • Quantitation Techniques

After raw data from an analysis is acquired, algorithms which use the parameters set in the Method (e.g., peak threshold and retention window) perform peak detection, retention time determination, and peak area calculations. From this basic information, the data can be further subjected to quantitation techniques to express it in terms of concentrations. All of these calculations occur after the run is ended.

The selection of a quantitation method should be based on its applicability to the sample material and the accuracy required. The quantitation methods discussed in Appendix C are those most frequently used today. Specifying a particular technique not only causes the data to be processed in a particular way, but also imposes certain restraints on the experimental procedure.

B.1 Response Factors

The response of any given detector or detector type varies from one chemical compound to another. This difference in response is the primary reason that it is necessary to calibrate your analytical system, although temperature drift and column degradation are also factors.

Part of the calibration process is to calculate response factors, which represent the specific detector response for each component. Run and Batch automatically calculate a response factor for each component in the calibration standard whenever you request an external or internal standard report in a Method. Each time you repeat a calibration run for a particular analysis, these factors are updated, either by averaging the new value with the previously stored value or by replacing the old value with the new one.

Response factors are a simplistic way of looking at calibration; they assume that the response is a direct linear function of amount with a 0 intercept value. Deviations from ideal behavior, caused by such factors as impure reagents, column overloading, and detector saturation, typically make it necessary to us more sophisticated techniques. Nevertheless, response factors can be a convenient tool for comparing components and for checking Method stability.

B.2 External Standard Quantitation

The external standard quantitation technique is used for analyses where the detector response for each component in the sample is different and independent of other components. When using external standards, the amount of each sample component is calculated with respect to the absolute response for that component.

External standard quantitation is also quite useful for trace analyses, where the error inherent in repeated sample injections is not critical. The use of external standard quantitation is especially attractive for use with an autosampler, where repetitive injection volumes are reproducible.

Since each response factor is independent of other components, response factors are needed only for components of interest. The presence of other components does not affect quantitative results, and not all components need be eluted or detected.

Requirements of external standard quantitation:

- The composition of the calibration mixture must be close to that anticipated for samples.
- Because this technique is dependent on sample size, the injection volumes for each calibration run and sample run must be known, or at least reproducible.
- Detector response should be very stable, or calibration should be repeated frequently to compensate for drift in the chromatographic system.

B.2.1 External Standard Calculations

For a single-level calibration, the absolute response factor for each component, i, is calculated as:

$$A_c = Function\ (R_c)$$

Where:

A_c	=	amount of the analyte in the calibration standard
Function	=	a form of the current calibration curve function
R_c	=	is the response of the analyte in the calibration standard

After the response factors for all of the components in the calibration standard have been determined, the sample can be injected and the response-corrected concentrations of the components calculated as:

$$A_S = Function\ (R_S)\ X\ \frac{V_C}{V_S}\ X\ D_S$$

Where:

A_S	=	the amount of the analyte in the Sample
Function	=	a form of the current calibration curve function
R_S	=	the response of the analyte in the sample
V_C	=	is the volume of standard injected
V_S	=	is the sample volume injected from the Method or Schedule
D_S	=	is the dilution factor from the Method or Schedule for the Sample

B.3 Internal Standard Quantitation

Like external standard quantitation, the internal standard quantitation technique is used for analyses where the detector response for each sample component is different. Because quantitation of an unknown peak is relative to the internal standard, the analysis is independent of variations in detector sensitivity, sample size, and other sample components.

Internal standard quantitation involves adding a known amount of a reference compound to each injection of the calibration standard and sample. This reference must elute in an open area of the chromatogram and must not interfere or chemically interact with any of the sample components. It should also exhibit chromatographic properties similar to those of the unknown component(s) to which it is compared.

Internal standard calculation allows the accurate quantitation of individual components despite changes in chromatographic conditions or in the injection volume, because all calculations are normalized to the response of the internal standard(s). Ideally, the amount of the internal standard component should be slightly larger than that of the peaks of interest. For best results, the area of the internal standard component should not vary by more than a factor of 10 from the areas of the peaks of interest.

B.3.1 Internal Standard Calculations

With Internal Standard Calibration, all samples and standards are spiked with a known amount of the internal standard component(s). A series of standards is injected, and a calibration plot is constructed in which the ratio of each component's amount to the amount of the internal standard component is related to the ratio of the component's response to the response of the internal standard component:

$$\frac{R_C}{R_I} = Function\left(\frac{A_C}{A_I}\right)$$

Where:

R_c	=	the response of the analyte in the calibration standard
R_I	=	the response of the internal standard component in the standard
Function	=	a form of the current calibration curve function
A_c	=	the amount of the analyte in the standard
A_I	=	the amount of the internal standard component in the standard

No correction factors for volume or dilution are used in the calculation. When samples are analyzed, each component's amount is determined from the ratio of the component's response to the response of the internal standard component, normalized against the amount of the internal standard component in the sample:

$$\frac{A_S}{A_I} = Function\left(\frac{R_S}{R_I}\right) X\, D_S$$

Where:

A_S	=	the amount of the analyte in the Sample
A_I	=	the amount of the Internal Standard component in the sample from the Method or Schedule
D_S	=	the dilution factor from the Method or Schedule for the Sample
Function	=	a form of the current calibration curve function
R_s	=	response of the analyte in the Sample
R_I	=	response of the internal standard component in the sample

B.4 Multilevel Calibrations

Single-level calibrations assume a linear detector response that passes through zero over the expected concentration range of each component in the sample. In the case where detector response is nonlinear or does not pass through zero, it is necessary to use multilevel calibration. For multilevel calibrations, several calibration standards covering the expected amount range are injected. A calibration curve for each component is determined from the data acquired for each different calibration level, using either a linear, quadratic, cubic, or point-to-point interpolation.

After the calibration curves are determined, the amounts of the components in the sample mixture can be calculated by relating the measured area to its corresponding calibration curve.

- When a linear fit is used, the calibration curve is determined by a least-squares calculation to fit a line through the calibration data points.
- When a quadratic fit is used, the calibration curve is drawn from a quadratic equation. A quadratic fit is most useful when detector response is known to “flatten out” toward one extreme of the concentration range or the other.
- A cubic fit is useful for curves that have both positive and negative inflections, such as electrochemical curves.
- When a point-to- point fit is used, the software determines which two calibration data points bracket the response of the unknown and uses a straight line between the two points to interpolate the concentration of the unknown.

B.4.1 Curve Fits

PeakNet software supports linear, point-to-point, quadratic, and cubic curve fits. Each of these curve fitting procedures is described below.

Linear Curve Fit

The linear curve fit models the detector response as a linear response factor. The response line does not assume a pass through the origin (zero), except with a single-level calibration or when the force zero option is selected.

The linear curve fit is also known as the least squares, or linear regression, technique. It may be used whenever the detector response is approximately linear and when the assumption of a linear response does not create a significant error. It can also be used for a narrow concentration range over which a somewhat linear detector response exists, or can be assumed, without producing substantial error.

This curve fit computes a relative or absolute response factor for each calibrated component in a calibration. The software then constructs a straight-line equation that best fits the response versus amount data points over all the levels. In a single-level calibration, this line is between the origin (0,0) and the calibration data point for the component. The response factor (amt/response) is then used in conjunction with the selected calibration formula to report the amount or concentration of each component in the sample.

The straight-line equation computes the response factor from the general straight-line equation in the slope-intercept form:

$$Y = K_0 + K_1 \times X$$

Where:

K_0 = the Y-axis intercept
K_1 = the slope of the response line

The response factor computed depends upon the calculation procedure selected. For external standard calibrations, an absolute response factor is computed. For internal standard calibrations, a relative response factor is derived.

For external standard calibrations, the slope, K_1, is computed according to the following formula:

$$K_1 = \frac{\sum_{j=1}^{n} [(CA)_j (Amt)_j] - \frac{[\sum_{j=1}^{n} (CA)_j][\sum_{j=1}^{n} (Amt)_j]}{n}}{\sum_{j=1}^{n} [(CA)_j]^2 - \frac{[\sum_{j=1}^{n} (CA)_j]^2}{n}}$$

Where:

$(Amt)_i$	=	the amount of a component in the calibration standard at level n
$(CA)_i$	=	the calibrated response (area or height) for a component at level n
n	=	the number of levels in which a component is calibrated

The Y-axis intercept, K_0, is computed according to the following formula:

$$K_0 = \frac{\sum_{j=1}^{n} [(Amt)_j] - K_1 [\sum_{j=1}^{n} (CA)_j]}{n}$$

For internal standard calibrations, the slope, K_1, is computed according to the formula:

$$K_1 = \frac{\sum_{j=1}^{n}\left[\frac{(CA)_j}{(CA)_{ISTD}}\cdot\frac{(Amt)_j}{(Amt)_{ISTD}}\right] - \frac{\left[\sum_{j=1}^{n}\frac{(CA)_j}{(CA)_{ISTD}}\right]\cdot\left[\sum_{j=1}^{n}\frac{(Amt)_j}{(Amt)_{ISTD}}\right]}{n}}{\sum_{j=1}^{n}\left[\frac{(CA)_j}{(CA)_{ISTD}}\right]^2 - \frac{\left[\sum_{j=1}^{n}\frac{(CA)_j}{(CA)_{ISTD}}\right]^2}{n}}$$

Where:

$(Amt)_i$	=	the amount of a component in the calibration standard for level n
$(CA)_i$	=	the calibrated response (area or height) for a component
$(CA)_{ISTD}$	=	the calibrated response (area or height) of the internal standard component
$(Amt)_{ISTD}$	=	the amount of the internal standard component
n	=	the number of levels in which a component is calibrated

The y-intercept, K_0, is then computed as:

$$K_0 = \frac{\sum_{j=1}^{n}\frac{(Amt)_j}{(Amt)_{ISTD}} - K_1\left[\sum_{j=1}^{n}\frac{(CA)_j}{(CA)_{ISTD}}\right]}{n}$$

Each component must be calibrated over at least two levels in order for this curve fit to work. If fewer than two levels exist, the calibration curve is forced through the origin (zero).

Forcing a nonlinear function should only be done when the resulting error produced would be minimal. This procedure can also be used when calibration is performed within a range where response is most linear.

When using an internal standard procedure, an internal standard component must be calibrated in each level.

Quadratic Curve Fit

The nonlinear curve fit produces a response factor from a quadratic equation of parabola that best fits a detector's second-order response. The general quadratic equation used to compute the response factor for each component in a multilevel calibration is:

$$Y = K_0 + K_1 \times X + K_2 \times X^2$$

The final equation produces the relative, or absolute, response factor, which is then used to compute the amount of the component according to the selected calibration formula.

At least three points are needed to fit a parabola; thus, the calibration must have at least three levels for all components. When using an internal standard calibration, an internal standard component must be calibrated in each level.

Cubic Curve Fit

The response factor produced from a cubic equation best fits a detector's third-order response. The equation used is shown below.

$$Y = K_0 + K_1 \times X + K_2 \times X^2 + K_3 \times X^3$$

At least four points are needed to fit the equation; thus, the calibration must have at least four levels for all components.

Point-to-Point Curve Fit

A point-to-point fit is often used to match an arbitrary response curve with the range of the identified calibration amounts. The segment of the response below the lowest calibrated amount is assumed to pass through the origin. Therefore, it is a good practice to calibrate at a point below the lowest expected sample amounts for any samples whose response curves do not pass through the origin or are unknown.

The segment above the highest calibrated amount is assumed to be a linear extrapolation of the segment between the second highest and highest calibrated amounts. If the actual response above the highest level is unknown or does not follow this behavior, make sure that the highest calibrated amount is greater than any expected sample amounts.

The formula used to compute a point-to-point calibration is:

$$Y = \frac{Y_2 - Y_1}{X_2 - X_1}(X - X_1) + Y_1$$

Where:

Y_2 = the calibrated amount of the component in the next level

Y_1 = the calibrated amount of the component in the present level

X_2 = the calibrated response of the component in the next level

X_1 = the calibrated response of the component in the present level

The response factor, K_1, is then computed from the following:

$$K_1 = \frac{Y_2 - Y_1}{X_2 - X_1}$$

The response factor, K_0, is then computed from the following:

$$K_0 = Y_1 - K_1 \, x \, X_1$$

If the response function is a second-order model, the quadratic fit method may be more desirable since it produces a more accurate response factor.

B.4.2 Average Response

When Average Response Factor is selected for a component, PeakNet uses a single-point, force zero, linear fit to calculate a separate response factor for each calibration point in all levels of the component. These response factors are then averaged to create the average response factor, which is used to calculate the amount of the component in samples.

B.5 Quantitation By Relative Response

When Relative Curve Fit is selected for a component, the component itself is not calibrated; the calibration equations of a Relative Response Component are used and then multiplied by a Relative Factor to obtain the response factor for the component. The relative curve fit is useful in situations where it is impractical to prepare a standard for a particular component, and the response of the component, relative to a calibrated component, is known.

You select the component to use as the Relative Response Component and enter a Relative Factor from the Calibration page of the Component Table.

B.6 Standard Addition Calibration

When analyzing samples with very low analyte amounts, it may not be possible to prepare standards with analyte amounts lower than those in the samples. In these cases, Standard Addition calibration often provides more accurate results than conventional calibration.

To perform Standard Addition calibration:

1. Prepare several similar aliquots of the sample (at least 2).
2. Add different amounts of analyte standard to each aliquot of sample.

   Quantities should be chosen such that final analyte amounts in the spiked samples are about 2x to 10x of the amounts in the unspiked sample.
3. In the Component Table - Calibration Tab Page, select Linear for Curve Fit Type and select Ignore for Origin.
4. Enter the amounts of the analytes added in each spiked sample into the Level cells (1 to n) in the Component Table - Calibration Standard Tab Page.
5. Analyze the spiked samples using Calibration Standard as the sample type and enter the Level of each (1 to n).
6. In Report Designer, select Amount By Standard Addition in the Peak Table.

   The analyte amount in the original sample will be shown as the amount by standard addition.

C • Troubleshooting Hardware Installation

C.1 Module(s) Not Controlled Correctly

1. Make sure the configuration is set correctly for the system components.
2. Make sure each module is connected to an RG-58U DX-LAN cable via a BNC tee connector. For installation instructions, see *Installing the Dionex PeakNet System* or the PeakNet on-line Help.
3. Verify that the current Moduleware is installed in each module.

C.2 Data Not Collected

1. Make sure the detectors are correctly connected to the DX-LAN computer interface card.
2. Make sure that **Begin Collection** is included in the detector Editor(s).
3. If the system includes an AD20 Absorbance Detector, verify that the lamp is on.
4. If the system includes an ED40 Electrochemical Detector operating in D.C. Amperometry mode, verify that the cell is on.

C.3 Relay Control Not Working

1. Use Dionex relay cables to make connections between the host computer and the RELAY connectors inside the DX-500 modules.
2. Make sure that the module Editors include a Timed Events step to turn on the relay.

C.4 Analog Detector Not Collecting Data

1. If the system includes a UI20 Universal Interface, make sure that the detector connected to the UI20 corresponds to the UI20 signal (Channel A and/or B) selected in the Method.
2. If the system includes a UI20, make sure the sensitivity settings selected from the detector and in the Method agree. A 1 mV or 10 mV full-scale signal from the detector provides barely enough signal for a usable record if the UI20 is set to 1 V or 10 V full-scale.

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