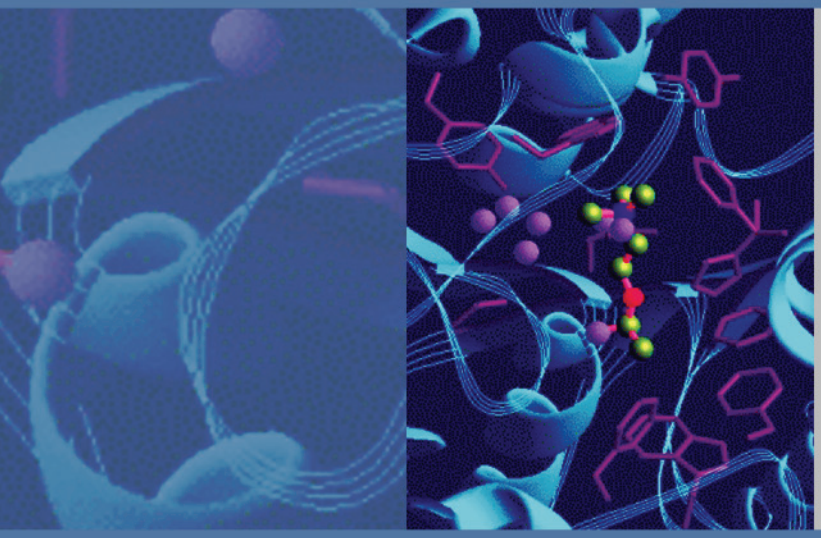


Thermo

TraceFinder

User Guide

Xcali-97281 Revision A October 2009

DOCUMENTATION SURVEY

Part of Thermo Fisher Scientific

Thermo SCIENTIFIC

Release history: Revision A

Minimum software requirements: Xcalibur 2.1.0; Microsoft Windows XP Professional SP 3; (optional) LC Devices 2.2.1

For Research Use Only. Not for use in diagnostic procedures.

Contents

Preface

Contents

❖ **To suggest changes to documentation or to Help**

- Complete a brief survey about this document by clicking the link below. Thank you in advance for your help.

Related Documentation

TraceFinder documentation includes Help and the *TraceFinder User Guide* as a PDF file.

❖ **To view the TraceFinder manual**

- Go to **Start > All Programs > Thermo TraceFinder > Manuals > TraceFinder User Manual.**

❖ **To open TraceFinder Help**

- From the TraceFinder window, choose **Help > TraceFinder Help**.

  To find a particular topic, use the Help Contents, Index, or Search panes.

For more information, including upcoming application notes, visit www.thermo.com.

Special Notices

This guide includes the following types of special notices:

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

System Requirements

Your system must meet these minimum requirements.

System	Requirements
PC	• 2 GHz processor dual core with 2 GB RAM • CD/R-ROM drive • Video card and monitor capable of 1280 × 1024 resolution (XGA) • 75 GB available on the C: drive • NTFS format
Instruments (supported or required)	Autosamplers • CTC PAL HTC-HTS • Accela™ • Surveyor™ • Agilent™ 1100 and 1200 LC Devices • Accela Pump • Agilent 1100 • Agilent 1200 • Surveyor MS Pump Plus • Surveyor LC Pump Plus Mass spectrometers • TSQ Quantum Access Max™ • TSQ Quantum Access™ • TSQ Quantum Ultra™ • TSQ Vantage™
Software	• Microsoft® Windows® XP Professional SP3 • Microsoft Office 2007 SP2 or Microsoft Office Excel 2007 SP2 • Dot Net 3.5 SP1 • Foundation 1.0.1 (available on the Xcalibur 2.1.0 CD) • Xcalibur 2.1.0.1139 and Xcalibur 2.1.0.1140QF03489 quick fix

Contacting Us

There are several ways to contact Thermo Fisher Scientific for the information you need.

❖ To contact Technical Support

Phone	800-532-4752
Fax	561-688-8736
E-mail	us.techsupport.analyze@thermofisher.com
Knowledge base	www.thermokb.com

Find software updates and utilities to download at mssupport.thermo.com.

❖ To contact Customer Service for ordering information

Phone	800-532-4752
Fax	561-688-8731
E-mail	us.customer-support.analyze@thermofisher.com
Web site	www.thermo.com/ms

❖ To copy manuals from the Internet

Go to mssupport.thermo.com and click **Customer Manuals** in the left margin of the window.

❖ To suggest changes to documentation or to Help

- Fill out a reader survey online at http://www.surveymonkey.com/s.aspx?sm=R7gKOvhLXn3NTkpK2BefHQ_3d_3d.
- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

Introduction

This chapter describes the general features of TraceFinder 1.0 quantitative software.

Contents

About the TraceFinder Application

The TraceFinder application is the next generation of Thermo Scientific quantitative software. The application focuses on environmental and food safety markets, creating the workflows that laboratories use.

In a single software package, the TraceFinder application provides a focused workflow for specific non-bioanalytical laboratory use and meets the need for a dynamic method development.

The TraceFinder application supports foreign language information systems and can export SRM data in .xml format so that other applications and foreign language systems can import the files into their databases.

The TraceFinder application can import the following file types:

- Sample lists in .csv or .xml format
- Processing (.pmd) and instrument (.meth) method files from Xcalibur
- Compounds from .xml files that use the datastore format

The TraceFinder application can continuously run acquisitions for 72 hours while processing batches of data and producing reports. It checks accuracy and precision of data against systems that have previously been certified against a standard processing program, such as the Statistical Analysis System (SAS).

Supported File Types

- Comma-separated values (CSV): A textual representation of value fields that are denoted as separated from a stream of alpha-numeric values that may be associated by a comma.
- Extensible Markup Language (XML): A generic framework for storing any amount of text or any data whose structure can be represented as a tree. The only indispensable syntactical requirement is that the document has exactly one root element (also called the document element). This means that the text must be enclosed between a root start-tag and a corresponding end-tag.
- METH: A proprietary file format for the Xcalibur software suite that contains specific instructions that let connected scientific instruments perform data acquisition.
- PMD: A proprietary file format for the Xcalibur software suite that contains specific instructions about processing data that has been acquired through the instruments attached to the system.
- RAW: A file type used for acquired samples on the system.

TraceFinder Directory Structure

The TraceFinder application creates folders for projects/subprojects/batches, methods, and templates in the ..\Thermo\TraceFinder directory. Within each batch folder, the application creates folders for data, methods, and reports.

IMPORTANT Users cannot rename or move the folders created by the TraceFinder application.

TraceFinder Feature Summary

The TraceFinder system provides a workflow-oriented approach to high-throughput quantitation. The system uses a batch-centric approach and tools to automate and speed up the processes of method creation, loading samples, automatically generating data, manually reviewing and editing results, and finalizing the data review and reporting process.

The TraceFinder software package includes data acquisition, processing, reviewing, and reporting capabilities designed to assist analysts in environmental and food safety applications. The application has a fully automated acquisition mode and a manual review mode. You can use the data acquisition system to create and submit batches and monitor real-time review of results.

The TraceFinder application uses a comprehensive processing method to provide improved handling of ion ratio calculations, review and reporting, a mass spectral comparison capability, and an integrated connection between the processes of data review and reporting.

Key features include the following:

- Role-based authorization for Lab Director, IT Administrator, Supervisor, Technician, and QAQC (quality assurance)
- Configuration mode with user administration, project administration, datastore administration, and application administration
- Method development mode with instrument method editor, processing parameters, QA/QC parameters, and reporting options
- Data Review mode with batch views, data review, local method views, and report views
- Acquisition mode
- Database-capable method development
- Quantification workflows, supporting capabilities present in LCquan and LabForms 2.5
- Pre defined, customized report formats

Features of the common workflow include the following:

- Acquisition and processing
- Peak detection
- Quantification to include calibration
- QA/QC analysis and flag setting
- Reporting
- Data persistence
- Raw data file handling

Reporting Features

The report engine can generate several different types of reports designed to meet the needs of the laboratory, the laboratory's customers, and key regulatory agencies that might review the results. The TraceFinder application can produce both standard reports and custom reports. The following types of reports meet the requirements of various methods and worldwide regulatory agencies and are designed to help track the performance of the GC/LC system and method:

Standard Reports

- Batch Report
- Blank Report
- Breakdown Report
- Calibration Density Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Confirmation Report
- Confirmation Report 2
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report
- Solvent Blank Report
- Surrogate Recovery Report

Custom Reports

- AltCalibrationReport
- Alternate BatchReport
- Alternate CalibrationReport
- Alternate ConfirmationReport
- Alternate MatrixSpikeReport
- Alternate SampleReport
- Alternate SummaryReport
- BatchReport
- BlankReport
- CalibrationDensityReport
- CalibrationReport
- CheckStandardReport
- CompoundCalibrationReport
- ConfirmationReport
- ConfirmationReport2
- HighDensitySampleReport1Long
- HighDensitySampleReport2Long
- HighDensitySampleReport3Long
- QuantitationReport

For additional information about custom and standard reports and a sample of each standard report type, see "Sample Reports" on page 221.

Getting Started

This chapter describes the basic TraceFinder workflow and the procedures for getting started with the TraceFinder application.

Contents

TraceFinder Workflow

The TraceFinder software is structured with a typical laboratory workflow in mind—the user creates a batch and the system injects samples into the instrument, runs the samples, analyzes the data, and generates a report. You can set up a master method for specific compound groups or assays you expect to run in your lab. When you are ready to run a particular type of sample, select the appropriate method and you are ready to start.

When using the TraceFinder application, follow these basic steps:

1. Create and save a master method.

   An instrument method defines only how raw data is acquired. A master method is a combination of instrument method and processing method that defines how the raw data is processed, how the QA/QC information evaluates the results, and how the results appear in reports.

2. Create and submit a batch.

   A batch is a list of samples for processing and reporting using a specified method. Each row of a batch represents a unique sample.

3. Monitor the status of the batch in the Real Time Status view.

   The real -time display is visible from the dashboard and all the TraceFinder modes. You can begin another batch while you watch the real-time display of the currently acquiring batch.

4. Evaluate the data in the Data Review mode.

   The Data Review mode includes views where you can review batches, batch data, reports, and local methods.

5. View and print reports in the Report View.

   Use the Report View to view or print the reports for the currently selected batch.

Installing the TraceFinder Application

Follow these instructions to install, start, and log on to the TraceFinder application.

❖ To install the TraceFinder application

1. Follow the instructions on the included CDs to install the Xcalibur 2.1 application and your TSQ instrument driver.
2. Install the driver for your LC pump and autosampler.
3. Insert the TraceFinder 1.0 CD in the drive, and follow the on-screen instructions.

   If the install windows do not automatically open, navigate to the Xinstall.exe file and launch it.

❖ To start the TraceFinder application

1. Configure your instruments.

   You cannot configure your instruments while the TraceFinder application is running.

2. Double-click the TraceFinder application icon on your desktop, or go to **Start > All Programs > Thermo TraceFinder 1.0 > TraceFinder 1.0**.

❖ To log on to the TraceFinder application

1. Enter your assigned user name.

   Before you can log on to the TraceFinder application, a system administrator must have set up a user account for you. The administrator will have assigned you a user name and password and given you permission to access specific modes.

2. Enter your password.

   If your user name and password do not match, the system reports this error:

   Correct the user name or password, or contact your system administrator.

3. Click **Login**.

   The TraceFinder dashboard opens. See "TraceFinder dashboard" on page 15.

4. To exit the TraceFinder application without logging on, click **Exit TraceFinder**.

TraceFinder log on screen

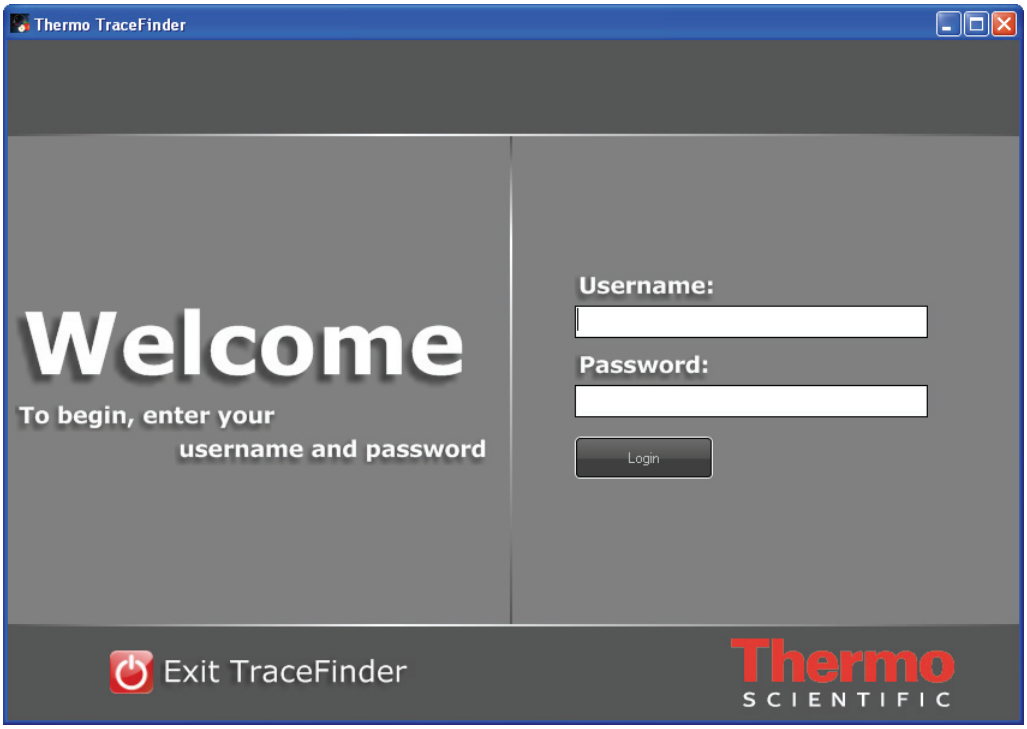


Table 1. Log on screen parameters

Parameters	Description
Username	The user's assigned user name.
Password	The assigned password for the user name.
Login	Verifies the user name and password, and displays the dashboard.
Exit TraceFinder	Quits the TraceFinder application.

Installing the QED and NIST Libraries

Follow these instructions to install the NIST and QED libraries.

❖ To install the NIST library

1. Launch the XInstall executable.
2. Click the **NIST Library** button.

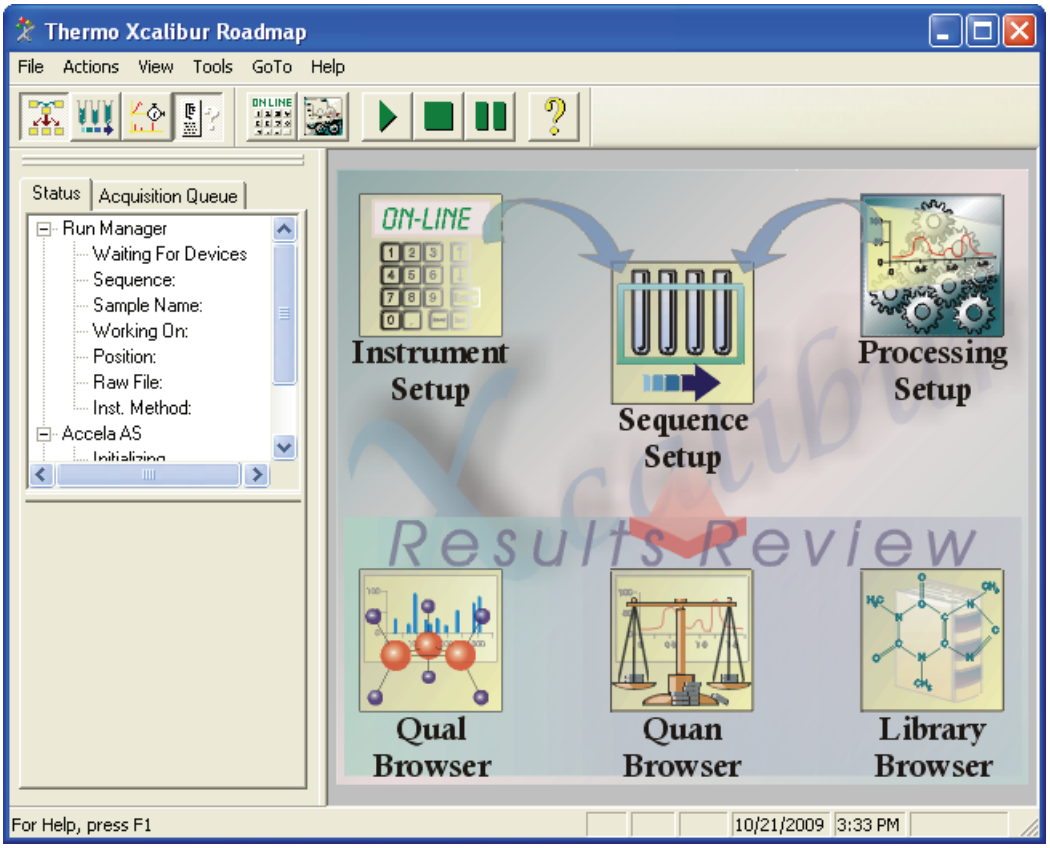
   The NIST 08 MS Search and AMDIS Setup wizard opens.
3. Follow the instructions in the setup wizard.
4. When the wizard prompts you to select a program folder, select **Thermo TraceFinder 1.0**.

❖ To install the QED library

1. On your desktop, double-click the Xcalibur icon, 

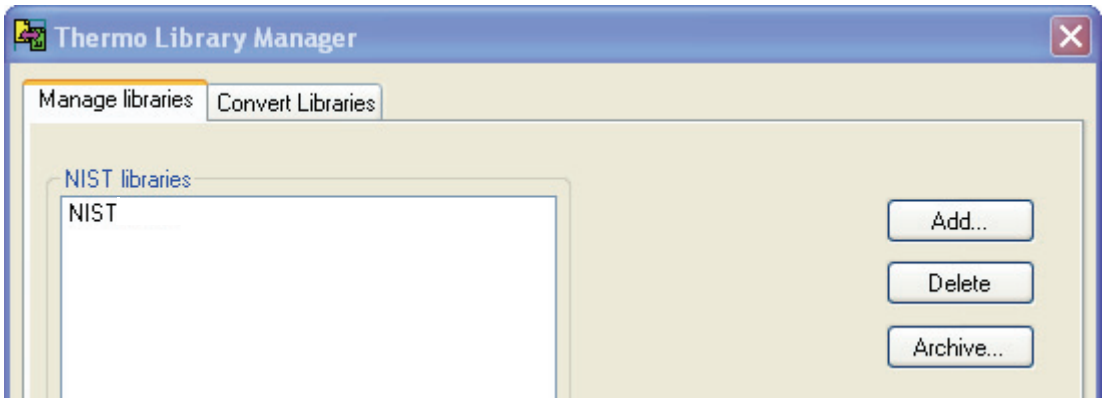
.

   The Thermo Xcalibur Roadmap opens.



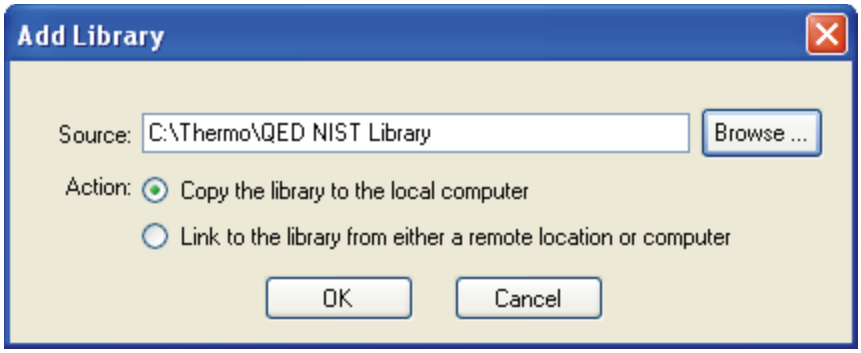
2. Select **Tools > Library Manager**.

   The Thermo Library Manager opens. The NIST library is displayed in the libraries list.



3. On the Library Manager, click **Add**.

   The Add Library dialog box opens.

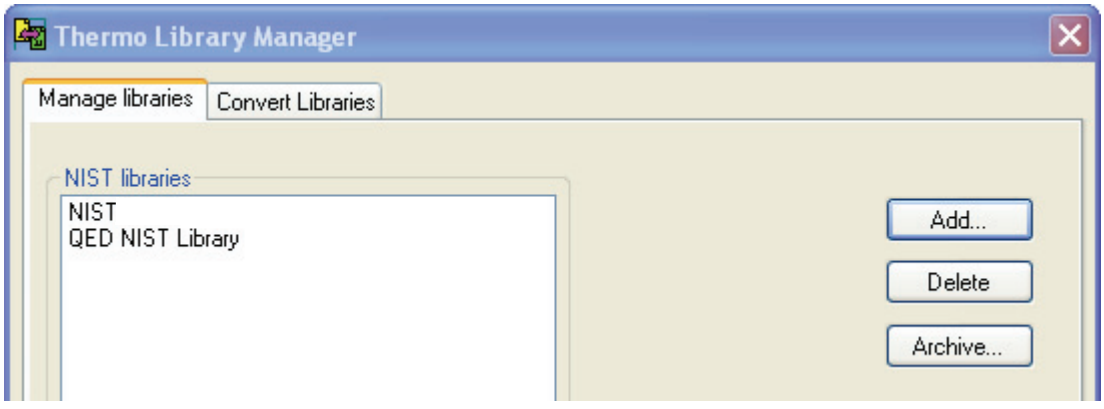


4. Click **Browse**, and locate your QED library in the C:\Thermo folder.
5. Click **OK**.

   The application reports that the library has been added to the NIST software.

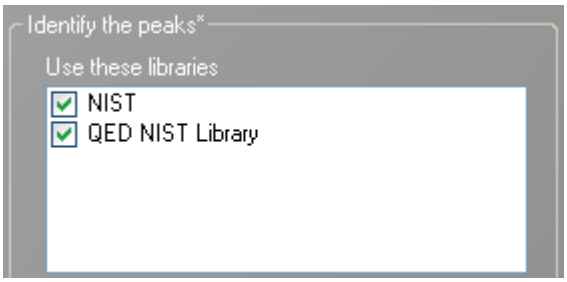
6. Click **Dismiss** to close the message box.

   The application adds the QED library to the NIST libraries list in the Library Manager.



7. Click **Exit** in the Thermo Library Manager.
8. Start the TraceFinder application.
9. Go to the Method Development mode.
10. Choose **File > New > Method template** from the main menu.

    The QED NIST Library is listed in the Use these libraries list on the Method Template Editor.



Choosing a Mode

The dashboard provides the current user with options applicable to assigned role of that user. The following table shows the available modes for each user role.

Table 2. User roles and permissions

User role	Method Development	Acquisition	Data Review	Configuration
Lab Director	×	×	×	×
IT Administrator				×
Supervisor	×	×	×	
Technician		×	×	
QAQC			×	

❖ To choose a mode

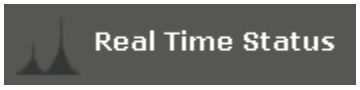
1. From the dashboard, click the mode in which you want to work.

   Your dashboard shows only the modes that you have permission to use. See "TraceFinder dashboard" on page 15.

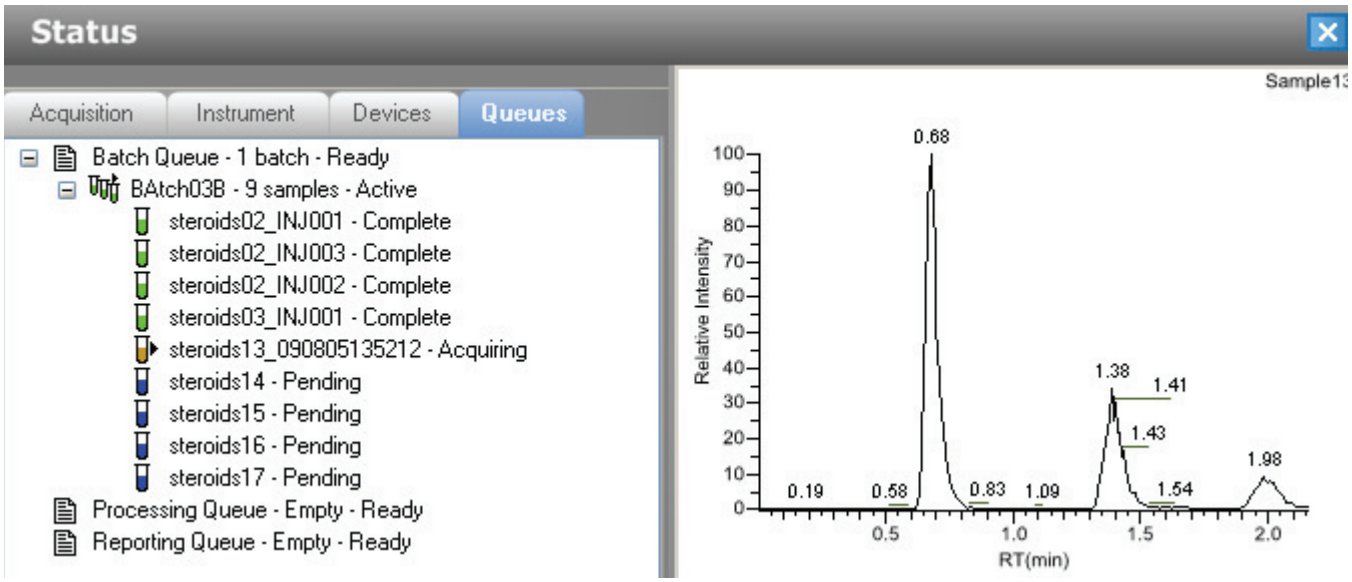
2. To change modes from within any of the TraceFinder application modes, click the mode buttons in the lower left corner of the window.

❖ To watch the real-time display from the dashboard

- Click **Real Time Status**.



The real-time status is displayed at the bottom of the dashboard.



For descriptions of all the features of the real-time display, see "Real-time Display" on page 176.

TraceFinder dashboard

A dashboard for a Lab Director, who has permission for all modes, looks like this:

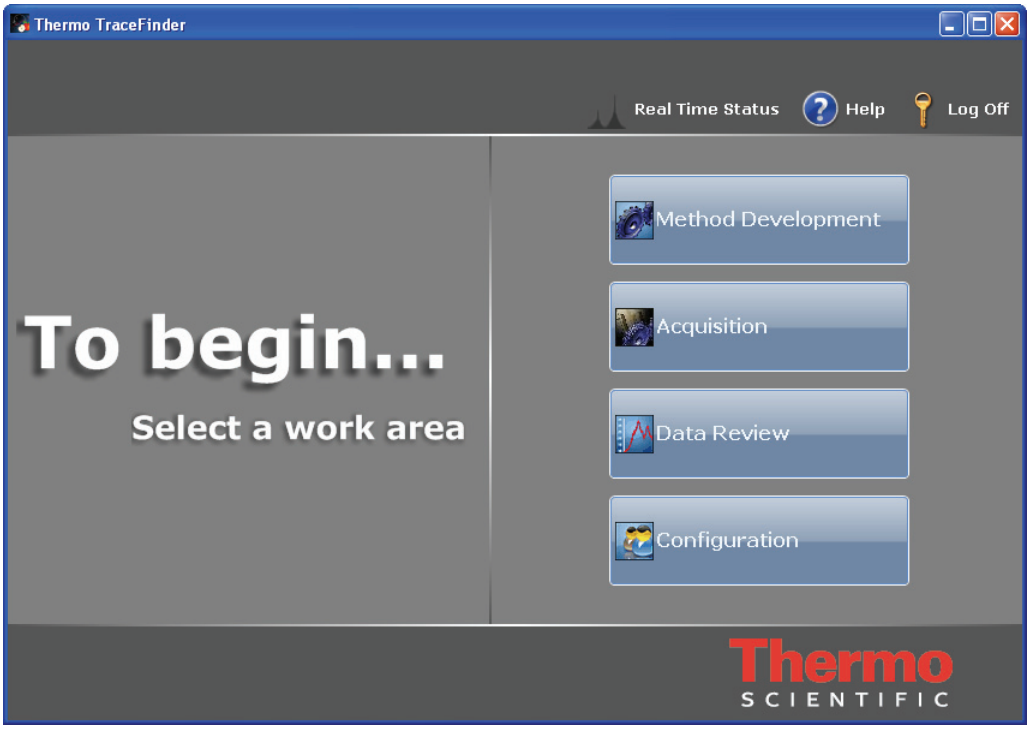


Table 3. TraceFinder dashboard parameters

Parameters	Description
Real Time Status	Opens the real-time display for the current acquisition. The acquisition progress is displayed within the current mode window.
Help	Opens the TraceFinder Help.
Log Off	Logs off the current user and displays the log on screen.
Method Development	Opens the Method Development mode where you can create a master method, an instrument method, or a development batch.
Acquisition	Opens the Acquisition mode where you can acquire and process a previously saved (.tbr) batch, create and acquire a new batch, reinject samples from a previously acquired batch, or create a batch template.
Data Review	Opens the Data Review mode where you can create and review batches, batch data, reports, and local methods.
Configuration	Opens the Configuration mode where you can set permissions, assign users to roles, configure available reports and import new reports, and maintain the various databases, including the Compound Datastore.

Using the Configuration Mode

This chapter discusses the configuration tasks assigned to the IT Administrator and Lab Director roles.

Contents

If your role is that of an IT Administrator or Lab Director, you are responsible for the following:

- Handling the databases
- Applying roles to users
- Understanding security, users, and groups
- Creating local users and network groups
- Creating projects and subprojects
- Maintaining compounds in the compounds datastore

❖ To access the Configuration mode

- Click **Configuration** from the dashboard or the navigation pane.

The Configuration navigation pane opens.

Figure 1. Configuration navigation pane

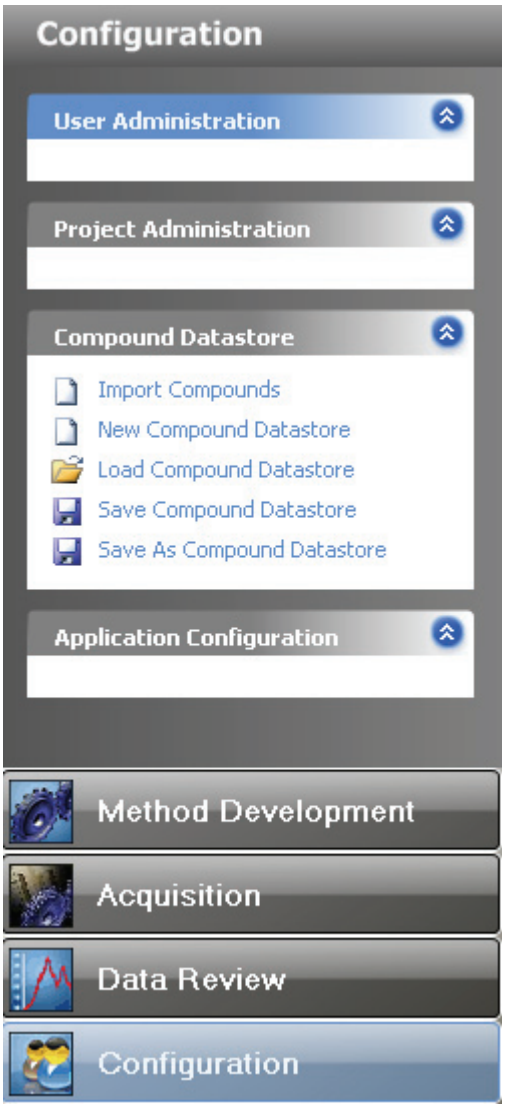


Table 4. Configuration navigation pane functions (Sheet 1 of 2)

Functions	Description
User Administration	Opens the User Administration view where you can add, remove, or edit user accounts and permissions. See "User Administration" on page 20.
Project Administration	Opens the Project Administration view where you can create and manage projects and subprojects. See "Project Administration" on page 28.

Table 4. Configuration navigation pane functions (Sheet 2 of 2)

Functions	Description
Compound Datastore	Opens the Compound Datastore view where you can manage the definition of compounds in the current datastore. See "Compound Datastore" on page 30.
Application Configuration	Opens the Application Configuration view where you can configure the TraceFinder application to operate as a Liquid Chromatography (LC) technology or as a Gas Chromatography (GC) technology and specify a compound datastore to use for that technology. See "Application Configuration" on page 37.

User Administration

In the User Administration view of the Configuration mode, in the role of Lab Director or IT Administrator, you can add, remove, or edit user accounts and permissions.

For detailed descriptions of each user role and the permissions and responsibilities for each role, see "User Roles" on page 25.

Use the following procedures:

- To open the User Administration view
- To add a user
- To edit user information
- To remove a user

❖ To open the User Administration view

1. Do one of the following:
   - From the dashboard, click **Configuration**.

     –Or–
   - Click **Configuration** in the navigation pane from any other mode.
2. Click the **User Administration** task pane.

   The User Administration view opens. See "User Administration view" on page 23.

❖ To add a user

1. Click the **Add user** icon,  .

   The parameters in the User area at the bottom of the view are enabled.
2. Enter a unique name in the Username field.
3. Select a role from the Role list.

   All users must be assigned to one of these defined roles. For detailed information about the permissions allowed for each role, see "User Roles" on page 25.
4. Enter the user's password.

   There is no confirmation for the encrypted password you enter, so carefully enter it and make sure to communicate it to the user.
5. (Optional) Enter the user's full name, account number, phone number, and e-mail address.

6. To enable this user login, select the **Enabled** check box.

   You can disable a user login without deleting the user's information. See To edit user information.

7. Do one of the following:

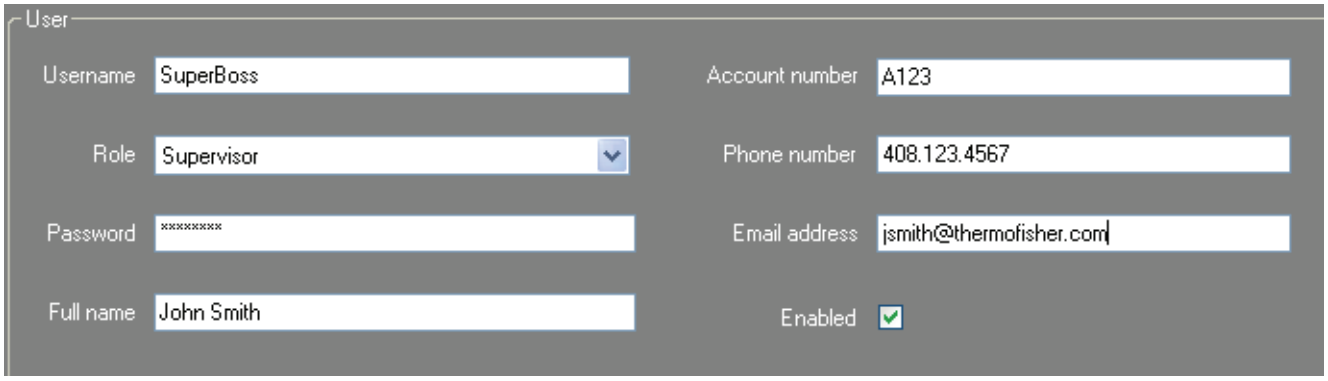
   - When all the user information is correct, click the **Save changes** icon,  .

     The TraceFinder application adds the new user to the User Listing table, and the parameters in the User area are unavailable.

     –Or–

   - To discard all information and not create a new user from the parameter values you entered, click the **Cancel changes** icon,  .

     All information is discarded and the parameters in the User area are unavailable.



❖ To edit user information

1. In the User Listing table, select a user.

   Note Clicking anywhere in the row selects the user.

   The user information populates the parameter fields in the User area.

2. Click the **Edit user** icon,  .

   The parameters in the User area are enabled.

3. Edit any of the parameter values.

   If you are editing your current user name, the Enabled check box is unavailable because you cannot make your own account unavailable.

4. Do one of the following:
   - When all the user information is correct, click the **Save changes** icon,  .

     The TraceFinder application adds the new parameter values to the User Listing, and the parameters in the User area are unavailable.

     – Or–
   - To discard all changes and not save the edits, click the **Cancel changes** icon,  .

     All changes are discarded, and the parameters in the User area are unavailable.

❖ To remove a user

1. In the User Listing table, select a user.

   Note Clicking anywhere in the row selects the user.

   The user information populates the parameter fields in the User area.

2. Click the **Remove user** icon,  .

   If you select your current user name, the Remove User icon is unavailable. You cannot remove yourself.

3. When prompted, confirm that you want to remove this user.

   If the user is currently logged on to the TraceFinder application, the user's current session is not affected.

4. Click **OK**.

   Note Rather than completely removing the user, you can disable a user login without removing all the user information from the system. See To edit user information.

User Administration view

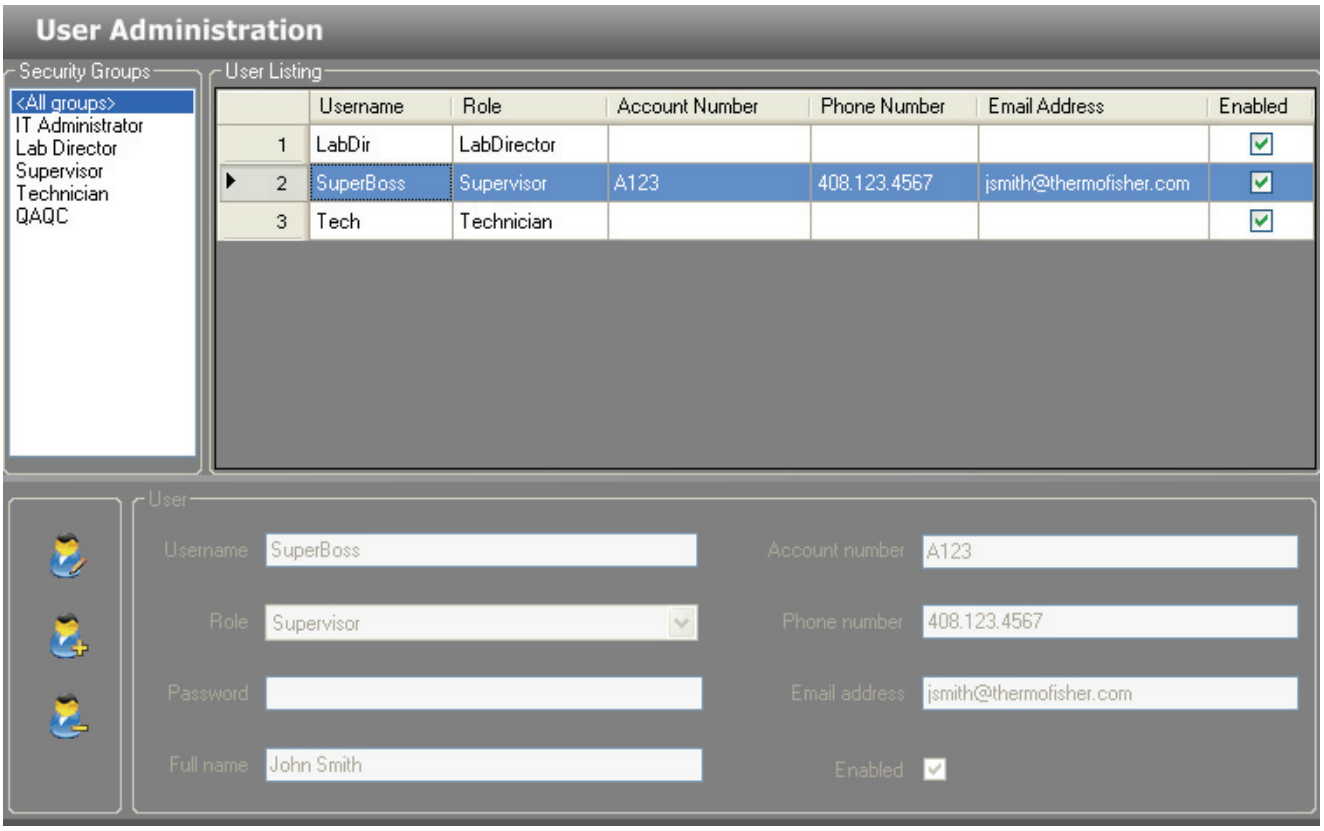


Table 5. User Administration parameters (Sheet 1 of 2)

Parameter	Description
Security Groups	All permission levels defined in the TraceFinder application. For detailed descriptions of user permissions, see "User Roles" on page 25.
User Listing	
Username	User login names.
Role	The security group that defines user permissions.
Account Number	User account numbers.
Phone Number	User telephone numbers.
Email Address	User e-mail addresses.
Enabled	Available or unavailable status for the user account.
User	
Username	Login name for this user.
Role	Security group that defines this user's permissions.
Password	Login password for this user.

Table 5. User Administration parameters (Sheet 2 of 2)

Parameter	Description
Full name	The user's actual name.
Account number	Optional account number for this user.
Phone number	Optional telephone number for this user.
Email address	E-mail address for this user. Used to notify user of a randomly generated password.
Enabled	Allows or disallows access for this user. When this user is currently logged on, disallowing takes effect after the user logs off.
Functions	
 Add user	Enables the fields in the User area where you can enter information for a new user.
 Remove user	Deletes all information for the selected user.
 Edit user	Enables the User area where you can edit any of parameters for the selected user.
 Save changes	Adds the new parameter values to the User Listing table and disables the parameters in the User area.
 Cancel changes	Discards all new or edited information.

User Roles

This section describes the responsibilities for five different types of users: Lab Director, IT Administrator, Supervisor, Technician, and QAQC.

User Permissions

A Lab Director or an IT Administrator assigns you to a role that gives you permission to access specific modes of the TraceFinder application. When you log on, the dashboard displays links to only the modes that you can access.

Table 6. User roles and permissions

User role	Method Development	Acquisition	Data Review	Configuration
Lab Director	×	×	×	×
IT Administrator				×
Supervisor	×	×	×	
Technician		×	×	
QAQC			×	

Lab Director

As a user in the role of Lab Director, you review graphically applicable data and manipulate data, batches, methods, and instruments.

A lab director is responsible for these tasks:

- Creating or editing methods for new levels of detection or adding new compounds to the existing database
- Reviewing data from the mass spectrometer
- Running samples and reviewing data collected by others
- Reporting the data
- Understanding the results and giving final approval of the released data before archiving

IT Administrator

As a user in the role of an IT administrator, you set security, manage users into roles, and manipulate the various databases. You are is responsible for adding compounds into the various compound databases.

An IT administrator is responsible for these tasks:

- Handling the databases
- Applying roles to users
- Understanding security, users, and groups
- Creating local users and network groups

Supervisor

As a user in the role of a supervisor, you are responsible for putting samples on the instrument and using previously built sequences and methods for processing and acquiring data. You also develop and edit methods for processing and acquiring data, review the data, and distinguish between the need to rerun samples or pass reports up to the lab manager or QAQC for final review. On a daily basis, you establish the priority for a list of samples to run and create the sequence of events.

A supervisor is responsible for these tasks:

- Submitting samples
- Creating and submitting batches
- Reporting the data to management
- Creating or editing methods for new levels of detection or adding new compounds to the existing database
- Reviewing data from the mass spectrometer
- Understanding the results, who ran the batch, and who passed along the results before you give intermediate approval and send the data to management
- Modifying new compounds or adjusting methods for specific result sets

Technician

A user in the role of a technician is responsible for putting samples on the instrument and using previously built sequences and methods for processing and acquiring data. A technician also edits existing methods for processing and acquiring data and is responsible for reviewing collected data and distinguishing between the need to rerun samples or pass reports up to the supervisor. On a daily basis, a technician is responsible for gathering the list of samples to run and creating the sequence of events.

A technician is responsible for these tasks:

- Submitting samples
- Creating and submitting batches
- Creating data to be reviewed by management
- Receiving instructions for new sets of samples for the TraceFinder application to analyze after finishing the current analysis
- Reviewing data from the mass spectrometer
- Understanding the resulting data, making integration changes, and passing those changes up for further approval.

QAQC

As a user in the role of a QAQC, you review graphically applicable data and interpret the data but you do not manipulate the data.

A QAQC user is responsible for these tasks:

- Reviewing data from the mass spectrometer
- Understanding the results and who ran and passed along the results before giving intermediate approval and sending the data on to management
- Receiving instructions for new sets of samples for the TraceFinder application to analyze after finishing the current analysis

Project Administration

In the role of Lab Director or IT Administrator, you can create and manage projects and subprojects in the Project Administration view of the Configuration mode.

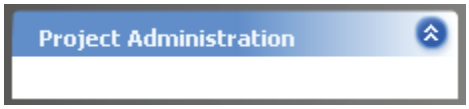
Use the following procedures:

- To open the Project Administration view
- To create projects or subprojects
- To delete projects or subprojects

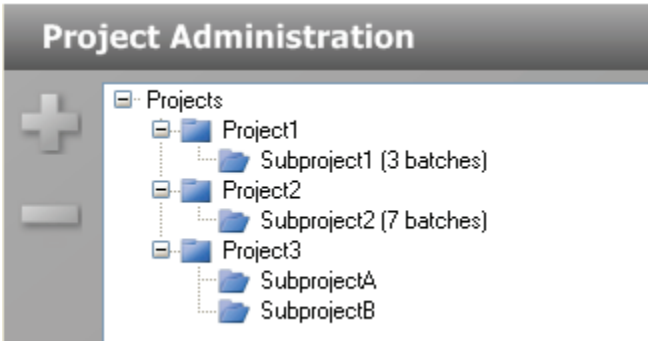
❖ To open the Project Administration view

1. Do one of the following:
   - From the dashboard, click **Configuration**.

     –Or–
   - Click **Configuration** in the navigation pane.
2. In the Configuration navigation pane, click **Project Administration**.



The Project Administration view opens.



All projects are created under a main Projects folder on the C: drive:

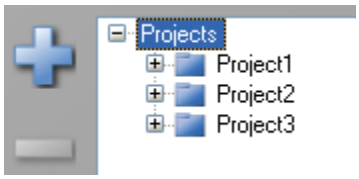
`C:\Thermo\TraceFinder\Projects`

❖ To create projects or subprojects

1. Select the top-level project.

   You can select the main Projects folder and create a new project under it, or you can select one of your existing projects and create a subproject under it.

   When you select a project folder, the plus sign is enabled.



2. Click the plus sign.

   The TraceFinder application creates a new, unnamed project folder under the selected project.

3. While the new project is still highlighted, type a new name.

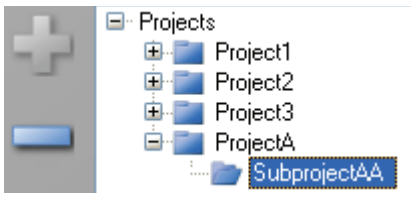
   Project names can contain spaces and special characters, except for the following special characters: \ / : * ? " < > |

4. To save the new name, press **Return** or click anywhere in the view.

❖ To delete projects or subprojects

1. Select the project or subproject you want to delete.

   You can delete any project that contains no subprojects. You can delete any subproject that contains no batches. When the selected project or subproject is available for deletion, the minus sign is enabled.



2. Do one of the following:

   - Click the minus sign.

     –Or–

   - Right-click and choose **Remove project** or **Remove subproject** from the shortcut menu.

3. At the prompt, click **Yes** to remove the selected project or subproject.

Compound Datastore

In the role of Lab Director or IT Administrator, you can manage the definition of compounds in the current datastore in the Compound Datastore view of the Configuration mode.

The current datastore is the datastore specified for the current technology in the Application Configuration view. See "Application Configuration" on page 37.

Use the following procedures:

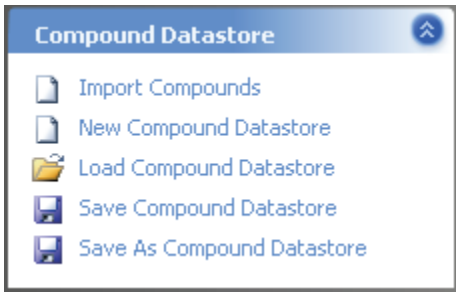
- To open the Compound Datastore editor
- To open a compound datastore
- To create a new compound datastore
- To import compounds
- To add a single compound
- To save a datastore
- To save a datastore to a new name
- To remove a compound or a compound's transition information
- To filter the compound list

❖ To open the Compound Datastore editor

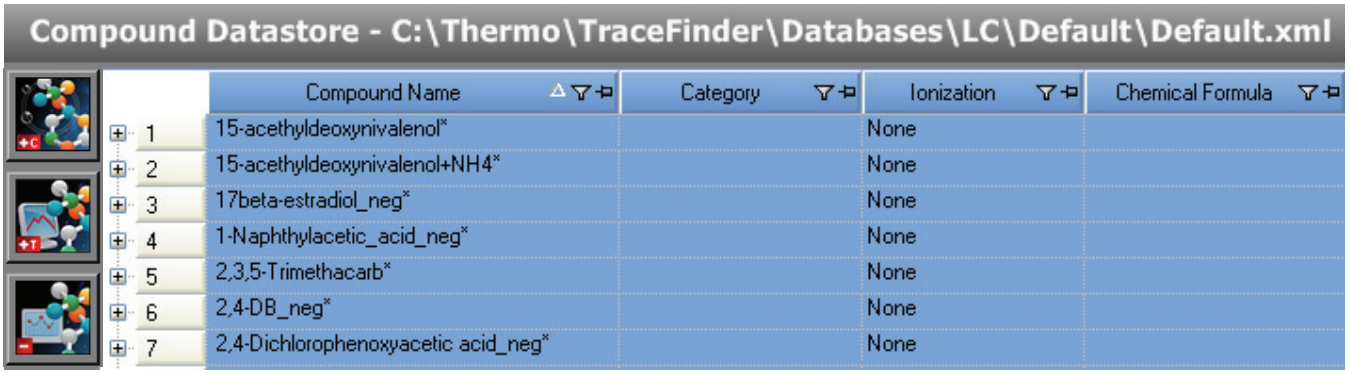
1. Do one of the following:
   - From the dashboard, click **Configuration**.

     –Or–

   - Click **Configuration** in the navigation pane.
2. Click the **Compound Datastore** task pane.



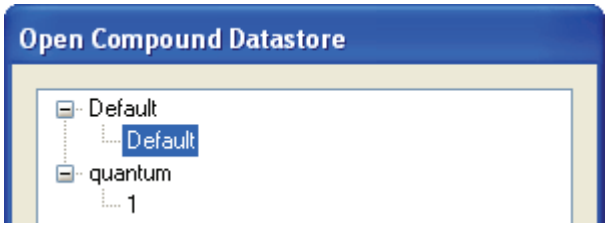
The current datastore opens in the Compound Datastore view.



❖ To open a compound datastore

1. Click **Load Compound Datastore** in the Compound Datastore task pane.

   The Open Compound Datastore dialog box opens.



2. To expand the folder, click the plus sign before the folder name.
3. Double-click the name of the datastore you want to open.

   The selected datastore opens in the Compound Datastore view. See "Compound Datastore view" on page 35.

❖ To create a new compound datastore

- Click **New Compound Datastore** in the Compound Datastore task pane.

  A new, empty datastore opens in the Compound Datastore view. You can import a file of compounds into the new datastore (see To import compounds), or you can manually add compounds one at a time (see To add a single compound).

❖ To import compounds

1. Click **Import Compounds** in the Compound Datastore task pane.
2. In the browser, locate a .csv or .xml compounds file and open the file.

   The TraceFinder application imports the compounds in the imported file, adds them to any compounds already in the datastore, and alphabetically sorts them.

❖ To add a single compound

1. To add a single compound to the datastore, do one of the following:
   - Click the **Add compound** icon,  .

     –Or–

   - Right-click in the compounds list and choose **Add compound** from the shortcut menu.

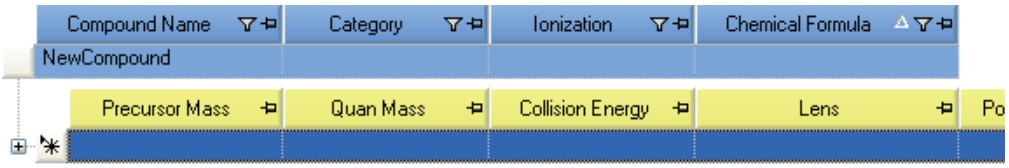
   A new empty compound row is added to the bottom of the compounds table.

2. Click the first table cell, and enter the required Compound Name parameter.
3. (Optional) Enter values for the Category, Ionization, or Chemical Formula columns.
4. To add a transition to the compound, select the compound and do one of the following:
   - Click the **Add transition information** icon,  .

     –Or–

   - Right-click and choose **Add transition information** from the shortcut menu.

   A new empty transition row is added to the compound. A transition includes quantitative values for the compound. Each compound requires at least one transition.



5. Enter all required parameters.

   For a list of required and optional parameters, see the list of Compound Datastore parameters.

   Tip You cannot add another new compound or save the compound datastore until you enter all required transition parameters or remove the transition from the compound. To remove a transition, right-click in the row and choose **Cancel**.

6. To save the new datastore, click **Save Compound Datastore** in the Compound Datastore task pane.

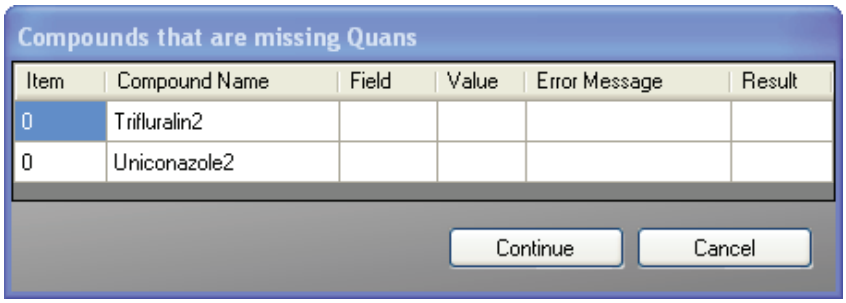
❖ To save a datastore

1. Click **Save Compound Datastore** in the Compound Datastore task pane.

   The database is stored as

   `..\Thermo\TraceFinder\Databases\<GC or LC>\`*`foldername`*`\`*`filename`*`.xml`

   If the datastore contains any compounds that do not have an associated transition, the Compounds that are missing Quans dialog box opens, listing the compounds.



2. Do one of the following:

   - To remove the listed compounds from the datastore and save the datastore, click **Continue**.

     –Or–

   - To keep the listed compounds and return to the datastore, click **Cancel**.

   Note You cannot save a compound that does not have an associated transition.

❖ To save a datastore to a new name

1. Click **Save As Compound Datastore** in the Compound Datastore task pane.

   The Save Compound Datastore dialog box opens.

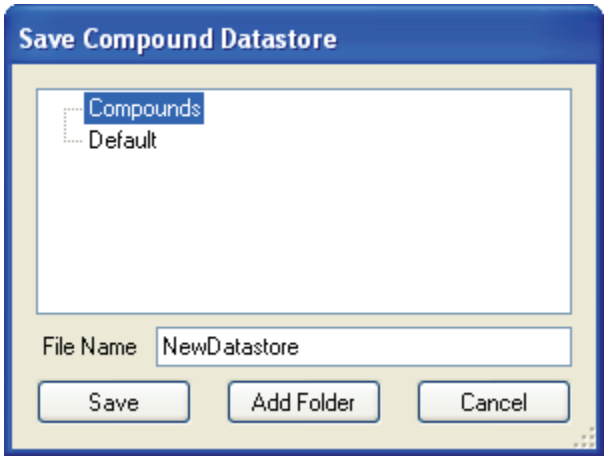


Table 7. Select Compound Datastore parameters

Parameter	Description
Compounds	Lists the datastores you have created for this technology.
Default	The default datastore defined for this technology.
File Name	File name for the new datastore.
Save	Writes the new datastore to the specified folder.
Add Folder	Adds a new folder where you can save the datastore.
Cancel	Closes the dialog box and makes no changes to the datastore for the current technology.

2. Enter a file name for the new compound datastore.
3. (Optional) Click **Add Folder** and enter the name for a new folder to be created in the ..\Thermo\TraceFinder\Databases\<GC or LC> folder.
4. Click **Save**.

   The database is stored as

   `..\Thermo\TraceFinder\Databases\<GC or LC>\`*`foldername`*`\`*`filename`*`.xml`

❖ To remove a compound or a compound's transition information

1. In the Compound Datastore view, select the row you want to delete.

   You can remove either of the following:

   - An entire compound, including all associated transition information.
   - A row of transition information.

2. Click the **Remove transition** icon,  , or right-click and choose **Remove transition** from the shortcut menu.
3. At the prompt, click **Yes** if you are sure you want to delete the selected row.

   The selected row and all items within it are deleted.

> **Tip** If you add a row of compound or transition information and do not complete all the required values, you can right-click and choose **Cancel** to remove the entire row. You can cancel only incomplete compound or transition rows.

❖ To filter the compound list

1. To display a filtered list of compounds, click the funnel icon,  , in the column header.

   For each column, a list of filterable criteria is displayed in a list box. On all list boxes, you can choose to filter by All, Blanks, NonBlanks, or by custom filter criteria. Other filter criteria are specific to the individual columns.
2. To create a custom filter based on column values, choose **Custom** from the menu.

   For detailed instructions about creating a custom filter, see Appendix C, "Using Filter Criteria."

Compound Datastore view

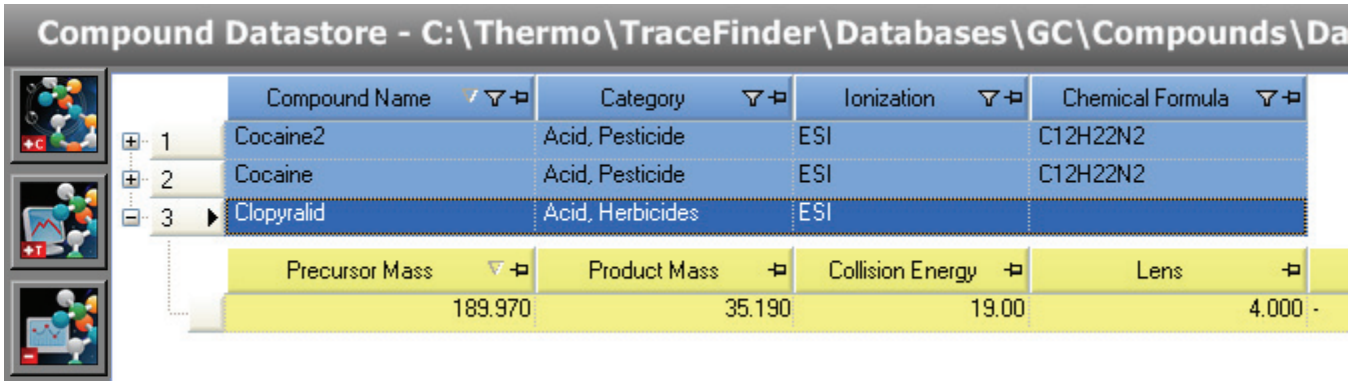


Table 8. Compound Datastore parameters (Sheet 1 of 2)

Parameter	Description
Function Icons	
	Adds a compound transition to the datastore.
	Adds a quantitation items row to the selected compound transition, or adds a confirming items row to the selected quantitation item.
	Deletes the selected compound transition.

Table 8. Compound Datastore parameters (Sheet 2 of 2)

Parameter	Description
Compound parameters	
Compound Name	Alphanumeric name assigned to the compound.
Category	(Optional) Alphanumeric identifier.
Ionization	(Optional) Alphanumeric identifier. Valid values: ESI, APCI, EI, CI, APPI
Chemical Formula	(Optional) Alphanumeric chemical identifier.
Precursor Mass	The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999
Product Mass	The mass-to-charge ratio of the quan ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Range: -250.00 to 250.00
Lens	(Optional) Range: -400 to 400
Polarity	**+** (positive) or **-** (negative)
RT (min)	Retention time. The application uses RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT - (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Window (sec)	Acquisition window. The application uses RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 499.50 Start time = RT - (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Energy Ramp	(Optional) Range: 0.00 to 200.00
Color coding	• Blue indicates a compound. • Yellow indicates a quantitative transition. • Green indicates a confirming transition. • Pink fields are editable when you import new transitions into the datastore from method editor.

Application Configuration

This section includes instructions for the following tasks:

- Specifying the General Configuration
- Specifying the Reports Configuration

Specifying the General Configuration

In the role of Lab Director or IT Administrator, you can configure the TraceFinder application as a Liquid Chromatography (LC) technology or as a Gas Chromatography (GC) technology in the Application Configuration view of the Configuration mode. Each technology uses a different compound datastore.

As a user in the role of Lab Director or IT Administrator, you can also choose a compound datastore to use with the LC or GC technologies.

Use the following procedures:

- To open the General page of the Application Configuration view
- To specify a technology
- To specify a datastore to use in method development

❖ To open the General page of the Application Configuration view

1. Do one of the following:
   - From the dashboard, click **Configuration**.

     –Or–
   - Click **Configuration** in the navigation pane.
2. Click **Application Configuration**.

The General page of the Application Configuration view opens. See "General page" on page 39.

❖ To specify a technology

1. In the Technology selection area, select a chromatography technique.
2. Click **Apply**.

   The TraceFinder software reminds you that you must restart the application when you change technologies.

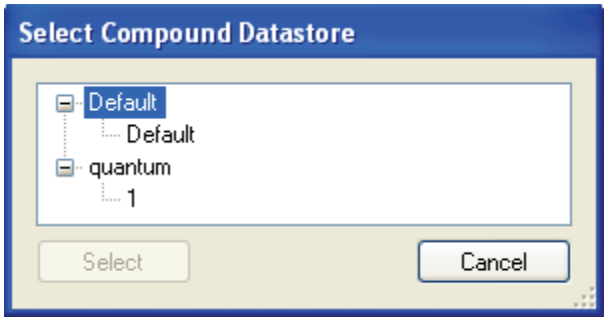
   - If you would like the TraceFinder application to restart for you, click **Yes**.
   - If you want to restart the TraceFinder application yourself, click **No**.

     Until you restart the TraceFinder application, you will not see the features specific to the new technology.

❖ To specify a datastore to use in method development

1. In the Compound Datastore selection area, click **Select**.

   The Select Compound Datastore dialog box opens.



   The list of available datastores is specific to the current chromatography technique (LC or GC). If you change the chromatography technique, you must restart the application to populate the compound datastore selection list with the appropriate datastores.

2. Do one of the following:

   - To use this datastore for all methods created for this technology, click **Select**.

     –Or–

   - To close the Select Compound Datastore dialog box and keep the currently specified datastore, click **Cancel**.

3. In the Application Configuration view, click **Apply**.

   When you switch between techniques, the TraceFinder application remembers the datastore assigned to each technique.

General page

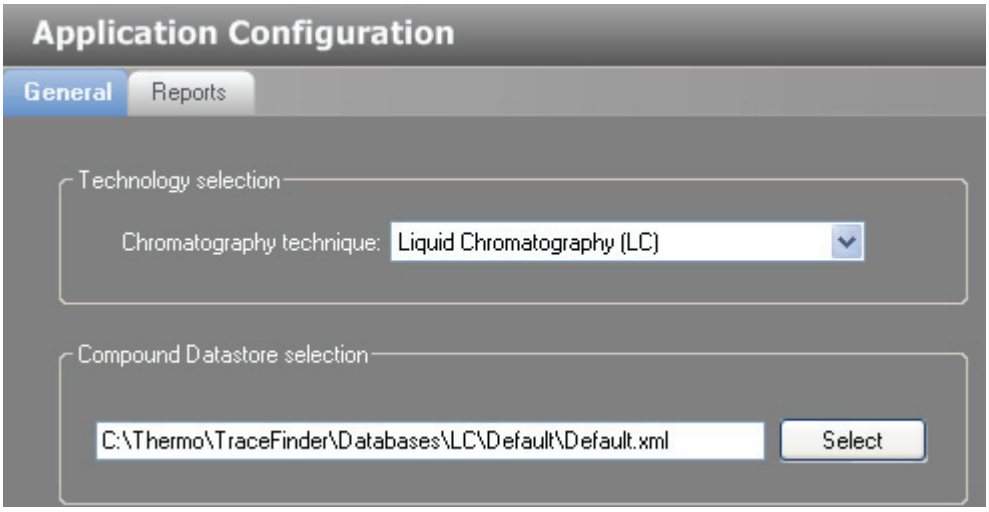


Table 9. General configuration parameters

Parameter	Description
Chromatography technique	Specifies Gas Chromatography or Liquid Chromatography.
Select	Opens a browser where you can select a saved datastore .xml file.

Specifying the Reports Configuration

In the Application Configuration view of the Configuration mode, as a user in the role of Lab Director or IT Administrator, you can configure a list of reports that are available to users when they generate reports from the Method Development or Acquisition modes. From the Reports page, you can configure standard reports or custom reports.

This section includes configuration instructions for the following reports:

- Standard Reports
- Custom Reports

❖ To open the Reports page of the Application Configuration view

1. Do one of the following:
   - From the dashboard, click **Configuration**.

     –Or–

   - Click **Configuration** in the navigation pane.
2. Click **Application Configuration**.

   The General page of the Application Configuration view opens.
3. Click the **Reports** tab.

   The Reports page of the Application Configuration view opens.

Standard Reports

The TraceFinder application supplies standard reports.

❖ To specify which standard reports are available

1. Click the **Standard reports** tab.

   The Standard report page opens. This page is the default when you first open the Reports page. See "Standard reports page" on page 42.

2. Use the directional arrows to move reports from the Available reports pane to the Configured reports pane.

   Tip Use the CTRL or SHIFT keys to select multiple reports.

   All reports in the Configured reports pane are available to users in the Method Development and Acquisition modes.

3. Do one of the following:

   - To return the report selections to their original state (when you first opened this page), click **Undo changes**.

     –Or–

   - To apply the current selections, do the following:

   a. Click **Apply**.

      A message reminds you that you must restart the TraceFinder application before your report selections are reflected in the reports available for the Method Development and Acquisition modes.

   b. In the message dialog box, click **Yes** to restart the TraceFinder application now or click **No** to remain on the Reports page.

❖ To import new standard report types

1. Click **Import**.

2. In the browser, locate a Crystal Reports .dll file and open the file.

   The application writes the imported report to the TraceFinder installation directory.

   The Available reports pane displays the new report.

Standard reports page

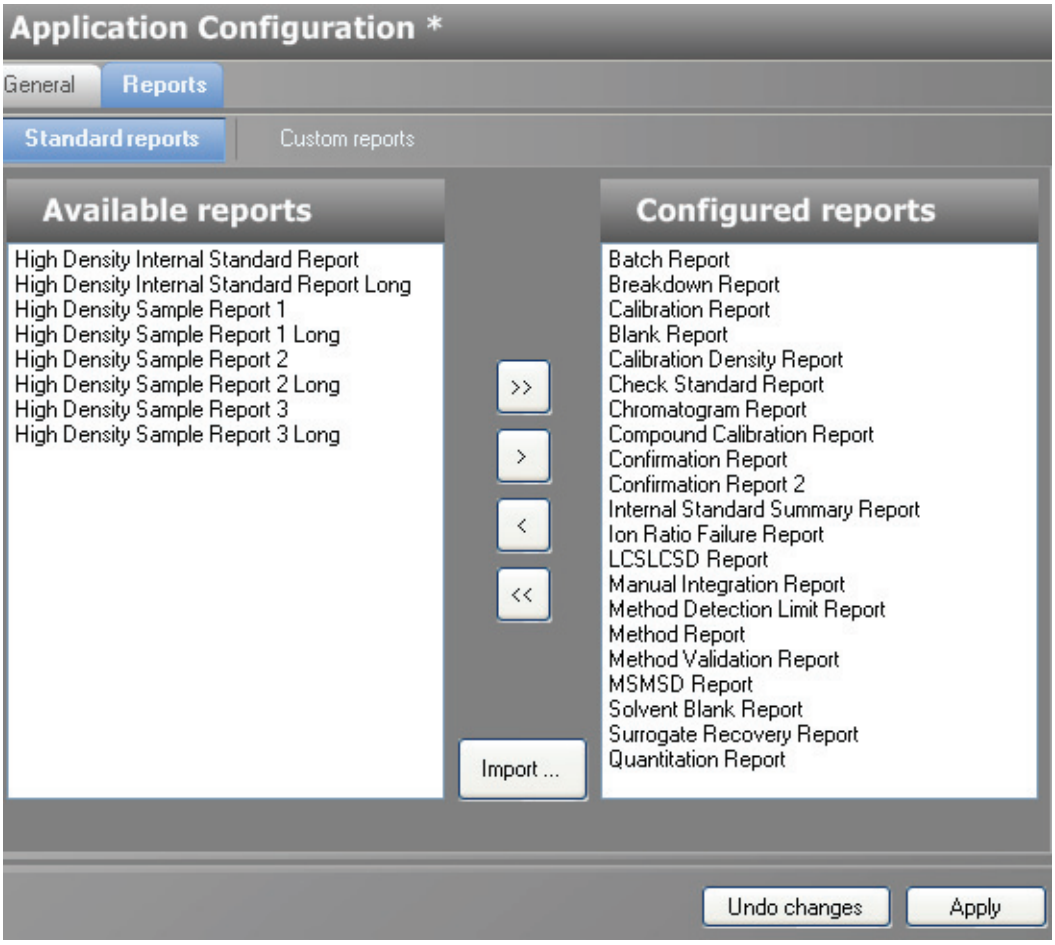


Table 10. Standard reports parameters (Sheet 1 of 2)

Parameter	Description
Standard reports	Displays all available standard reports.
Custom reports	Displays all available custom reports.
Available reports	All reports listed in the Available reports pane are potentially available for this application but have not been selected for the Method Development or Acquisition modes.
Configured reports	All reports listed in the Configured reports pane have been selected for the Method Development and Acquisition modes.
>>	Moves all reports from the Available reports list to the Configured reports list.
>	Moves the selected reports from the Available reports list to the Configured reports list.
<	Moves the selected reports from the Configured reports list to the Available reports list.

Table 10. Standard reports parameters (Sheet 2 of 2)

Parameter	Description
<<	Moves all reports from the Configured reports list to the Available reports list.
Import	Opens a browser where you can choose a report file to add to the Available reports list.
Undo changes	Returns the report selections to their original state (when you first opened this page).
Apply	Applies the current selections, and reminds you that you must restart the application before the report selections are available for the Method Development and Acquisition modes.

Custom Reports

The TraceFinder application lets you configure and import custom reports.

❖ To specify which custom reports are available

1. Click the **Custom reports** tab.

   The Custom reports page opens. See "Custom reports page" on page 45.

2. Use the directional arrows to move reports from the Available reports pane to the Configured reports pane.

   Tip Use the CTRL or SHIFT keys to select multiple reports.

   All reports in the Configured reports pane are available to users in the Method Development and Acquisition modes.

3. To create a single report for an entire batch (rather than separate reports for each sample), select the **Batch level report** check box for the report type.

   Rather than creating separate reports for each sample, this uses data from only the last sample to create a single report for the entire batch.

4. Do one of the following:

   - To return the report selections to their original state, click **Undo changes**.

     –Or–

   - To apply the current selections, do the following:

   a. Click **Apply**.

      A message reminds you that you must restart the TraceFinder application before your report selections are reflected in the reports available for the Method Development and Acquisition modes.

   b. In the message dialog box, click **Yes** to restart the TraceFinder application now or click **No** to remain on the Reports page.

❖ To import new custom report types

1. Click **Import**.
2. In the browser, locate a Custom Reports .xltm file and open the file.

   The application writes the imported report to the following folder:

   `..\Thermo\TraceFinder\Templates\Reports`

   The Available reports pane displays the new report.

Custom reports page

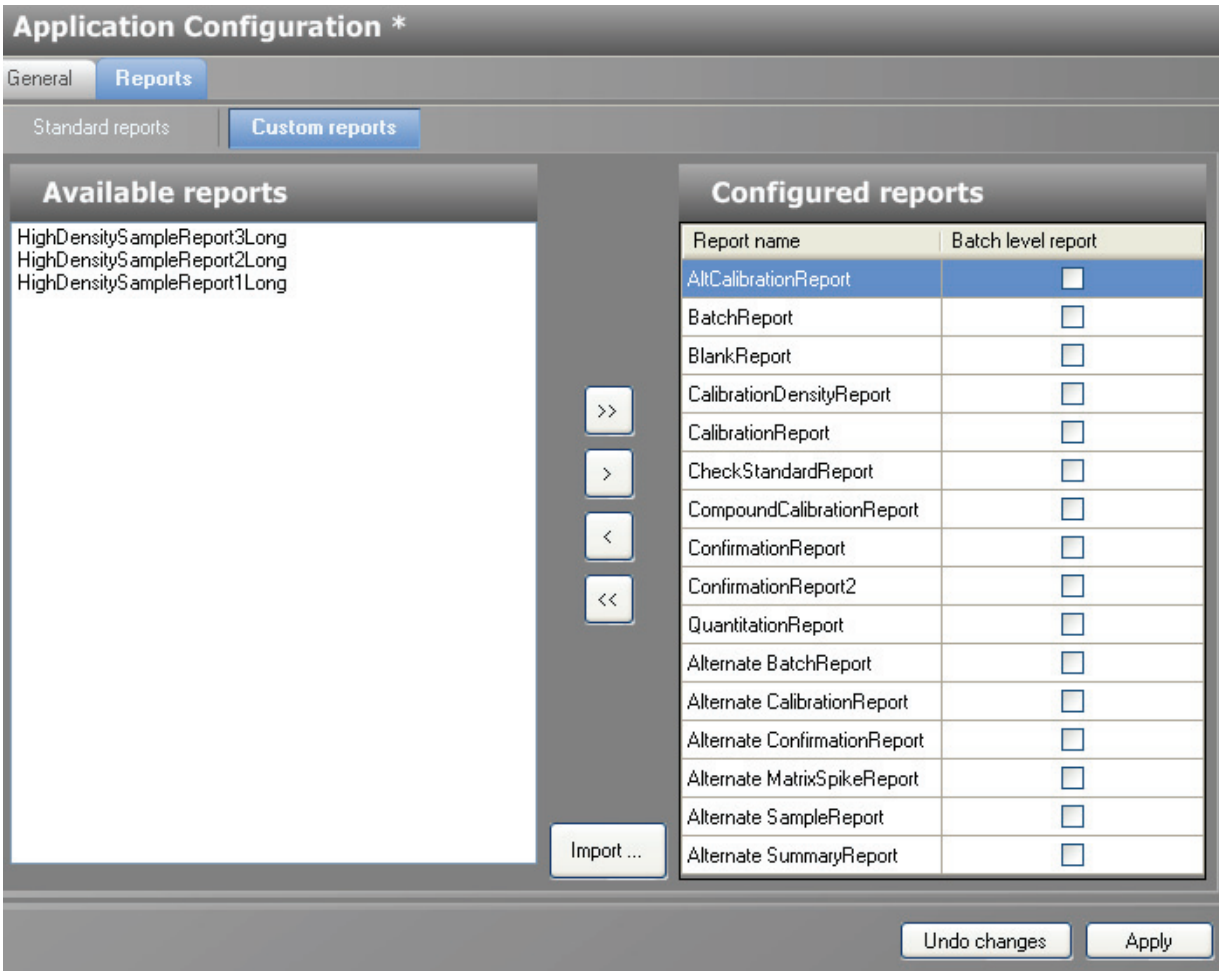


Table 11. Custom reports parameters (Sheet 1 of 2)

Parameter	Description
Standard reports	Displays all available standard reports.
Custom reports	Displays all available custom reports.
Available reports	All reports listed in the Available reports pane are potentially available for this application but have not been selected for the Method Development or Acquisition modes.
Configured reports	All reports listed in the Configured reports pane have been selected for the Method Development and Acquisition modes.
>>	Moves all reports from the Available reports list to the Configured reports list.
>	Moves the selected reports from the Available reports list to the Configured reports list.

Table 11. Custom reports parameters (Sheet 2 of 2)

Parameter	Description
<	Moves the selected reports from the Configured reports list to the Available reports list.
<<	Moves all reports from the Configured reports list to the Available reports list.
Batch level report	Rather than creating separate reports for each sample, this uses data from only the last sample to create a single report for the entire batch.
Import	Opens a browser where you can choose a report file to add to the Available reports list.
Undo changes	Returns the report selections to their original state (when you first opened this view).
Apply	Applies the current selections, and reminds you that you must restart the application before the report selections are available.

Using the Method Development Mode

This chapter includes method development tasks assigned to the Supervisor or Lab Director roles.

Contents

❖ To access the Method Development mode

- Click **Method Development** from the dashboard or the navigation pane.

The Method Development navigation pane opens.

Method Development navigation pane

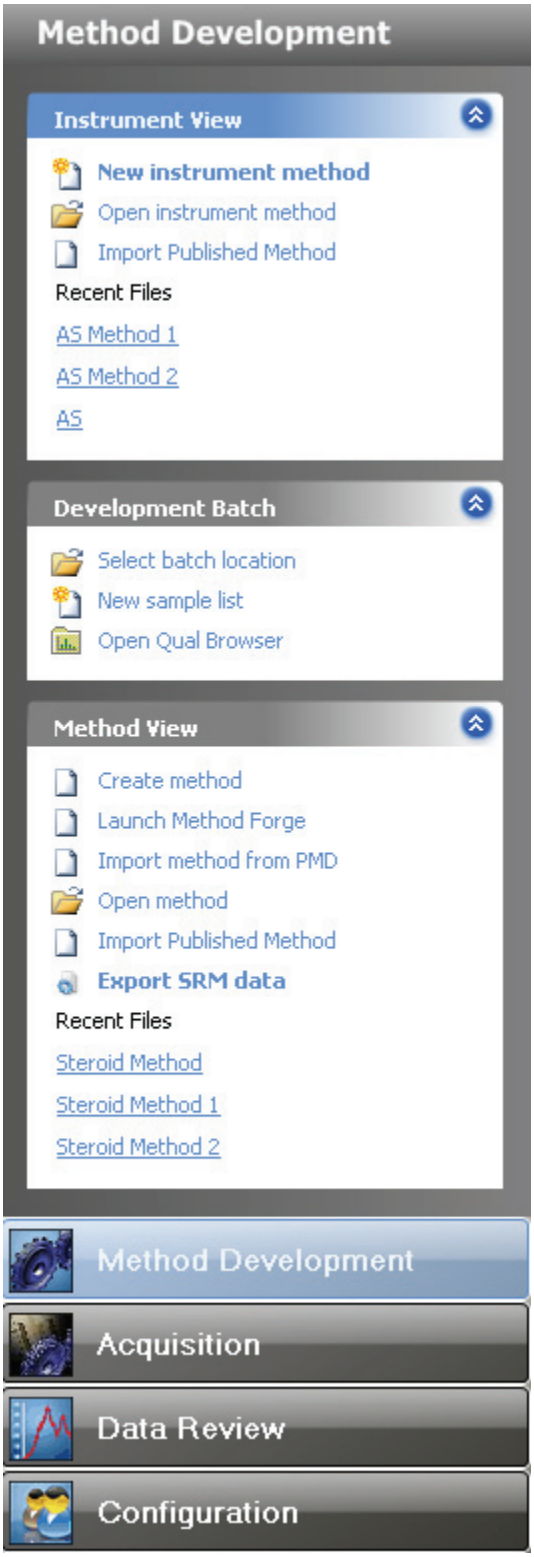


Table 1. Method Development navigation pane functions

Functions	Description
Instrument View	See "Working with Instrument Methods" on page 51.
New instrument method	Opens the Instrument View where you can specify instrument settings for your configured instruments. If the instrument you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the TraceFinder application. You cannot configure an instrument while the TraceFinder application is running.
Open instrument method	Opens a browser where you can choose an instrument method to open.
Import Published Method	Imports an instrument method (.meth) from the Published Methods folder.
Recent Files	Displays recently saved instrument methods.
Development Batch	See "Working with Development Batches" on page 55.
Select batch location	Specifies a location to store temporary development batch raw data files.
New sample list	Removes acquired samples from your development batch so you can begin a new sample list.
Open Qual Browser	Opens the Qual Browser where you can monitor the acquisition of your samples.
Method View	See "Working with Master Methods" on page 62.
Create method	Creates a new, empty master method.
Launch Method Forge	Opens the Method Forge dialog box where you can create a new master method.
Import method from PMD	Import a processing method created by Xcalibur or LCquan applications.
Open method	Opens the Open Master Method dialog box where you can choose a master method to open.
Import Published Method	Imports a processing method (.mmx) from the Published Methods folder.
Export SRM data	Writes the data in the SRM table to the following file: `..\Thermo\TraceFinder\Methods\`*`methodname`*`.xml` You can use the data in this file in the instrument method editor when you open the TSQ 2.1 application.
Recent Files	Displays recently saved master methods.

Using Published Methods

Published instrument and processing methods reside in the C:\Thermo\Published Methods folder. All method files in this folder are accessible when you use the Import published method command in the Instrument view or Method view of the Method Development mode.

The instrument (.meth) and processing (.mmx) methods in your Published Methods folder can originate in any of the following ways:

- Create a method in the TraceFinder application and copy it to the C:\Thermo\Published Methods folder on any computer.
- Create a method in the Xcalibur or LCquan applications and copy it to your C:\Thermo\Published Methods folder.
- Install sample methods when you install the TraceFinder application. The application automatically writes these methods to your C:\Thermo\Published Methods folder.
- Download methods from the TraceFinder Web site to your C:\Thermo\Published Methods folder.

❖ To download a method from the TraceFinder Web site

1. Choose **Help > TraceFinder Online > Published Methods**.

   The Customer Download Web site opens.

2. Do one of the following:

   - If you are not a registered user, fill in all required fields and click **Submit**.

     –Or–

   - If you are a registered user, enter your user name and password and click **Sign In**.

3. On the Customer Download page, locate the method file you want to download.
4. Save the method file to the following folder:

   `..\Thermo\Published Methods`

Working with Instrument Methods

An instrument method is a set of experiment parameters that define the operating settings for an autosampler, liquid chromatograph (LC), gas chromatograph (GC), mass spectrometer, and so on. Instrument methods are saved as file type .meth.

IMPORTANT Do not open the Thermo Foundation Instrument Configuration tool while the TraceFinder application is running.

Use the following procedures:

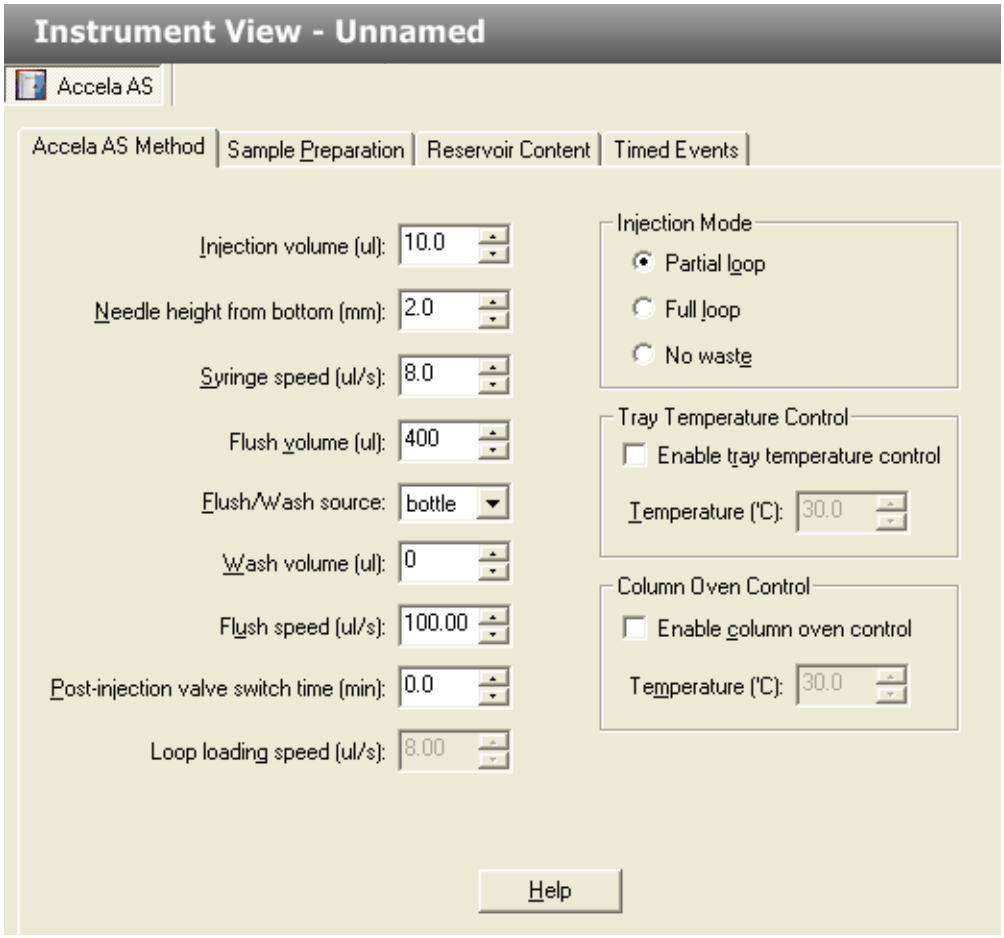
- To open the Instrument View
- To create a new instrument method
- To open an instrument method
- To import a published method

❖ To open the Instrument View

1. Do one of the following:
   - From the dashboard, click **Method Development**.

     –Or–
   - Click **Method Development** in the navigation pane from any other mode.
2. Click the **Instrument View** task pane.

The Instrument View opens. All configured instruments are displayed on separate pages. This example shows the instrument page for the Accela autosampler (Accela AS).

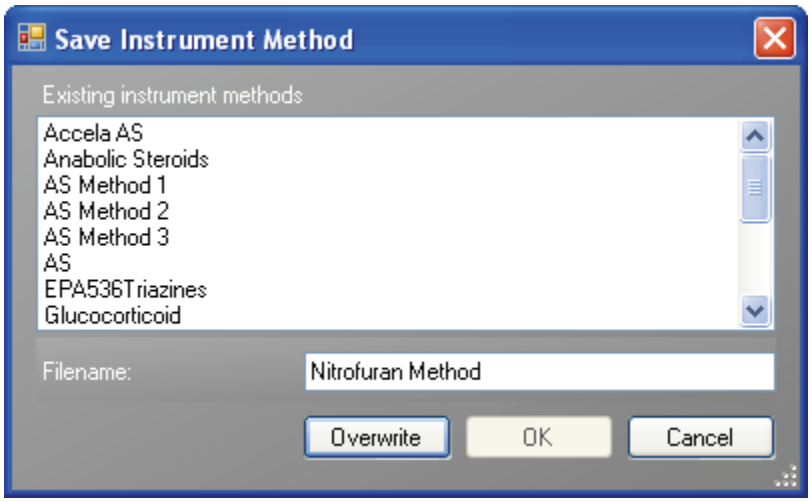


Note To open Help for any of your configured instruments, click **Help** on the instrument page.

❖ To create a new instrument method

1. Click **New instrument method** in the Instrument View task pane.
2. In the Instrument View, click the tab for the instrument you want to use for the method.
3. Edit the values on the instrument page.
4. From the main menu, choose **File > Save As**.

   The Save Instrument Method dialog box opens.



5. Do one of the following:
   - Type a new name for the instrument method and click **OK**.

     –Or–

   - Select an instrument method name to overwrite and click **Overwrite**.

   The TraceFinder application saves the new instrument method in the following folder:

   `..\Thermo\TraceFinder\InstrumentMethods`

❖ To open an instrument method

1. Click **Open instrument method** on the Instrument View task pane.

   A browser opens.

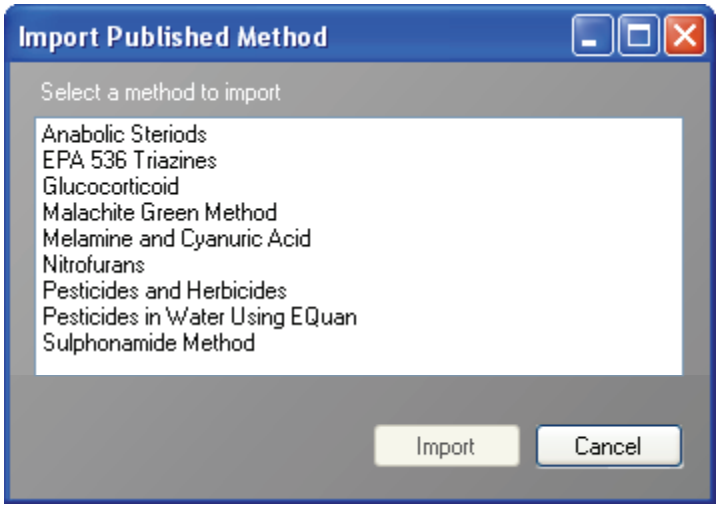
2. In the browser, select an instrument method from the list and open the file.

   The selected method opens in the Instrument View. You can edit this method and save the changes, or you can save this method to another name.

❖ To import a published method

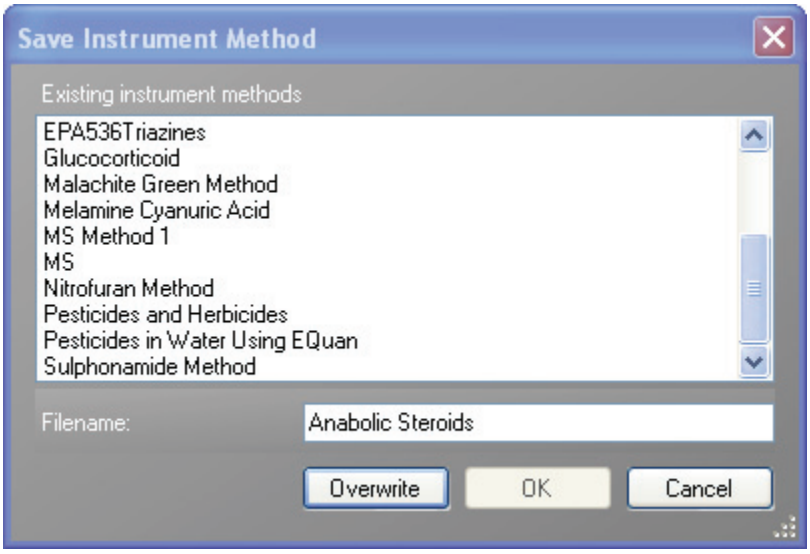
1. Click **Import published method** in the Instrument View task pane.

   The Import Published Method dialog box opens, displaying all the methods in the Published Methods folder.



2. Select the method you want to import and click **Import**.

   The Save Instrument Method dialog box opens.



3. Do one of the following:

   - Type a new name for the instrument method and click **OK**.

     –Or–

   - Select an instrument method name to overwrite and click **Overwrite**.

   The TraceFinder application reports that the method imported successfully. Published methods reside in the C:\Thermo\Published Methods folder.

Working with Development Batches

In the Development Batch view, you can test your instrument method in real time by creating and acquiring test samples. Development batches let you test different instrument methods and optimize parameters, such as LC gradients, MS source parameters, and autosampler variables, to find the best conditions for a master method. Development batches are not designed for high throughput in everyday analysis.

This section includes instructions for the following tasks:

- Creating a Development Batch
- Editing Samples in a Development Batch
- Acquiring Samples in a Development Batch

Creating a Development Batch

You create a development batch to test your instrument method and use it to acquire samples only once. You cannot save a development batch.

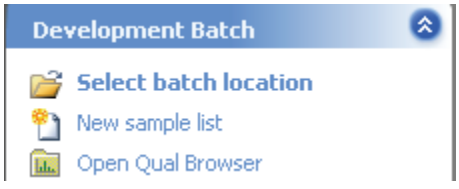
Use the following procedures:

- To a open the Development Batch view
- To add samples to the development batch
- To insert samples into the development batch
- To copy a sample

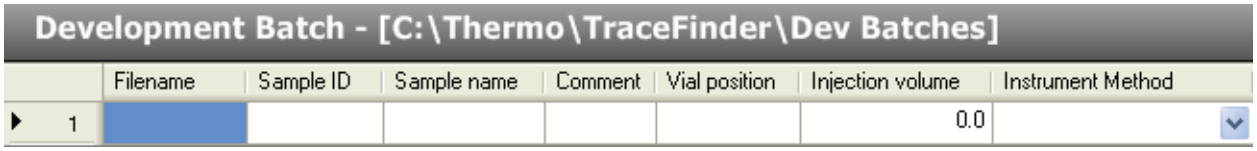
❖ To a open the Development Batch view

1. Do one of the following:
   - From the dashboard, click **Method Development**.

     –Or–
   - Click **Method Development** in the navigation pane of the current mode.
2. In the Method Development navigation pane, click **Development Batch**.



The Development Batch view opens a new, empty batch.



❖ To specify a location for development batch data

1. To specify a location for the files, click **Select batch location** in the Development Batch task pane.

   By default, the TraceFinder application writes the temporary files, raw data files, and .sld method file to the following folder:

   `../Thermo/TraceFinder/Temp`

2. In the browser, do one of the following:

   - Locate the folder you want to use for the development batch files and click **OK**.

     –Or–

   a. Locate and select the folder where you want to create a new folder for the batch files.

   b. Click **Make New Folder**.

      The application creates a new folder in the selected folder.

   c. Right-click the New Folder filename and choose **Rename** from the shortcut menu.

   d. Type the name for the folder.

   e. Click **OK**.

   The TraceFinder application creates all development batch files in the specified folder.

❖ To add samples to the development batch

- Do one of the following:

  - Right-click and choose **Add sample** from the shortcut menu.

    –Or–

  - Use the spin box to select the number of rows and click the **Add Sample** icon to add multiple sample rows.

  New, empty samples appear at the end of the sample list.

❖ To insert samples into the development batch

1. Select the sample above which you want to insert empty samples.
2. Do one of the following:
   - Right-click and choose **Insert sample** from the shortcut menu.

     –Or–

   - Use the spin box to select the number of rows and click the **Insert Sample** icon to insert multiple sample rows.

   New, empty samples appear above the selected sample.

❖ To copy a sample

1. Select the sample you want to copy.
2. Right-click and choose **Insert copy sample** from the shortcut menu.

   The copy of the sample appears above the selected sample.

Editing Samples in a Development Batch

A development batch requires fewer parameters than a real batch, but the mechanism for managing the information is the same.

For detailed instructions about using Copy down or Fill down to enter column values, see Appendix B, "Using Copy Down and Fill Down."

Use the following procedures:

- To enter column values
- To resize or reorganize the columns
- To remove selected samples from the list
- To remove all samples from the list

❖ To enter column values

1. Double-click the Filename column and type a file name for the raw data file.
2. (Optional) Enter values for the Sample name, Sample ID, or Comment columns.
3. Enter a vial position for each sample.
4. Enter an injection volume for each sample.
5. To enter an instrument method for each sample, click the down arrow in the Instrument method column and select a method from the list.

   This list contains all the available instrument methods.

❖ To resize or reorganize the columns

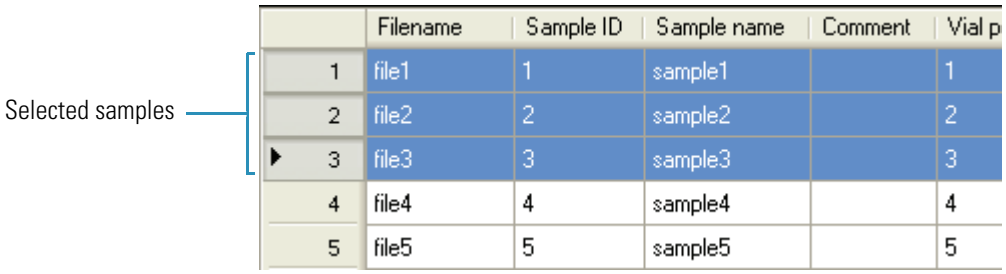
1. To resize a column, drag the header separator on the right side of the column.
2. To move a column, drag the column header.

   You cannot move the Filename column.

❖ To remove selected samples from the list

1. Select the samples you want to remove.

   Make sure the first column indicates that the samples are selected.



2. Right-click and choose **Remove selected samples** from the shortcut menu.

❖ To remove all samples from the list

1. Click **New sample list** in the Development Batch task pane.
2. One of the following happens:
   - If the samples in the current batch have all been acquired, the list is cleared.
   - If the samples in the current list have not been acquired, a message confirms that you want to clear them and start a new list.
3. To create a new empty list, click **Yes**.

Note You cannot save a development batch when you create a new one; you can only create, acquire, and discard each batch after you use it. The application saves only the generated raw files in the specified batch location.

Acquiring Samples in a Development Batch

In a development batch, you can submit the entire batch for acquisition or submit only selected samples.

Use the following procedures:

- To acquire selected samples
- To acquire the batch
- To open the Qual Browser

❖ To acquire selected samples

1. Select the samples you want to acquire.
2. Do one of the following:
   - Right-click and choose **Submit selected samples** from the shortcut menu.

     –Or–
   - Click the **Submit selected samples** icon,  .

   The TraceFinder application creates a raw data file for each selected sample. It writes the raw files and all temporary working files to the following folder:

   `../Thermo/TraceFinder/Temp`

   When the acquisition is complete, the application deletes all the temporary working files. Only the raw files and a MethodDevelopment.sld file remain in the folder.

   If a sample is acquired more than once, the subsequent raw data files are timestamped with the acquisition time.

❖ To acquire the batch

- Do one of the following:
  - Right-click and choose **Submit batch** from the shortcut menu.

    –Or–
  - Click the **Submit batch** icon,  .

  The TraceFinder application creates a raw data file for each sample in the batch and a .sld method file. The TraceFinder application writes the raw data files, the .sld method file, and all temporary working files to the specified folder.

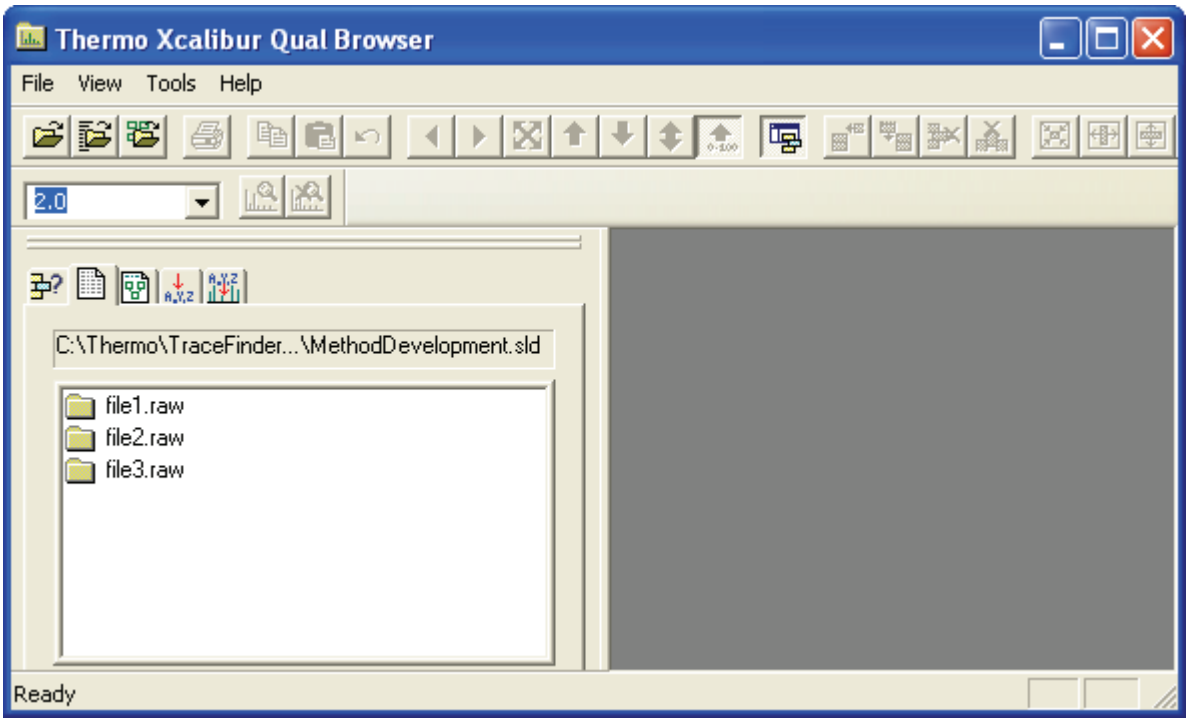
  When the acquisition is complete, the application deletes all the temporary working files. Only the raw files and a MethodDevelopment.sld file remain in the folder.

  If a sample is acquired more than once, the subsequent raw data files are time-stamped with the acquisition time.

❖ To open the Qual Browser

- In the Development Batch task pane, click **Open Qual Browser**.

  The Thermo Xcalibur Qual Browser opens.



For detailed instructions about using the Qual Browser, refer to the Qual Browser Help.

Working with Master Methods

The TraceFinder application uses a master method to specify the nature and types of acquisition, processing, and reporting that occur with a batch of samples. When you are testing for compounds in an assay, you can create a method designed specifically for that type of application.

When you create a master method, the TraceFinder application uses the method to determine how the software works with a set of samples to provide a set of meaningful results. The application uses an instrument method to define how raw data is acquired, while the rest of the master method defines how the raw data is processed, how the flags information evaluates the results, and how the reporting functionality defines the way your data and results are output into reports.

The TraceFinder application applies your master method to a batch, which is a list of one or more samples to be processed and reported. Together, the master method and batch provide a workflow-oriented approach to the processing of data and the reporting of information for small and large sets of samples.

To speed up the creation of master methods, you can create a method template. Using a method template helps you to develop methods faster because all of your commonly used method settings, such as number of confirming ions, are saved in a template.

This section includes instructions for the following tasks:

- Creating a New Method
- Creating a Method with Method Forge
- Importing an Xcalibur Method
- Importing a Published Method
- Exporting SRM Data
- Creating a Method Template
- Editing a Master Method

Creating a New Method

You can create a new, empty method that has no compounds associated with it. You can then add compounds one at a time.

Use the following procedures:

- To open the Method View
- To open a new method
- To add compounds to the method
- To save the new method

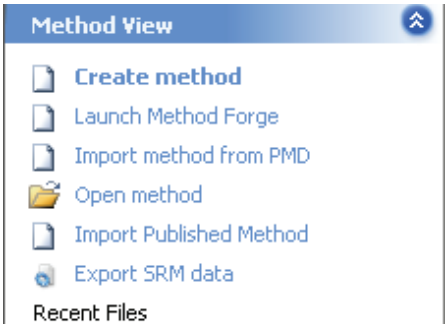
❖ To open the Method View

- Do one of the following:
  - From the dashboard, click **Method Development**.

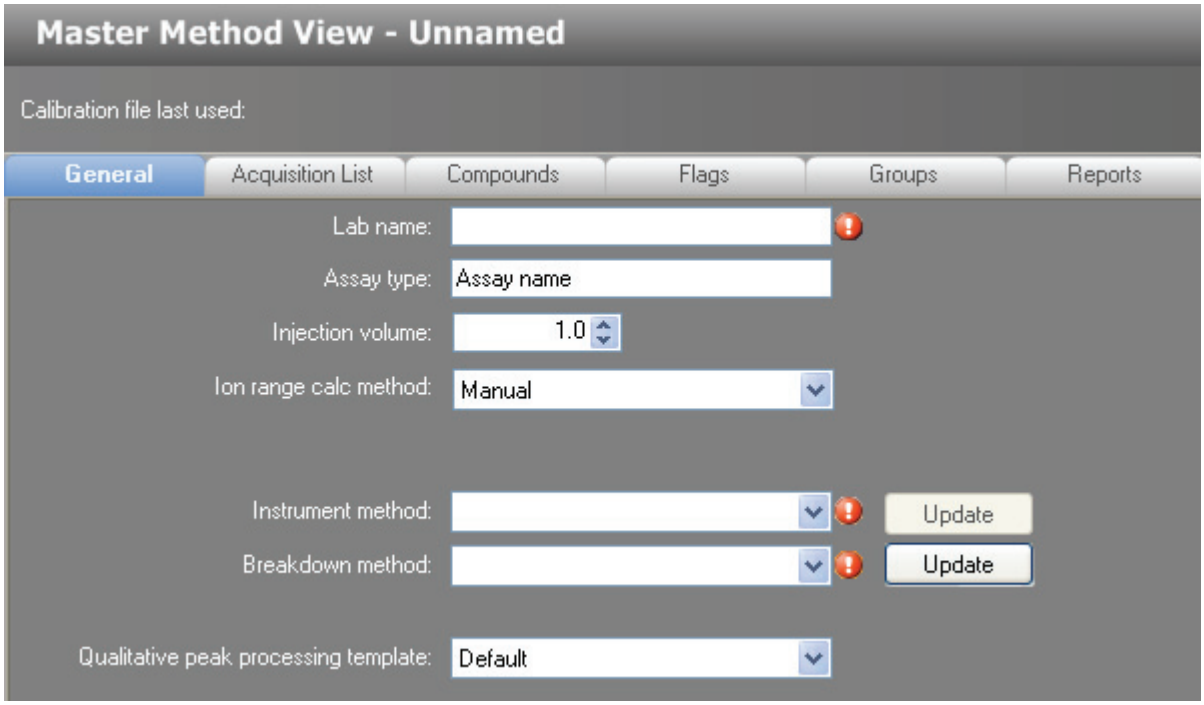
    –Or–
  - Click **Method Development** in the navigation pane from the current mode.

❖ To open a new method

1. From the Method View task pane, click **Create method**.



A new, empty master method view opens.

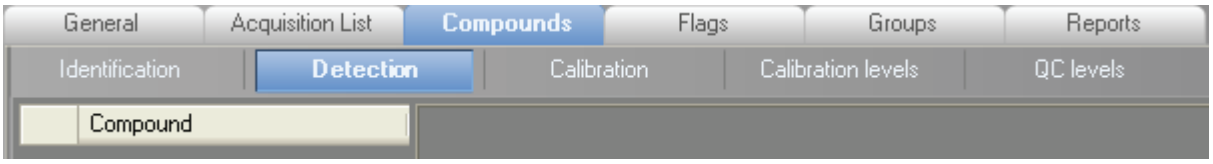


2. In the Labname box, type your laboratory name.
3. From the Instrument method list, select an instrument method.
4. (GC only) Select a breakdown method (if different from your instrument method).
5. (Optional) Enter any other parameters for the new method.

   For detailed descriptions of all parameters on the General page, see "Editing the General Page" on page 88.

❖ To add compounds to the method

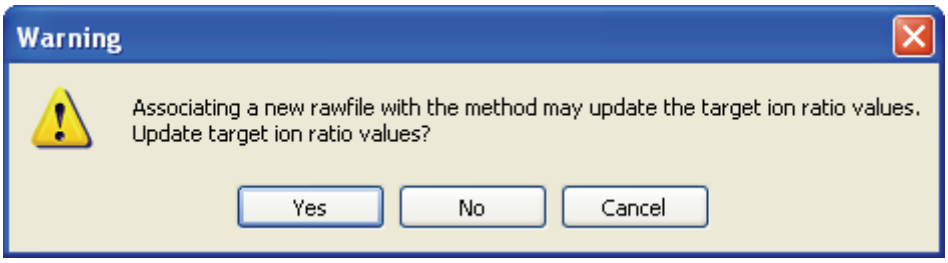
1. Click the **Compounds** tab.
2. Click the **Detection** tab.



   The Detection page shows an empty Compound list.

3. From the main menu, choose **Master method > Associate a raw file**.

   A warning informs you that associating a new raw file with the method can update the target ion ratio values.



4. Do one of the following:

   - To associate a raw data file and update the ion ratio values, click **Yes**.

     –Or–

   - To associate a raw data file without updating the ion ratio values, click **No.**

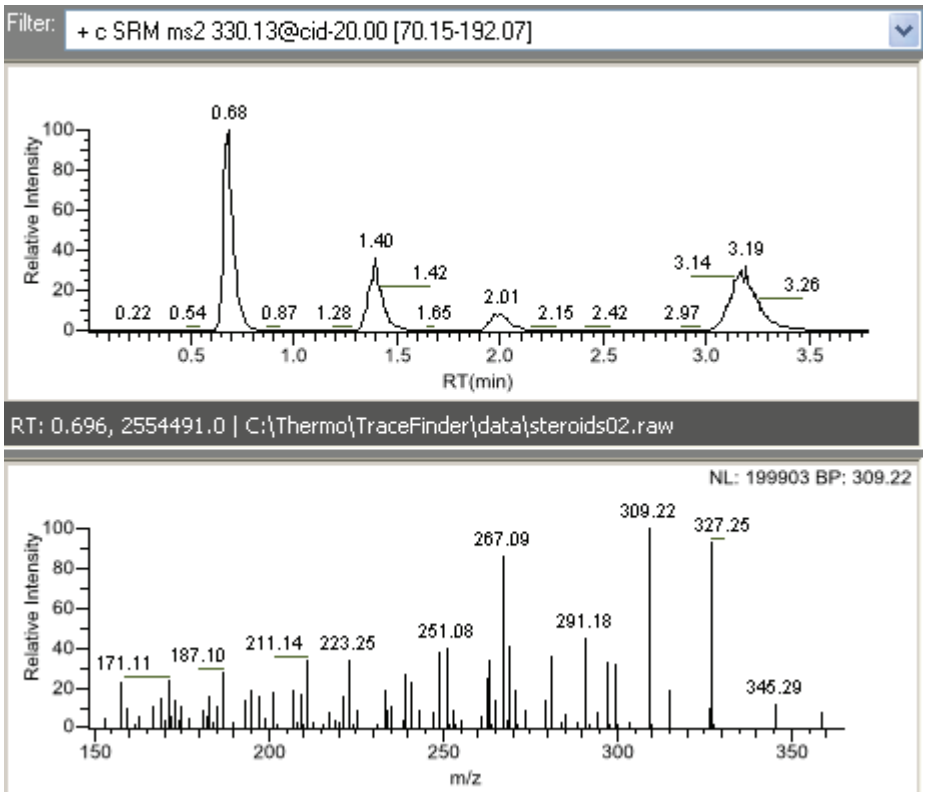
     –Or–

   - To stop this action and not associate a raw data file, click **Cancel.**

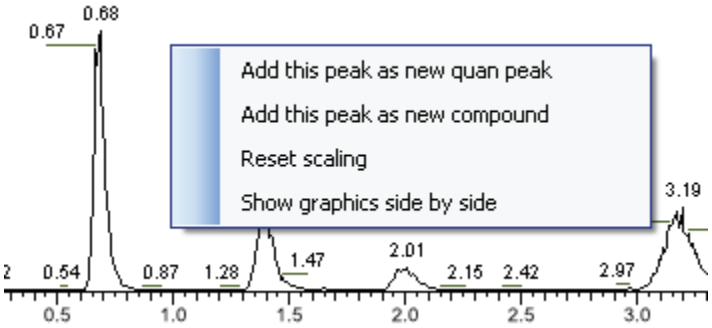
   Unless you cancel the operation, the What raw file would you like to use? dialog box opens.

5. Locate the raw file you want to use to identify compounds for this method and open the file.

   The TraceFinder application displays the chromatographic and spectrum data for the compounds in the selected raw file.



6. Select a filter from the Filter list.
7. Click the peak in the chromatogram that represents the compound you want to add to the method.
8. Right-click and choose **Add this peak as new compound** from the shortcut menu.



The TraceFinder application adds a new compound named Peak@*RetentionTime* and displays the quantitation peak information for the compound. If you have a NIST library installed and the compound is found in the library, the compound name is displayed instead.

9. Repeat these steps for each compound you want to add to the method.

For detailed descriptions of all parameters on the Detection page, see "Editing the Compounds Page" on page 95.

❖ To save the new method

1. Choose **File > Save**.

   The Save Master Method dialog box opens.

2. Do one of the following:

   - Type a new name for the master method and click **OK**.

     –Or–

   - Select a method name to overwrite and click **Overwrite**.

   The TraceFinder application saves the new method data in the following folder:

   `..\Thermo\TraceFinder\Methods`

Creating a Method with Method Forge

With Method Forge, you can create a master method by manually selecting peaks, cutting and pasting peak names, selecting multiple compounds, renaming peaks, or comparing mass spectra from the datastore searches, or the TraceFinder application can automatically create a master method for you.

When the TraceFinder application automatically creates a master method for you, it performs the following functions:

- Reviews your raw data file and identifies compounds that are present in your sample.
- Uses your mass spectral reference libraries to assign a compound name and CAS number.
- Uses mass spectral information to select potential quantification and confirming ions and a reference mass spectrum for the compound.

A master method contains a list of compounds and an initial set of information for detecting, processing, and reporting those compounds.

Use the following procedures:

- To automatically create a method
- To manually select compounds to create a method

❖ To automatically create a method

1. From the Method View task pane, click **Launch Method Forge**.

   The Method Forge dialog box opens. See "Method Forge" on page 71.

   Use the Method Forge to create a master method from an existing raw data file or create a new raw data file to use for the master method.

2. In the Method Forge dialog box, do one of the following:

   - Select the **Use the default template** option.

     –Or–

   - Select the **Select a custom template** option and highlight your custom template in the Method template table.

     For detailed instructions on creating a custom method template, see "Creating a Method Template" on page 78.

3. Select the **Name the master method** check box and type a name for your master method.

   You can enter an existing method name and overwrite it when you create the method. If you do not specify a name, the method is named for the raw file used to create the method.

4. Select the **Automatically create the master method** check box.
5. Do one of the following:
   a. In the Raw file selection area, choose **Use an existing raw data file**.
   b. Click the browse button and locate a raw data file to use for the method.

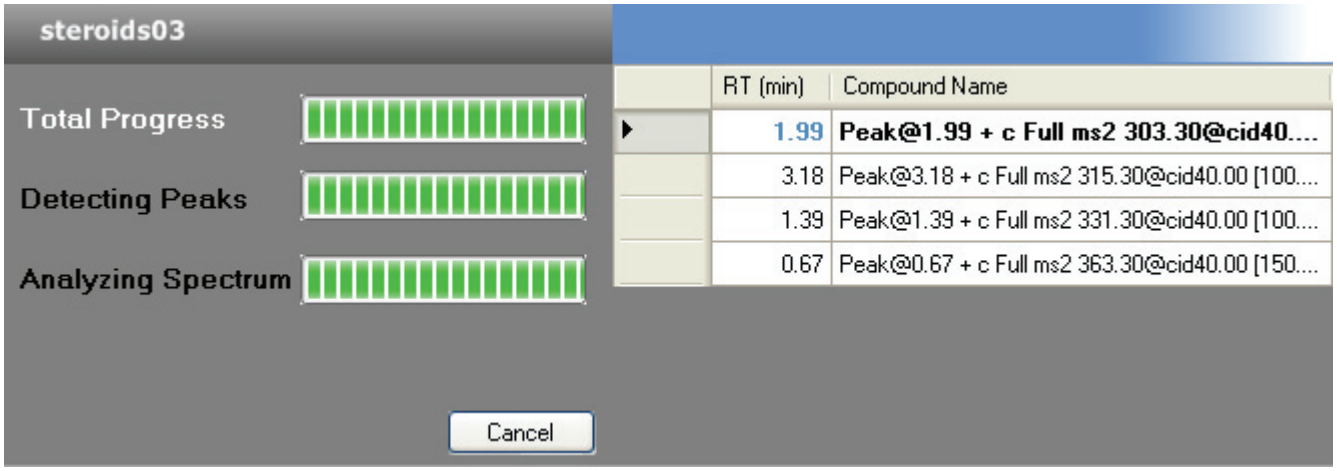
   –Or–

   a. In the Raw file selection area, choose **Acquire a new raw data file**.
   b. From the Instrument method list, select a method (.meth) file to use for acquiring the data.
   c. In the Raw filename box, type the name of the file where the application will write the raw data.
   d. In the Path box, type a path or click the browse button and locate a folder where the application will save the raw data file.
   e. (Optional) Type a comment about the acquired sample or the data file.
6. Do one of the following:
   - Choose **Manual injection**.

   –Or–

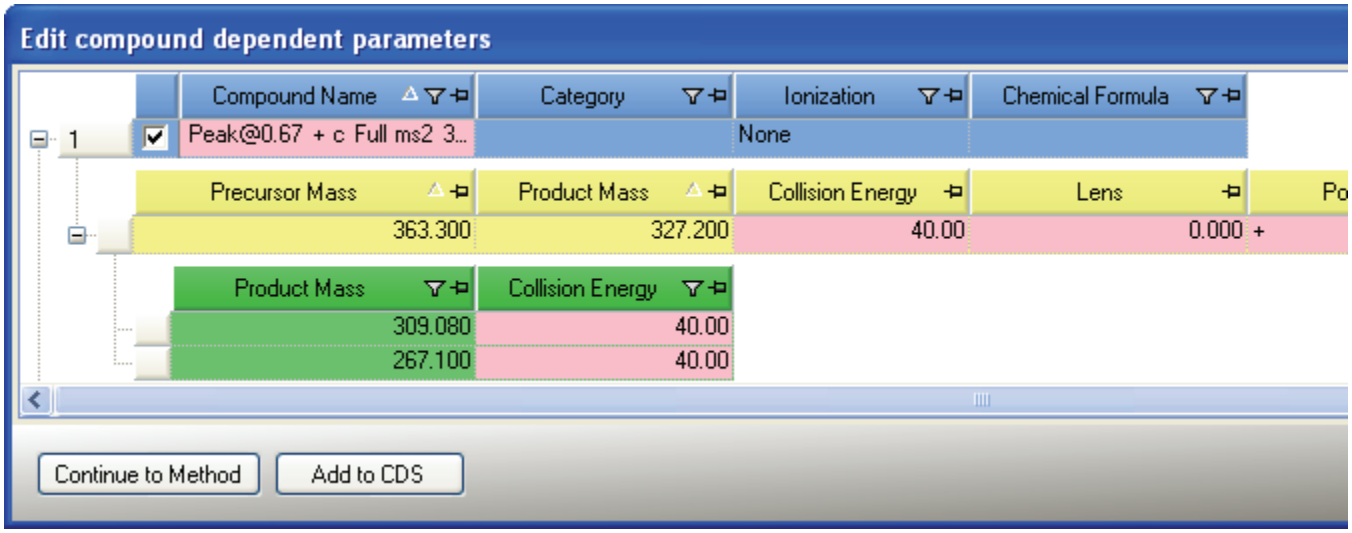
   a. Choose **Use autosampler**.
   b. In the Vial position box, type a vial position.
   c. In the Injection volume box, type an injection volume.
7. To automatically create the master method, click **OK** (or **Overwrite**).

   As the Method Forge creates the method, it displays the following status:



When the acquisition completes, Method Forge performs peak detection, datastore searching, and characteristic ion and reference spectrum identification and then loads this information into a new master method. This process occurs immediately if you selected a previously acquired raw file.

Method Forge displays the detected compounds in the Edit compound dependent parameters dialog box.



8. (Optional) Select the compounds that you want to add to the compound datastore and click **Add to CDS**.

   The selected compounds are added to the current compound datastore.

   Note To add these compounds to the datastore, you must use this command before you continue to the method.

9. To use these compounds in your method and close the dialog box, click **Continue to Method**.

   All compounds in the imported processing method are used in your method. The TraceFinder application displays the General page of the Master Method View.

10. From the Instrument method list, choose an Instrument method to use for your master method.

❖ To manually select compounds to create a method

1. From the Method View task pane, click **Launch Method Forge**.

   The Method Forge dialog box opens. See "Method Forge" on page 71.

2. In the Method Forge dialog box, do one of the following:

   - Select the **Use the default template** option.

     –Or–

   - Select **Select a custom template** and highlight your custom template in the Method template table.

     For detailed instructions about creating a custom method template, see "Creating a Method Template" on page 78.

3. Select the **Name the master method** check box and type a name for your master method.

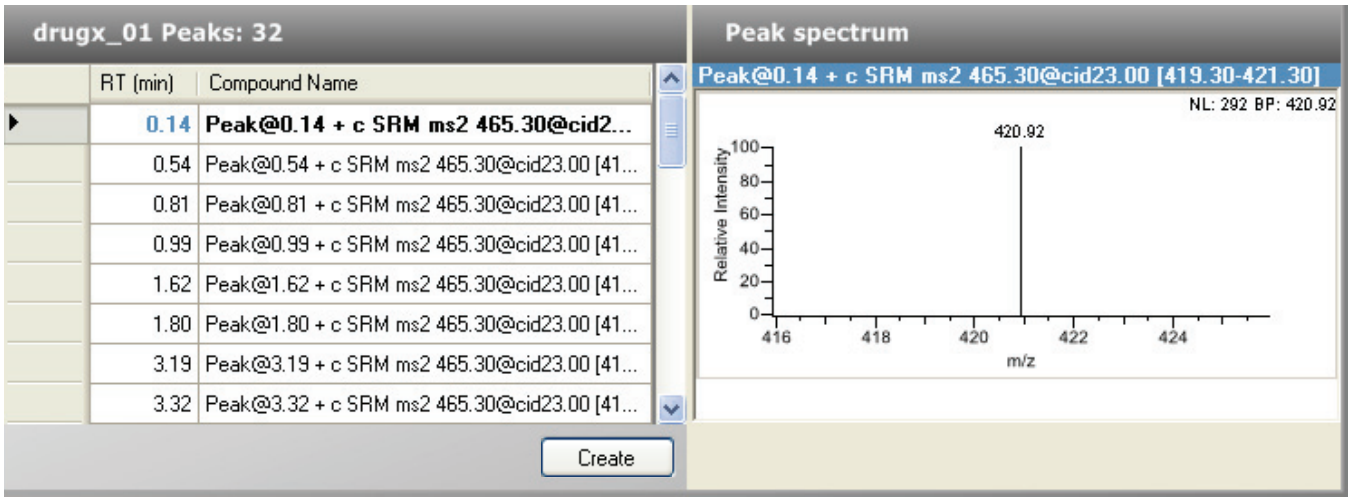
   You can enter an existing method name and overwrite it when you create the method. If you do not specify a name, the method is named for the raw file used to create the method.

4. Make sure the **Automatically create the master method** check box is not selected.

5. To select a raw data file, click the browse button and locate the file.

6. To manually create the master method, click **OK** (or **Overwrite**).

   The Master Method view displays a list of compounds in the data file.

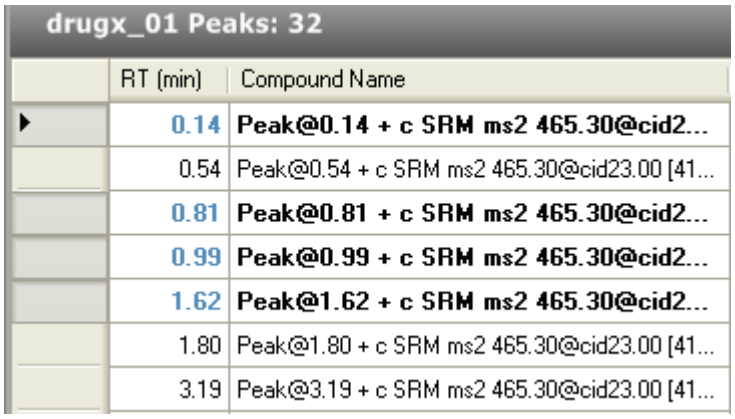


When you select a peak in the Compound Name list, the peak spectrum is displayed in the right pane. When multiple peaks are selected, the peak spectrum display is blank.

7. Select a group of peaks to be included in your master method.

   Hold down **SHIFT** to select a range of peaks or **CTRL** to select multiple, individual peaks.

Selected peaks are indicated with blue RT values and bold compound names.



8. After you manually select your peaks, click **Create** to create the master method.

   The results are displayed in the Master Method View.

9. To save the new method, choose **File > Save** from the main menu.

Method Forge

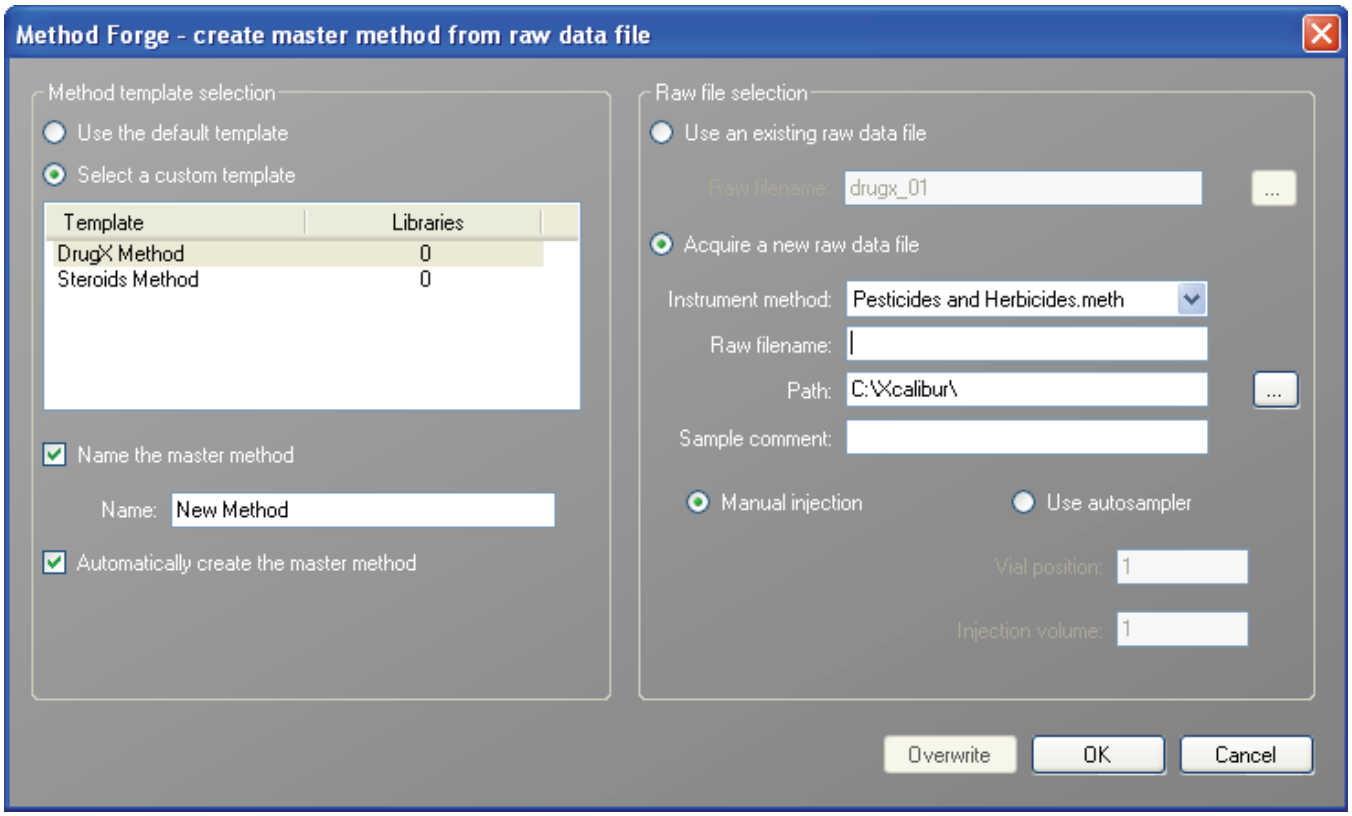


Table 2. Method Forge parameters

Parameter	Description
Method template selection	
Use the default template	Creates a new method with the default template.
Select a custom template	Lists all the available method templates. For detailed instructions about creating a custom method template, see "Creating a Method Template" on page 78.
Name the master method	The name for the new master method.
Automatically create the master method	When the acquisition completes, Method Forge performs peak detection, datastore searching, and characteristic ion and reference spectrum identification. This information is loaded into a new master method. This process occurs immediately when you select a previously acquired file.
Raw file selection	
Use an existing raw data file	Enables the Raw filename box where you can select a raw data file to use to create the master method.
Acquire a new raw data file	Enables functions to acquire data to create a raw file to use to create the master method.
Instrument method	Saved method (.meth) file to use for acquiring the data.
Raw filename	File name where the application will write the raw data.
Path	Location where the application will save raw data file.
Sample comment	(Optional) Comment about the acquired sample or the data file.
Manual injection	Performs a manual acquisition.
Use autosampler	Performs an autosampled acquisition.
Vial position	The tray vial number used for the autosampler acquisition.
Injection amount	The volume (in milliliters) injected by the autosampler acquisition.
Function buttons	
Overwrite	Overwrites the specified master method name. This function is enabled only when the specified master method name already exists.
OK	Creates a master method using the data and parameters you specified.
Cancel	Closes the Method Forge and does not create a master method.

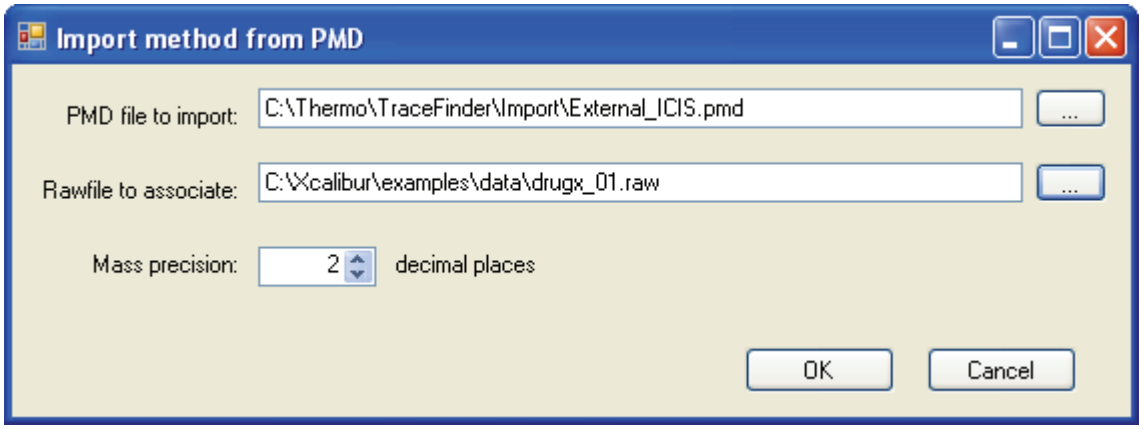
Importing an Xcalibur Method

You can create a new method from an existing Xcalibur processing method.

❖ **To import a method**

1. From any mode, click **Method Development**.
2. In the Method View task pane, click **Import method from PMD**.

   The Import method from PMD dialog box opens.

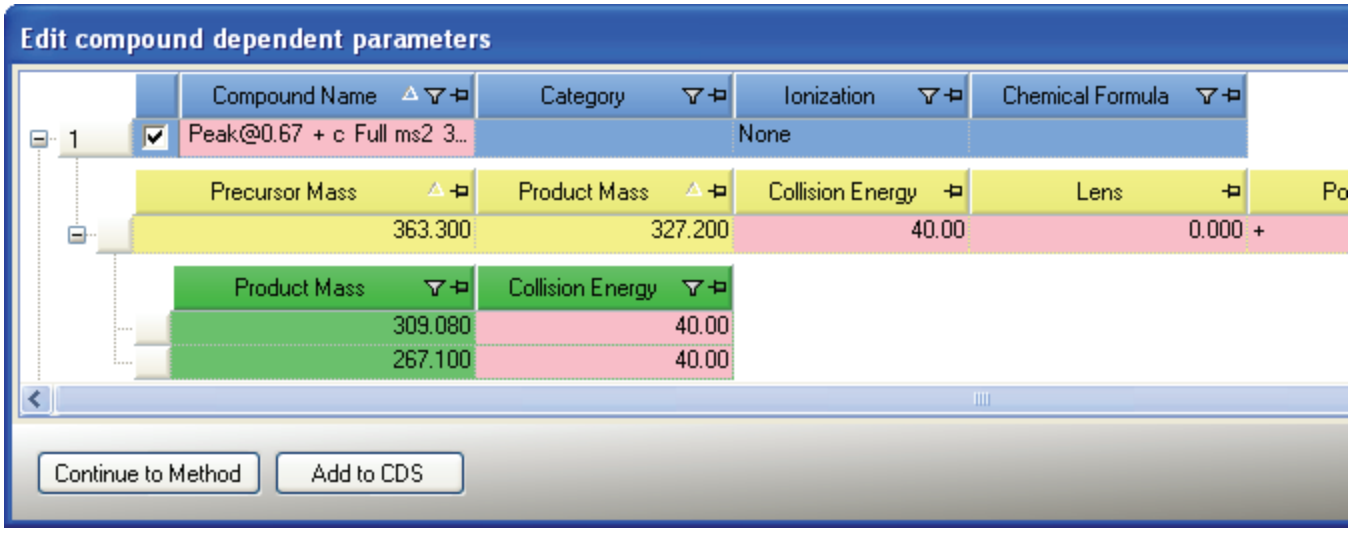


3. To select an Xcalibur processing method file to import, click the browse button for the **PMD file to import** box.
4. In the browser, locate the Xcalibur processing method file and open the file.

   The TraceFinder application imports the compound information from the Xcalibur method file.
5. To associate a raw data file with this method, click the browse button for the **Rawfile to associate** box.
6. In the browser, locate the raw data file and open the file.
7. (Optional) Change the number of decimal places in the Mass precision box.

   You can set the mass precision decimal places to an integer between 0 and 3.
8. Click **OK**.

   If the compounds in the imported method file are not in the Compound Datastore, the TraceFinder application displays the compounds in the Edit compound dependent parameters dialog box.



9. (Optional) Select the compounds you want to add to the Compound Datastore and click **Add to CDS**.
10. To add these compounds to your method and close the dialog box, click **Continue to Method**.

    The TraceFinder application adds the compounds in the imported method to your new method.
11. Specify an Instrument method to use for the master method.
12. (GC only) Specify a Breakdown method to use for the master method.
13. To edit the imported compounds, follow the instructions in "Editing a Master Method" on page 87.
14. Choose **File > Save As** and specify a name for your new method.

Importing a Published Method

In the TraceFinder application, you can import processing methods from the Published Methods folder. For information about the methods in the Published Methods folder, see "Using Published Methods" on page 50.

❖ To import a published processing method

1. In the Method View task pane, click **Import published method**.

   The Import Published Method dialog box opens.

2. Choose the method you want to import and click **Import**.

   The TraceFinder application reports that the processing method (and any associated instrument method) imported successfully and displays the imported processing method in the Master Method View.

Exporting SRM Data

In the TraceFinder application, you can export your selected reaction monitoring (SRM) data to an XML file.

❖ To export SRM data

1. Open the master method from which you want to export SRM data.
2. From the Method View task pane, click **Export SRM data**.

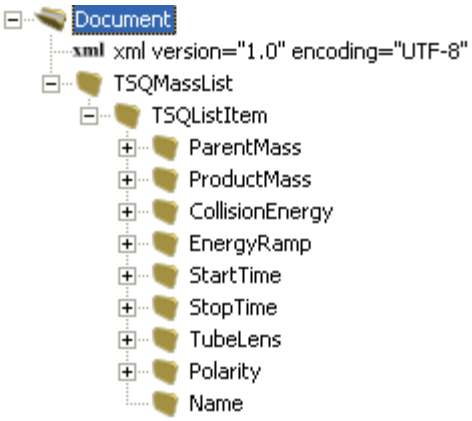
   The TraceFinder application writes the data in the SRM table to the following file:

   `..\Thermo\TraceFinder\Methods\`*`methodname`*`.xml`

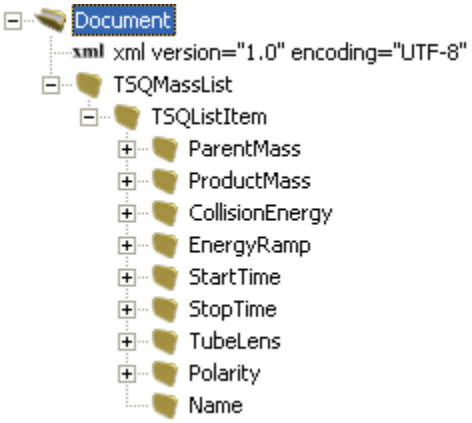
   The data in this file matches the TSQ .xml data and can be used in the instrument method editor when you use the TSQ 2.1 application.

SRM data examples

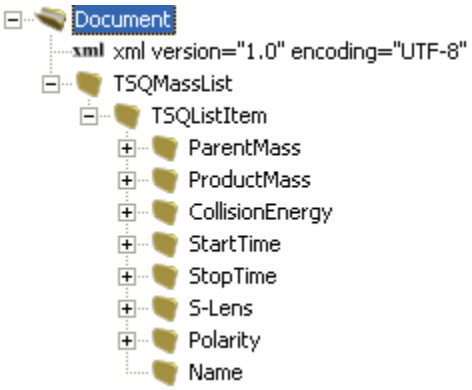
TSQ Quantum (LC) example



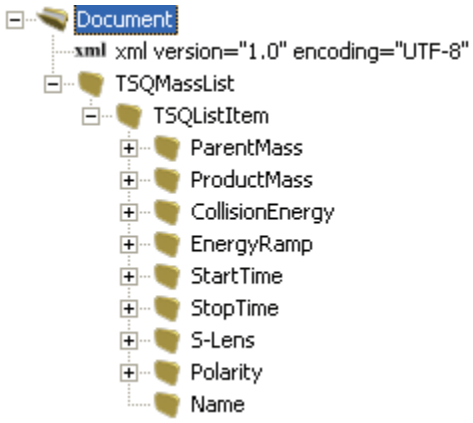
TSQ Quantum QED (LC) example



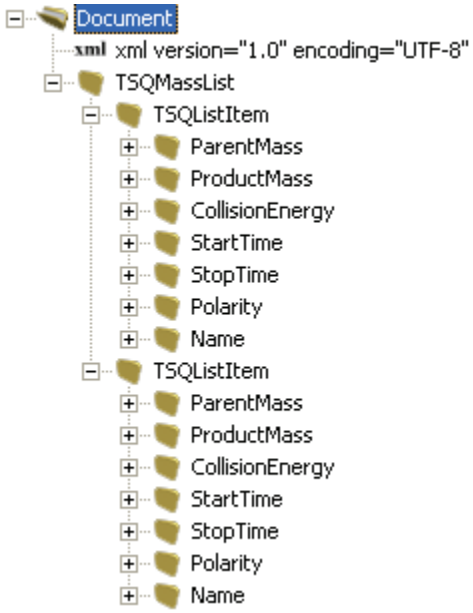
TSQ Vantage (LC) example



TSQ Quantum QED (LC) example



TSQ Quantum™ (GC) example



Creating a Method Template

In the TraceFinder application, you can create a processing method using a method template that contains the basic settings as defined by a user in the role of Lab Director or Supervisor.

Use the following procedures:

- To create a method template
- To specify peak criteria
- To choose a library
- To specify confirming ions
- To calibrate the compounds
- To enter a note for the method
- To save the method template

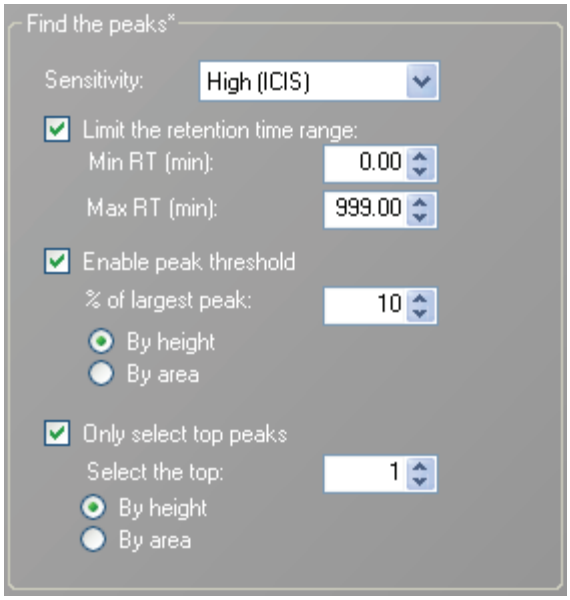
❖ To create a method template

1. Do one of the following:
   - From the dashboard, click **Method Development**.

     –Or–
   - Click **Method Development** in the navigation pane from the current mode.
2. Click **Method View** in the navigation pane.
3. From the main menu, choose **File > New > Method template**.

   The Method Template Editor opens. See "Method Template Editor" on page 84.

❖ To specify peak criteria



1. In the Find the peaks area, choose a sensitivity level.

   In selecting the degree of sensitivity, you define how extensively the peak detector algorithm searches for low-level peaks.

   - The High (ICIS) peak detection algorithm is designed for MS data and has superior peak detection efficiency at low MS signal levels.
   - The Standard (Genesis) peak detection algorithm is provided for backward compatibility with Xcalibur 1.0 studies.

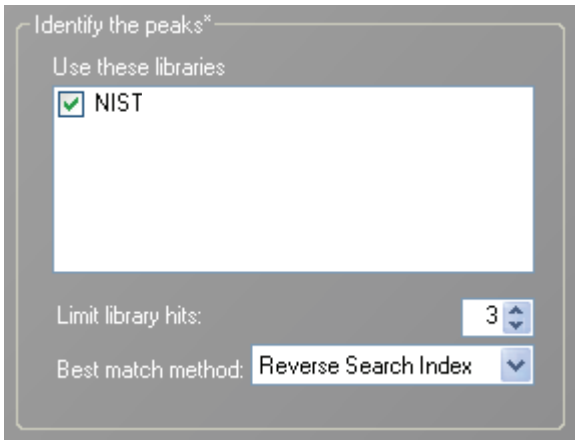
2. To look for peaks only in a certain range of the entire chromatogram, select the **Limit the retention time range** check box and specify a retention time (RT) range.

3. To indicate whether to select peaks by relative height or area and the percentage of the highest peak that will result in compound selection, select the **Enable peak threshold** check box.

   To consider a peak for a processing method, the application uses the Enable peak threshold filter to determine which peaks meet the specified percentage of the largest peak.

4. To display a specific number of the largest peaks by height or area, select the **Only select top peaks** check box.

❖ To choose a library



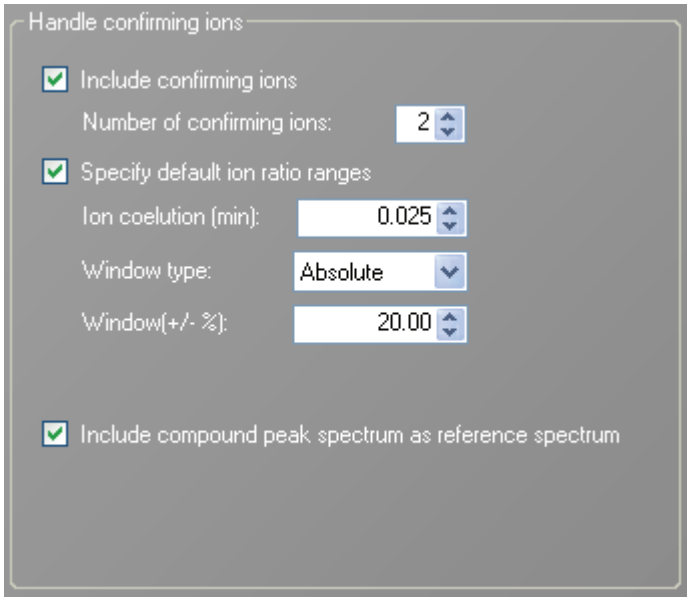
1. In the Use these libraries box, select the libraries you want to search.

   All libraries loaded on your instrument are displayed in the Use these libraries box.

2. To limit the number of hits returned when the system searches a spectrum against the selected libraries, set a value in the Limit library hits box.

3. To specify how to sort the library searches, choose a value for the Best match method list box.

❖ To specify confirming ions



1. To set the number of confirming ions, select the **Include confirming ions** check box and set a value in the Number of confirming ions box.

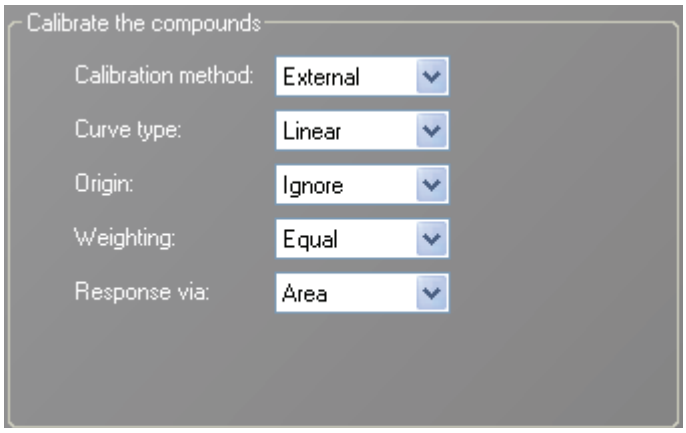
This value is the number of other ions in the spectrum whose ratio is compared to the quantitation ion. Using this ratio, you can then determine if it is the target compound or something else. This value defaults to **2** because you typically perform a 3-ion experiment with one quan mass and two confirming ions.

The system selects the most intense ion to use as the quantitation mass and uses this mass for the mathematical operations.

2. To define the criteria for evaluating confirming or qualifying ions, select the **Specify default ion ratio ranges** check box and set the following values:
   a. To specify the maximum difference in retention time between a confirming ion peak and the quantification ion peak, set a value in the Ion coelution (min) box.
   b. To specify an absolute or relative calculation approach for determining the acceptable ion ratio range, select **Absolute** or **Relative** from the Window type list.
   c. To specify the acceptable ion ratio range, set a value in the Window (+/– %) box.
3. To include the peak spectrum in the processing method, select the **Include compound peak spectrum as reference spectrum** check box.

   Use this setting to perform a spectra comparison in Data Review mode.

❖ To calibrate the compounds



1. From the Calibration method list, select **Internal** or **External**.
2. From the Curve type list, select one of the following:
   - Linear: All other settings are available with this exception: When **Include** is selected in the Origin list, all weighting values are unavailable except for **Equal**.
   - Quadratic: All other settings are available with this exception: When **Include** is selected in the Origin list, all weighting values are unavailable except for **Equal**.
   - Average RF: No selections in the Weighting or Origin lists are available. The Weighting list is set to **Equal**, and the Origin list is set to **Ignore**.

3. From the Origin list, select one of the following:
    - Ignore: Specifies that the origin is not included as a valid point in the calibration curve when the curve is generated. When you select **Ignore**, the calibration curve might or might not pass through the origin.
    - Force: Specifies that the calibration curve passes through the origin of the data point plot when the calibration curve is generated.
    - Include: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select **Include**, the calibration curve might or might not pass through the origin.
4. From the Weighting list, select one of the following:
    - Equal: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select **Equal**, the calibration curve might or might not pass through the origin.
    - 1/X: Specifies a weighting of 1/X for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their quantity.
    - 1/X^2: Specifies a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity.
    - 1/Y: Specifies a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio).
    - 1/Y^2: Specifies a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).
5. From the Response via list, choose **Area** or **Height**.
    - Area: Specifies that the application use this area value in response calculations.
    - Height: Specifies that the application use this height value in response calculations.

❖ To enter a note for the method

- Type in the Notes box, or paste text from another application using CTRL-V.

  You can add a note to your method template so that there is a record of what makes this template unique.

❖ To save the method template

1. Choose **File > Save** from the Method Template Editor menu.

   The Save Method Template dialog box opens.

2. Do one of the following:

   - Type a new name for the master method and click **OK**.

     –Or–

   - Select a method name to overwrite and click **Overwrite**.

   The TraceFinder application saves the new method template in the following folder:
   `..\Thermo\TraceFinder\Templates\Methods`

Method Template Editor

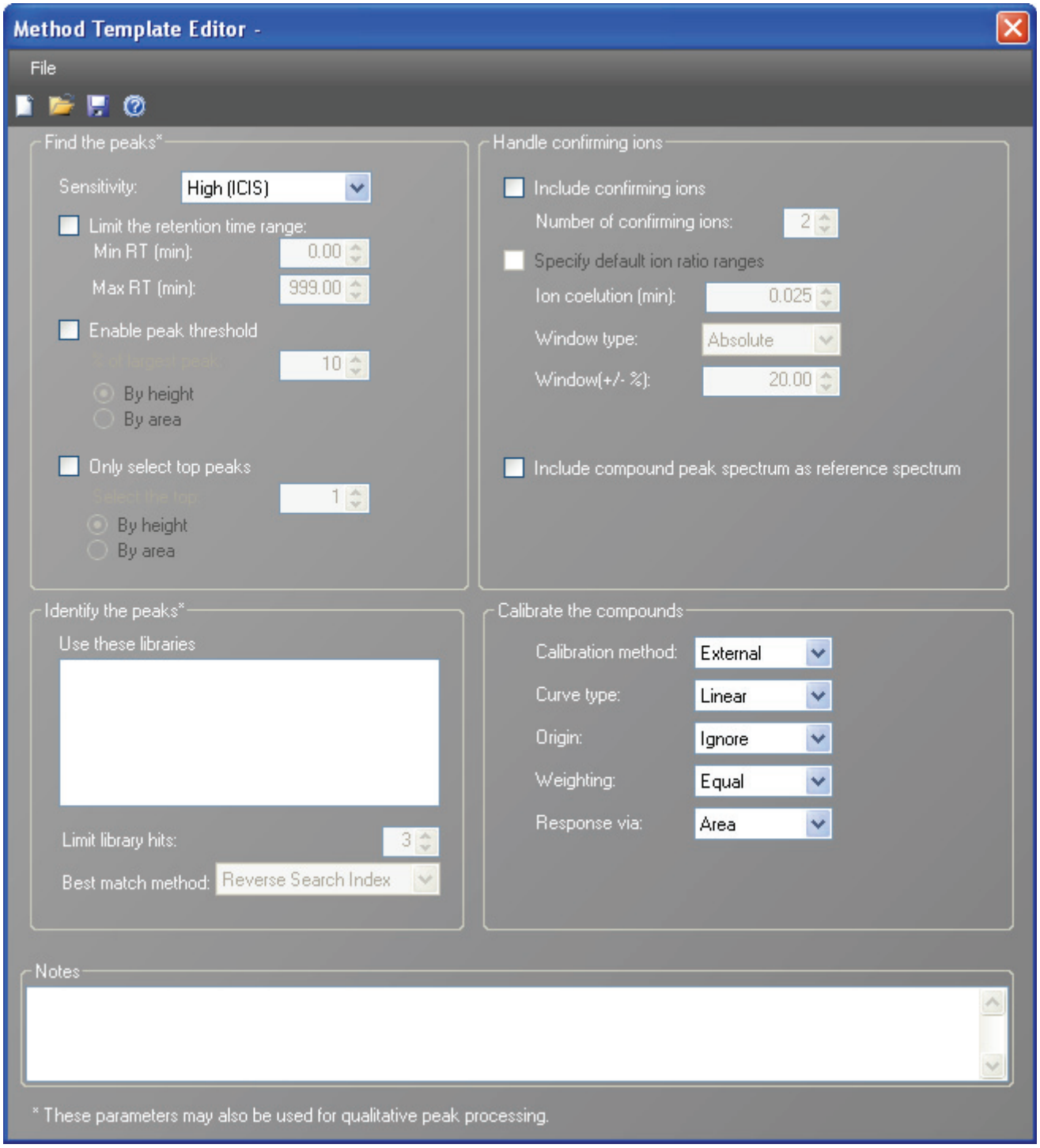


Table 3. Method Template Editor parameters (Sheet 1 of 2)

Parameter	Description
Find the peaks	
Sensitivity	Defines how extensively the peak detector algorithm searches for low-level peaks.
Limit the retention time range	Min RT specifies the beginning of the range, and Max RT specifies the end of the range.
Enable peak threshold	Specifies whether to select peaks by relative height or area and the percentage of the highest peak that will result in compound selection.
Only select top peaks	Displays a specific number of the largest peaks by height or area.
Identify the peaks	
Use these libraries	Lists the libraries you can search.
Limit library hits	Specifies the number of hits returned when the system searches a spectrum against the selected libraries.
Best match method	Specifies how to sort the library searches.
Handle confirming ions	
Include confirming ions/ Number of confirming ions	Specifies the number of confirming ions, which are other ions in the spectrum whose ratio is compared to the quantitation ion to identify the compound. This value defaults to 2 because you typically perform a 3-ion experiment with one quan mass and two confirming ions.
Specify default ion ratio ranges	Enables the ion ratio range features.
Window type	An Absolute or Relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	The acceptable ion ratio range.
Ion coelution	The maximum difference in retention time between a confirming ion peak and the quantification ion peak
Include compound peak spectrum as reference spectrum	Includes the peak spectrum in the processing method. Use this setting to perform a spectra comparison in Data Review.
Calibrate the compounds	
Calibration method	Specifies an internal or external calibration method.
Curve type	Specifies a linear, quadratic, or average RF curve type.

Table 3. Method Template Editor parameters (Sheet 2 of 2)

Parameter	Description
Origin	Specifies that the origin is ignored, forced, or included in the generated calibration curve. • Ignore: Specifies that the origin is not included as a valid point in the calibration curve when the curve is generated. When you select **Ignore**, the calibration curve might or might not pass through the origin. • Force: Specifies that the calibration curve passes through the origin of the data point plot when the calibration curve is generated. • Include: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select **Include**, the calibration curve might or might not pass through the origin.
Weighting	Specifies the weighting for the calibration data points. • Equal: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select **Equal**, the calibration curve might or might not pass through the origin. • 1/X: Specifies a weighting of 1/X for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their quantity. • 1/X^2: Specifies a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity. • 1/Y: Specifies a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio). • 1/Y^2: Specifies a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).
Response via	Specifies if the application uses area or height in response calculations. • Area: Specifies that the application use this peak area value in response calculations. • Height: Specifies that the application use this peak height value in response calculations.

Editing a Master Method

You can open a master method to view or edit the compounds, method instructions, and reporting options in the method.

This section includes instructions for the following tasks:

- Opening a Master Method
- Editing the General Page
- Editing the Acquisition List
- Editing the Compounds Page
- Editing the Flags Page
- Editing the Groups Page (GC only)
- Editing the Reports Page

Opening a Master Method

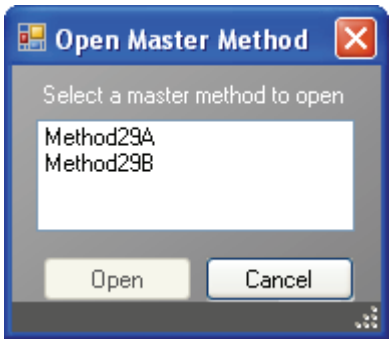
Use the following procedures:

- To open a master method
- To open a master method from the Recent Files list

❖ To open a master method

1. From any view, click **Method Development**.
2. In the Method View task pane, click **Open Method**.

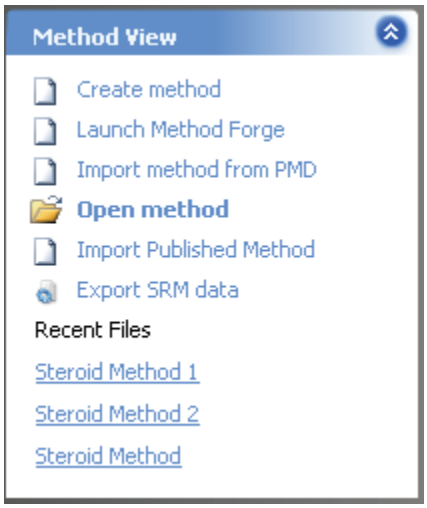
   The Open Master Method dialog box opens where you can select a master method to open.



3. Select a master method and open the file.

   The selected master method opens in the Master Method View.

❖ To open a master method from the Recent Files list



1. From any view, click **Method Development**.

   When you save a method, it is added to the Recent Files list. The Recent Files list displays a list of your most recently saved master method files.

2. Click the method name in the Recent Files list. Do not double-click.

   The selected method opens in the Method View.

Editing the General Page

The General page defines basic information about the master method.

Use the following procedures:

- To specify general information for a master method
- To update the instrument method parametersTo delete a compound from the list

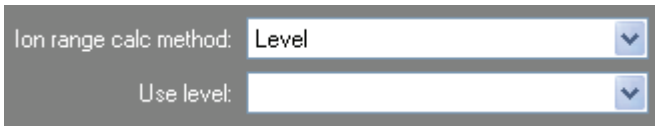
❖ To specify general information for a master method

1. In the Lab name box, type the name to be displayed on the top of each printed, saved, or exported report.
2. In the Assay type box, type the assay type to be targeted by the method.
3. From the Injection volume box, select the injection volume (in µL) to be used for sample injection.

   Use either the up/down arrows to change the volume in increments/decrements of 1 µL, or the keyboard to enter non-integer injection volumes.

4. From the Ion range calc method box, select a method for calculating the ion ratio range windows.

   If you select **Level**, an additional list box is displayed where you can choose a calibration level. These calibration levels are defined on the Compounds page. See "Editing the Compounds Page" on page 95.



5. From the Qualitative peak processing template box, select a template for performing peak detection on quantitative samples following target compound analysis.

   These templates are defined by a user in the role of IT Administrator or Lab Director.

❖ To update the instrument method parameters

1. To update any changes in the instrument method after you created this master method, click **Update**.
2. (GC only) To update any changes in the breakdown method after you created this master method, click **Update**.

General page

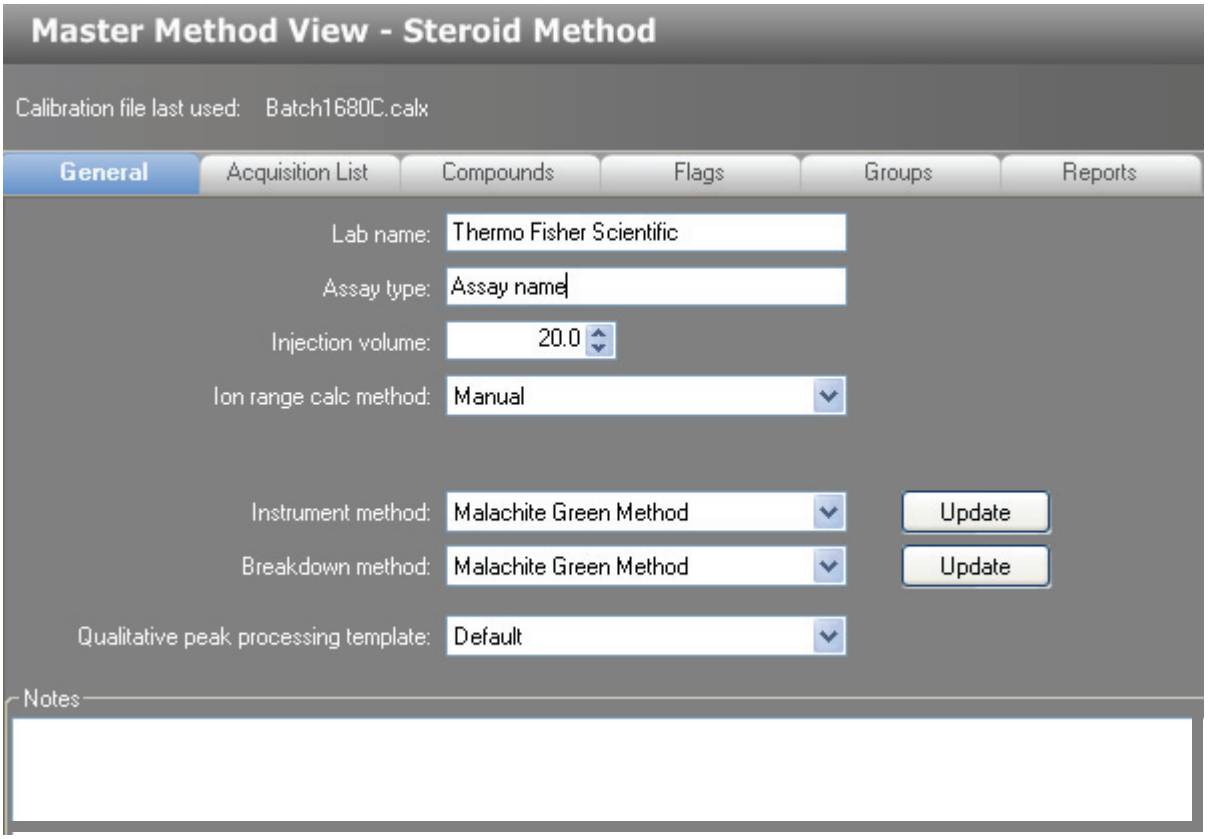


Table 4. General parameters

Parameter	Description
Lab name	(Optional) The laboratory name to be displayed on the top of each printed, saved, or exported report.
Assay type	The name for the analysis type to be targeted by the method. The assay type associates the method with the analysis of a compound or specific class of compounds (for example, an assay type of PAH might be used for the analysis of Polynuclear Aromatic Hydrocarbons). The TraceFinder application uses this assay type in the batch template. You can also select an appropriate combination of method and batch template.
Injection volume	The system use the injection volume (in µL) for sample injection. Certain autosamplers, such as the AI/AS 3000, use the injection volume specified in the associated instrument method. For those autosamplers, the value entered in this field is ignored and the instrument uses a default method injection volume. Other autosamplers, such as the TriPlus, use the TraceFinder application method injection volume for sample analysis and override the instrument method. For a more detailed explanation, refer to the documentation for the autosampler.
Ion range calc method	The application uses the ion range calc method to calculate the ion ratio range windows: Manual (default), Average, Level, or Weighted average. When you select **Level**, an additional list box is displayed where you can choose a calibration level amount. These calibration levels are defined on the Compounds page. See "Editing the Compounds Page" on page 95.
Instrument method	Instrument method used for processing samples.
Breakdown method (GC only)	Breakdown method used for processing samples.
Update	Updates any changes to the instrument or breakdown methods after you created this master method.
Qualitative peak processing template	The application uses the qualitative peak processing template to perform peak detection on quantitative samples following target compound analysis.
Notes	User-added notes about the method.

Editing the Acquisition List

The Acquisition List page displays all compounds defined for the current method. From this page, you can add or delete compounds from the method. See "Acquisition List page" on page 93.

❖ To filter the compound list

1. To display a filtered list of compounds, click the funnel icon,  , in the column header.

   For each column, a list of filterable criteria is displayed in a list box. On all list boxes, you can choose to filter by All, Blanks, NonBlanks, or by custom filter criteria. Other filter criteria are specific to the individual columns.

2. To create a custom filter based on compound values in a specific column, choose **Custom** from the column list box.

   For detailed instructions about creating a custom filter, see Appendix C, "Using Filter Criteria."

❖ To delete a compound from the list

1. Select the compound to remove from the list.
2. Do one of the following:
   - Click the **Remove compound transition** icon,  .

     –Or–

   - Right-click and choose **Remove compound transition** from the shortcut menu.

   A confirmation dialog box opens, listing the compound to be removed.
3. To confirm the deletion, click **Yes**.

   The selected compound is removed from the acquisition list.

❖ To add a compound transition to the list

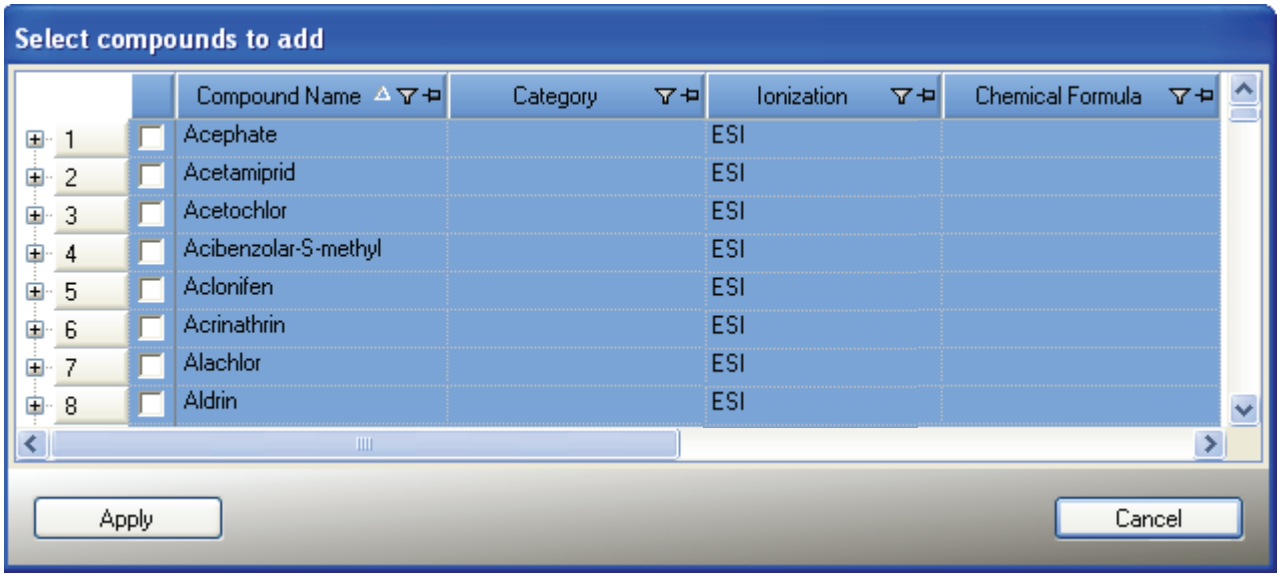
1. Do one of the following:
   - Click the **Add compound transition** icon,  .

     –Or–

   - Right-click and choose **Add compound transition** from the shortcut menu.

   The Select compounds to add dialog box opens, listing all the compounds defined in the compound datastore specified for the current technology (LC or GC).

Figure 1. Select compounds to add dialog box



2. Select the check box for each of the compounds you want to add to the method and click **Apply**.

   The compounds are added to the Acquisition List page and the Compounds page of the Master Method View.

Acquisition List page

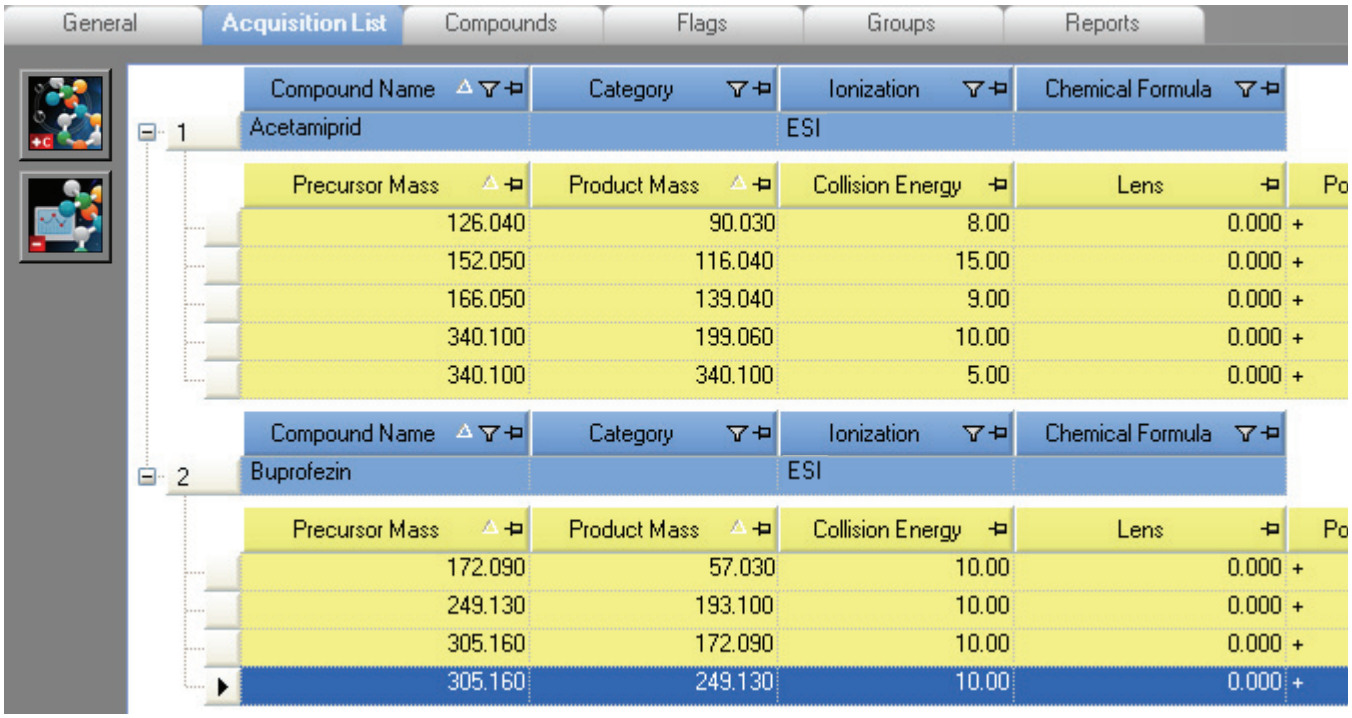


Table 5. Acquisition List parameters (Sheet 1 of 2)

Parameter	Description
Function Icons	
	Adds a confirming items row to the selected quantitation item. The icon is unavailable when adding a quantitation items or confirming items row is not feasible (a confirming item row is selected).
	Deletes the selected compound transition. The icon is unavailable when no row is selected.
Compound parameters	
Compound Name	Alphanumeric name assigned to the compound.
Category	(Optional) Alphanumeric identifier.
Ionization	(Optional) Alphanumeric identifier. Valid values: ESI, APCI, EI, CI, APPI
Chemical Formula	(Optional) Alphanumeric chemical identifier.
Precursor Mass	The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999

Table 5. Acquisition List parameters (Sheet 2 of 2)

Parameter	Description
Product Mass	The mass-to-charge ratio of the quan ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Range: –250 to 250
Lens	(Optional) Range: –400 to 400
Polarity	+ (positive) or – (negative)
RT (min)	Retention time. RT and Window values are used to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Window (sec)	Acquisition window. RT and Window values are used to determine the start and stop time for the acquisition. Range: 0.00 to 499.50 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Energy Ramp	(Optional) Range: 0.00 to 200.00

Editing the Compounds Page

The Compounds page sets all parameters for the identification, detection, and quantification for the target compound list. From the Compounds page of the Master Method View, you can access the following pages:

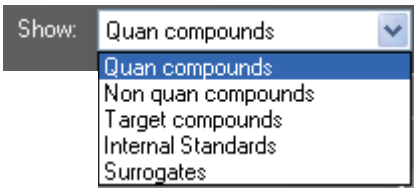
- Identification
- Detection
- Calibration
- Calibration Levels
- QC Levels

Identification

The Identification page lists the compounds that are targeted for analysis, reporting, and other compound-specific values.

❖ To filter the displayed compounds

- From the **Show** list box, select the type of compounds you want to display in the compounds list.



Compound Types	Description
Quan compounds	Displays only quan compounds, such as target compounds, internal standards, and surrogates.
Non quan compounds	Displays only non quan compounds, such as native and breakdown compounds.
Target compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.
Surrogates	Displays only surrogate compounds.

Identification page

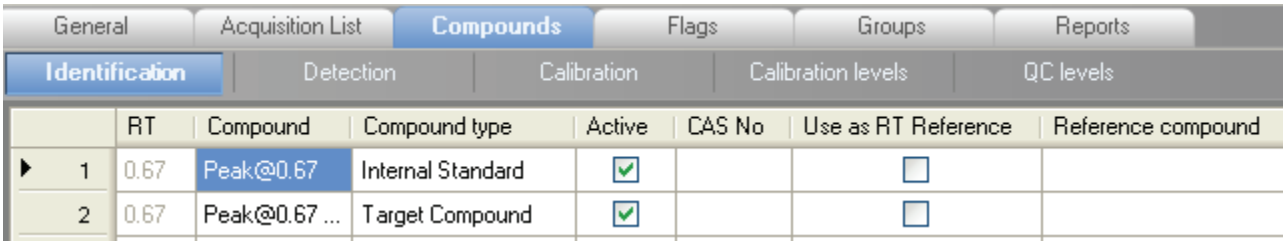


Table 6. Identification parameters

Parameter	Description
RT	Retention time. RT and Window values are used to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Compound	A list of compounds that have been identified. To customize the compound names, click the cell and type a new name. To display a filtered list of compounds, use the Show list box.
Compound type	Compound types are Target Compound, Internal Standard, Surrogate, Native, or Breakdown. The application uses target compounds, internal standards, and surrogates in quantitative analysis, and it uses native and breakdown compound types in system evaluation, as defined on the Breakdown page for the GC technology.
Active	Identifies each compound to be included in data review and reporting. By default, all added compounds are set to active.
CAS No	The Chemical Abstract Service (CAS) number that the TraceFinder application matched with each compound. To change or add a number, click the CAS No cell and enter a new number.
Use as RT Reference (GC only)	When performing peak detection with retention time standards, the application first identifies those compounds identified as retention time standards and then uses their observed retention times to adjust any associated target compound.
Reference compound (GC only)	Reference compound to be used for retention time adjustment for a compound. This list includes all compounds that are selected in the Use as RT Reference column.

Detection

Use the Detection page to customize peak detection and integration for any ions that define peaks and compounds.

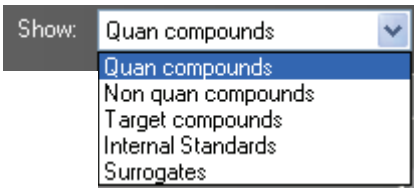
On the Detection page, you can configure how characteristic ions for targeted compounds are detected and integrated. You can also edit the list of characteristic ions for a specific compound. Refining these parameters in the master method for each compound and its ions can reduce the degree of manual integration that would otherwise be required.

The Detection page includes these additional pages:

- Times
- Signal
- Detect
- Spectrum
- Ratios

❖ To filter the displayed compounds

- From the **Show** list box, select the type of compounds you want to display in the compounds list.



Compound types	Description
Quan compounds	Displays only quan compounds, such as target compounds, internal standards, and surrogates.
Non quan compounds	Displays only non quan compounds, such as native and breakdown compounds.
Target compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.
Surrogates	Displays only surrogate compounds.

Detection page

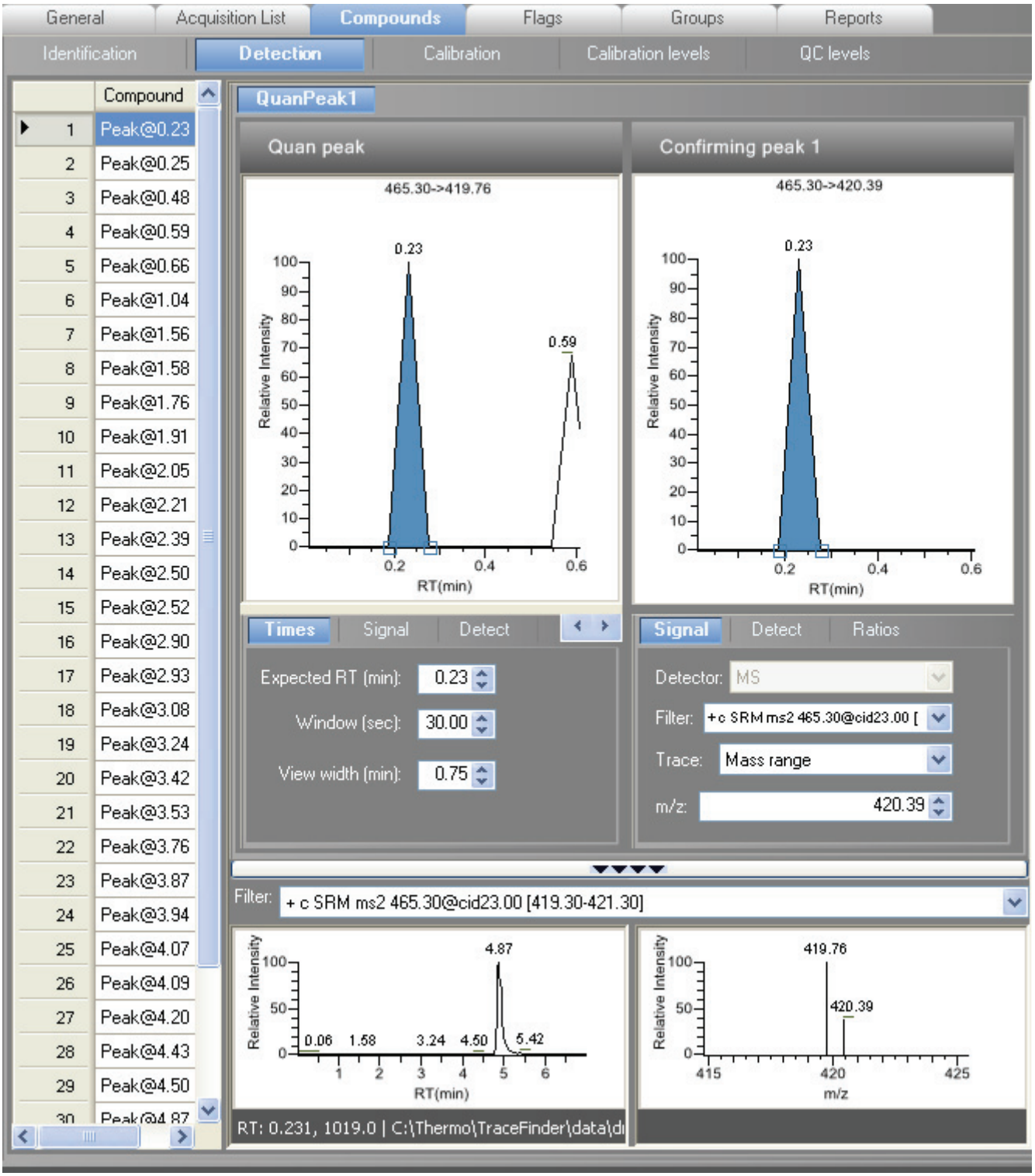


Table 7. Additional detection pages

Pages	Description
Times	Page to define the retention time and window for a quan peak.
Signal	Page to define the detector and its parameters used to display each chromatogram trace.
Detect	Page to define the peak detection algorithm and its options.
Spectrum	Page to define a reference mass spectrum for a quan peak or compound.
Ratios	Page to define the criteria for evaluating, confirming, or qualifying ions.

Times

Use the Times page to define the retention time and window for a quan peak.

Times page

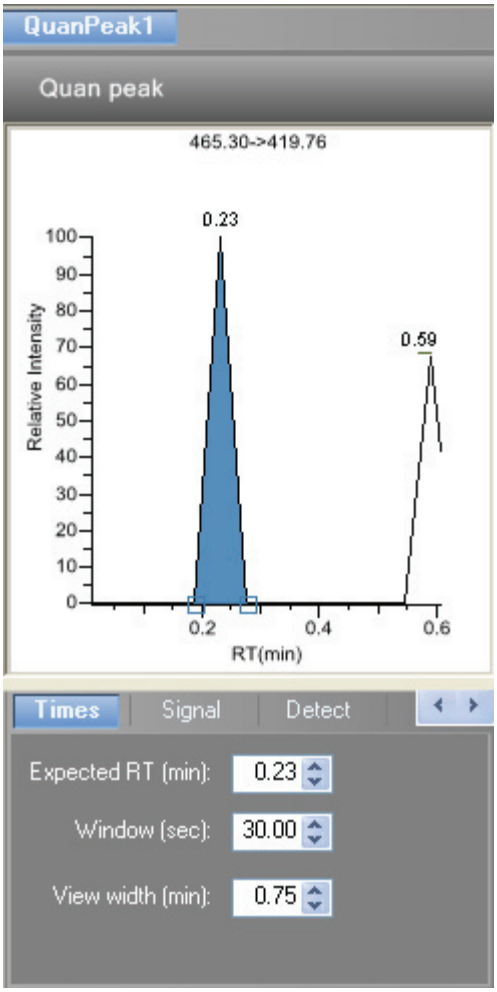


Table 8. Times parameters

Parameter	Description
Expected RT (min)	Expected retention time.
Window (sec)	Width of the window (in seconds) of how far around the expected retention time the system will look for a peak apex.
View width (min)	Viewable size of the ion chromatogram display. Changing the view width does not affect the process of peak detection; the TraceFinder application uses it only for graphical display.

Signal

Use the Signal page to define the detector and its parameters as you display each chromatogram trace.

Signal page

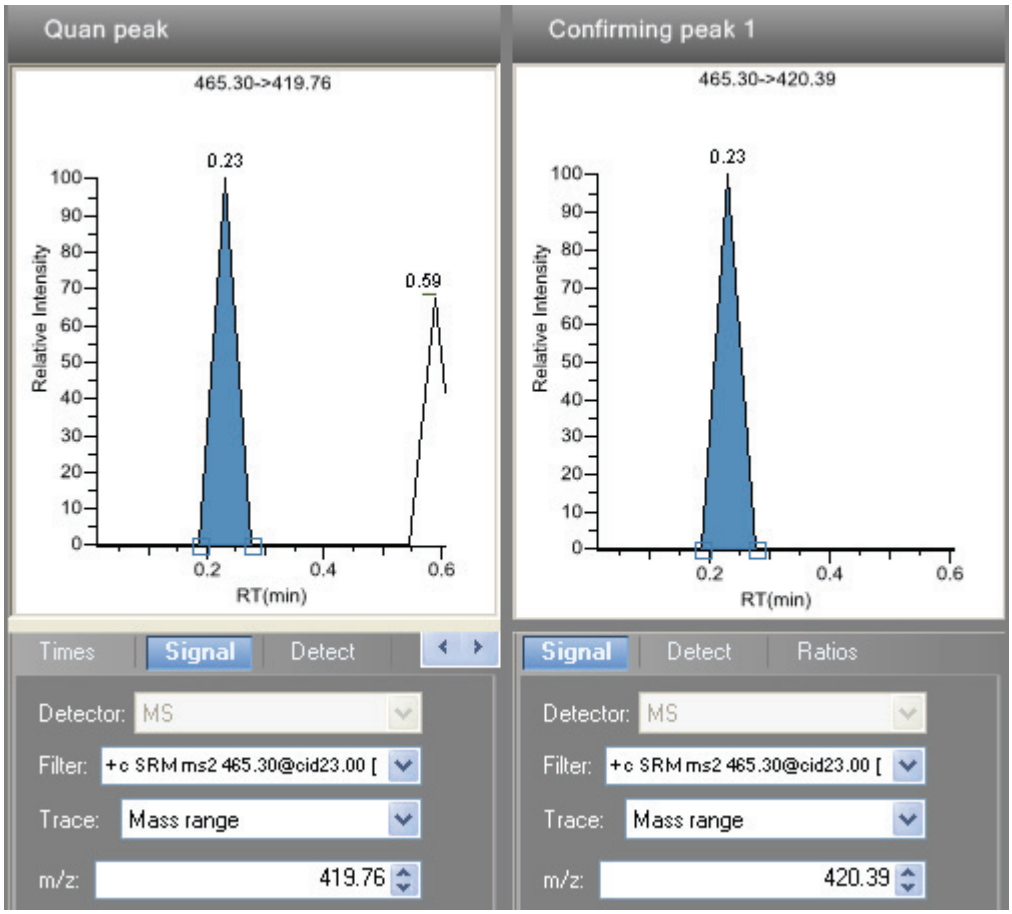


Table 9. Signal parameters (Sheet 1 of 2)

Parameter	Description
Detector	MS: Mass spectrometers. Analog: Supplemental detectors (for example, FID, ECD). AD card: If you have a detector not under data system control, you can capture the analog signal and convert it to digital using an interface box (for example, SS420X) for storage in the raw file. PDA (photo diode array): Detectors used for LC. UV (Ultra-violet): Detectors used for LC.
Filter	Represents a particular data acquisition channel. For example, the filter option + c Full ms [35.00-500.00] represents a positive ion centroid signal acquired in single-stage, full-scan mode from *m/z* 35 to 500.

Table 9. Signal parameters (Sheet 2 of 2)

Parameter	Description
Trace	Represents a specific range of the data. In conjunction with the filter, the application uses the trace to identify the characteristic ions for a compound. The options are: Mass range, TIC, or Base peak.
m/z	The initial mass value.

Detect

Use the Detect page to define the peak detection algorithm and its options and to determine the area under a curve. There are two different modes - Standard (Genesis) and High (ICIS). On this page, you can choose how you want each mode to run.

Detect page for Standard (Genesis)

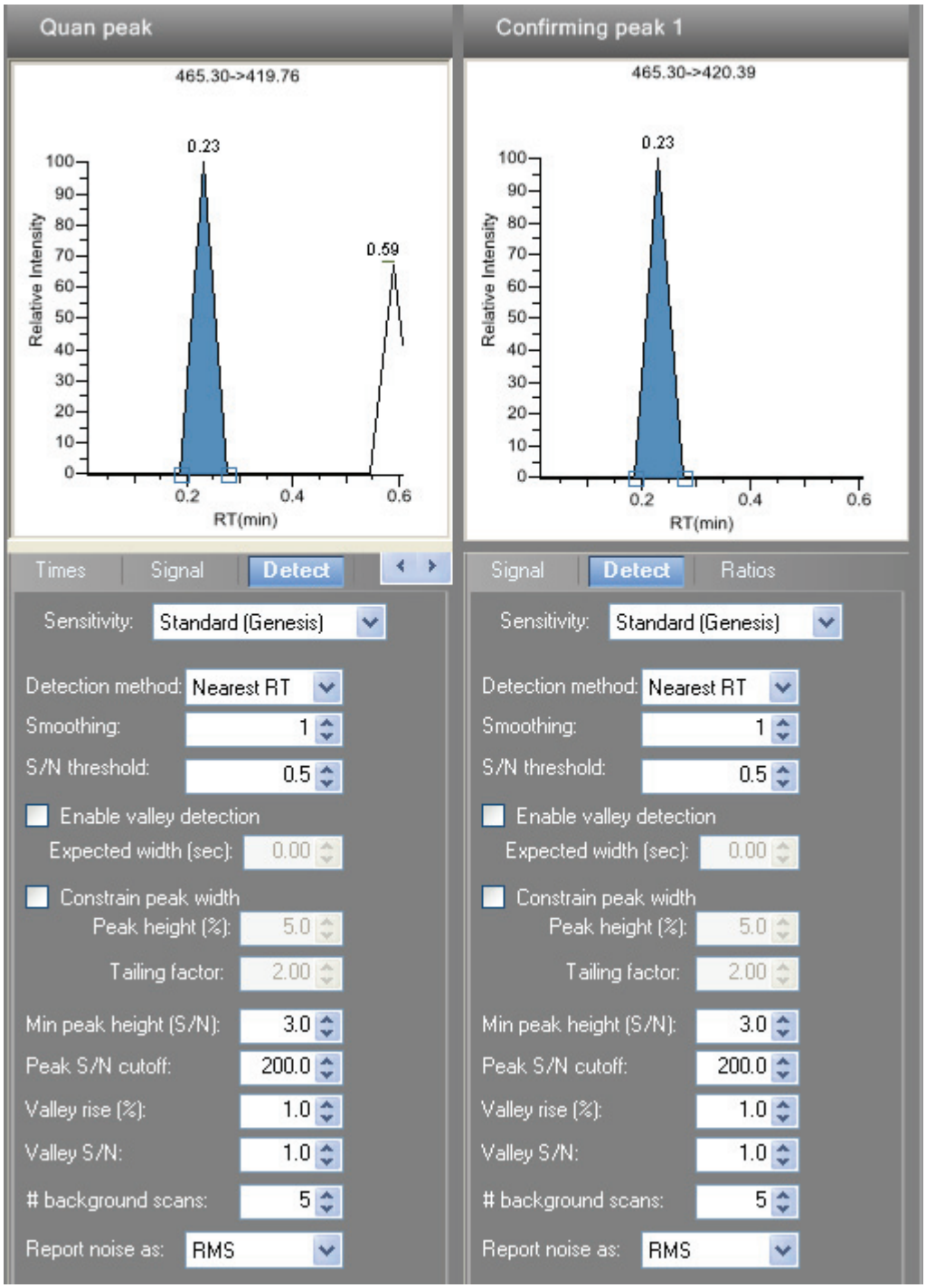


Table 10. Detect parameters for Standard (Genesis) (Sheet 1 of 3)

Parameter	Description
Sensitivity	Specifies the Standard (Genesis) peak detection algorithm.
Detection method	Highest peak: Uses the highest peak in the chromatogram for component identification. Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value. Range: Any odd integer from 1 through 15 points Default: 1
S/N threshold	Current signal-to-noise threshold for peak integration. Peaks with signal-to-noise values less than this value are not integrated. Peaks with signal-to-noise values greater than this value are integrated. Range: 0.0 to 999.0
Enable valley detection	Uses the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Expected width (sec)	The expected peak width parameter (in seconds). This controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the [expected width]/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the application terminates the peak at that point. The TraceFinder application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. Range: 0.0 to 999.0
Constrain peak width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain peak width check box enables the Peak Height (%) and Tailing Factor options.

Table 10. Detect parameters for Standard (Genesis) (Sheet 2 of 3)

Parameter	Description
Peak height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when the Constrain peak width check box is selected. Range: 0.0 to 100.0%
Tailing factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when the Constrain the Peak Width check box is selected. Range: 0.5 through 9.0
Min peak height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0
Peak S/N cutoff	The peak edge is set to values below this signal-to-noise ratio. This test assumes it has found an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio. When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 10000.0

Table 10. Detect parameters for Standard (Genesis) (Sheet 3 of 3)

Parameter	Description
Valley rise (%)	The peak trace can rise above the baseline by this percentage after passing through a minimum (before or after the peak). This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. When the trace exceeds rise percentage, the TraceFinder application applies valley detection peak integration criteria. This test is applied to both the left and right edges of the peak. The rise percentage criteria is useful for integrating peaks with long tails. Range: 0.1 to 500.0
Valley S/N	Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher. Range: 1.0 to 100.0 Default: 2.0
# background scans	Number of background scans performed by the application.
Report noise as	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or peak-to-peak resolution threshold. Options are RMS or Peak to Peak.

Detect page for High (ICIS)

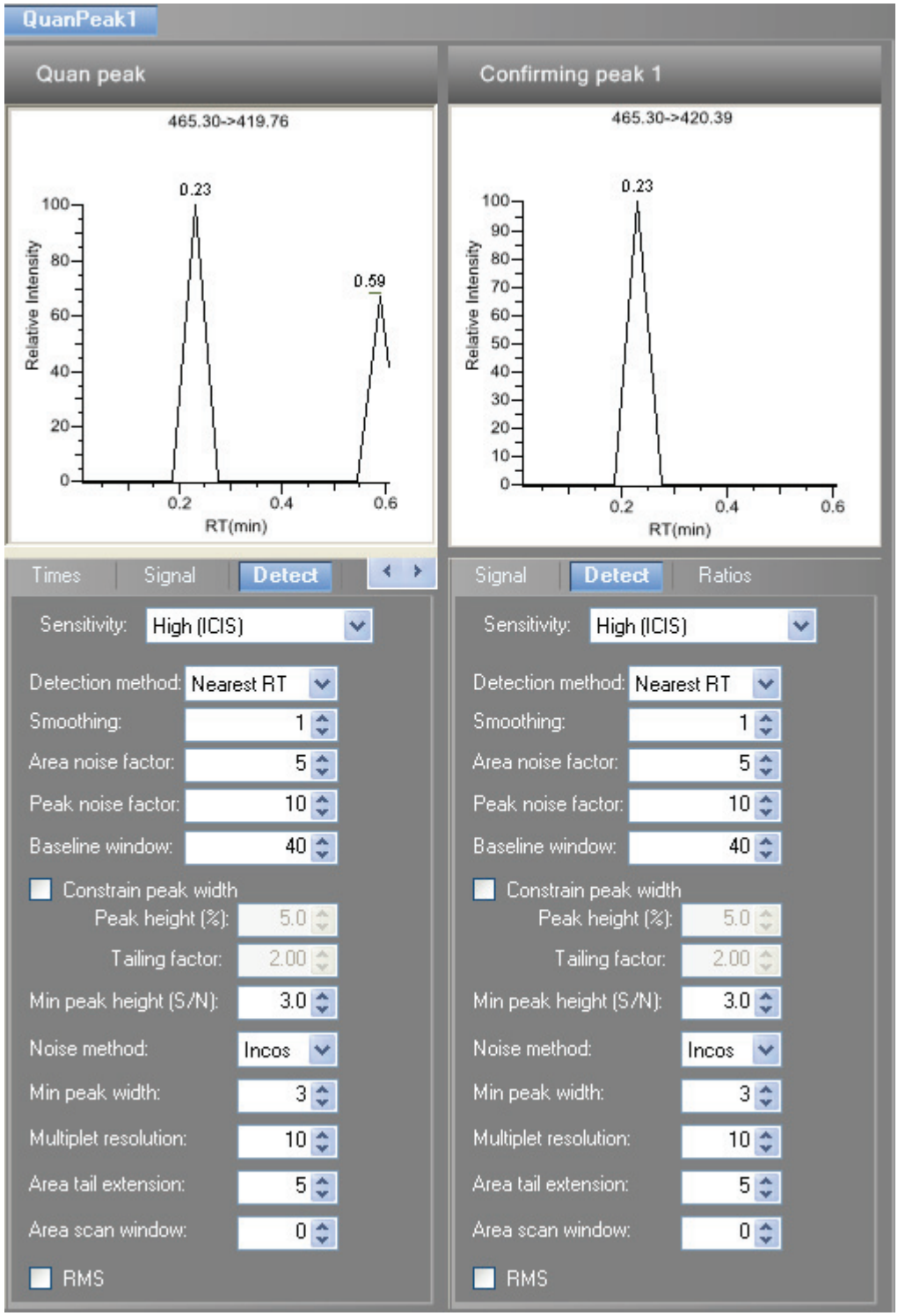


Table 11. Detect parameters for High (ICIS) (Sheet 1 of 3)

Parameter	Description
Sensitivity	Specifies the High (ICIS) peak detection algorithm.
Detection method	Highest peak uses the highest peak in the chromatogram for component identification. Nearest RT uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value. Range: Any odd integer from 1 through 15 points Default: 1
Area noise factor	The noise level multiplier used to determine the peak edge after the location of the possible peak. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 5
Peak noise factor	The noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value. Range: 1 through 1000 Default: 10
Baseline window	The TraceFinder application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 40
Constrain peak width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain peak width check box enables the Peak Height (%) and Tailing Factor options.
Peak height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when the Constrain peak width check box is selected. Range: 0.0 to 100.0%

Table 11. Detect parameters for High (ICIS) (Sheet 2 of 3)

Parameter	Description
Tailing factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when the Constrain the Peak Width check box is selected. Range: 0.5 through 9.0
Min peak height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0
Noise method	The options are INCOS or Repetitive. INCOS uses a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. Repetitive uses a multiple pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but it takes longer.
Min peak width	The minimum number of scans required in a peak. The ICIS peak detection algorithm uses this value. Range: 0 to 100 scans Default: 3
Multiplet resolution	The minimum separation in scans between the apexes of two potential peaks. This is a criteria to determine if two peaks are resolved. The ICIS peak detection algorithm uses this value. Range: 1 to 500 scans Default: 10
Area tail extension	The number of scans past the peak endpoint to use in averaging the intensity. The ICIS peak detection algorithm uses this value. Range: 0 to 100 scans Default: 5

Table 11. Detect parameters for High (ICIS) (Sheet 3 of 3)

Parameter	Description
Area scan window	The number of allowable scans on each side of the peak apex. A zero value defines all scans (peak-start to peak-end) to be included in the area integration. Range: 0 to 100 scans Default: 0
RMS	Specifies that the TraceFinder application calculate noise as RMS. By default, the application uses Peak To Peak for the noise calculation. RMS is automatically selected if you manually determine the noise region.

Spectrum

Use the Spectrum page to store a reference mass spectrum for a quan peak or compound.

Use the following procedures:

- To update confirming ion ratios
- To change the quantitation mass used for a quan peak
- To add ions together to get an accumulated signal
- To add a quan peak to an existing compound
- To add one or more confirming ions to an existing compound
- To zoom in the chromatogram or spectrum displays

❖ To update confirming ion ratios

1. Click a peak in the chromatogram pane.

   The mass spectrum for the peak is displayed in the spectrum pane.

2. Right-click the spectrum pane and choose **Update confirming ion ratios with this spectrum** from the shortcut menu.

❖ To change the quantitation mass used for a quan peak

1. Click a peak in the chromatogram pane.

   The mass spectrum for the peak is displayed in the spectrum pane.

2. In the spectrum pane, click the ion.

   A red box around the ion's relative intensity value indicates that the ion is selected.

3. Right-click and choose **Set this mass as quan mass** from the shortcut menu.

❖ To add ions together to get an accumulated signal

1. Click an ion in the spectrum pane.

   A red box around the ion's relative intensity value indicates that the ion is selected.

2. Right-click and choose **Add this mass to existing quan mass range** from the shortcut menu.

   You can now update the ion ratios to adjust the confirming ion comparisons to the new summed quan peak signal.

❖ To add a quan peak to an existing compound

1. Click the peak in the chromatogram pane.

   The mass spectrum for the peak is displayed in the spectrum pane.

2. In the spectrum pane, click the ion.

   A red box around the ion's relative intensity value indicates that the ion is selected.

3. Right-click and choose **Set this mass as new quan peak** from the shortcut menu.

❖ To add one or more confirming ions to an existing compound

1. Click the peak in the chromatogram pane.

   The mass spectrum for the peak is displayed in the spectrum pane.

2. In the spectrum pane, click the ion.

   A red box around the ion's relative intensity value indicates that the ion is selected.

3. Right-click and choose to **Add this mass as new confirming ion** from the shortcut menu.

❖ To zoom in the chromatogram or spectrum displays

1. Drag your cursor to delineate a rectangle.

   The display zooms into the specified rectangle.

2. To return to the original display, right-click and choose **Reset Scaling** from the shortcut menu.

Spectrum page

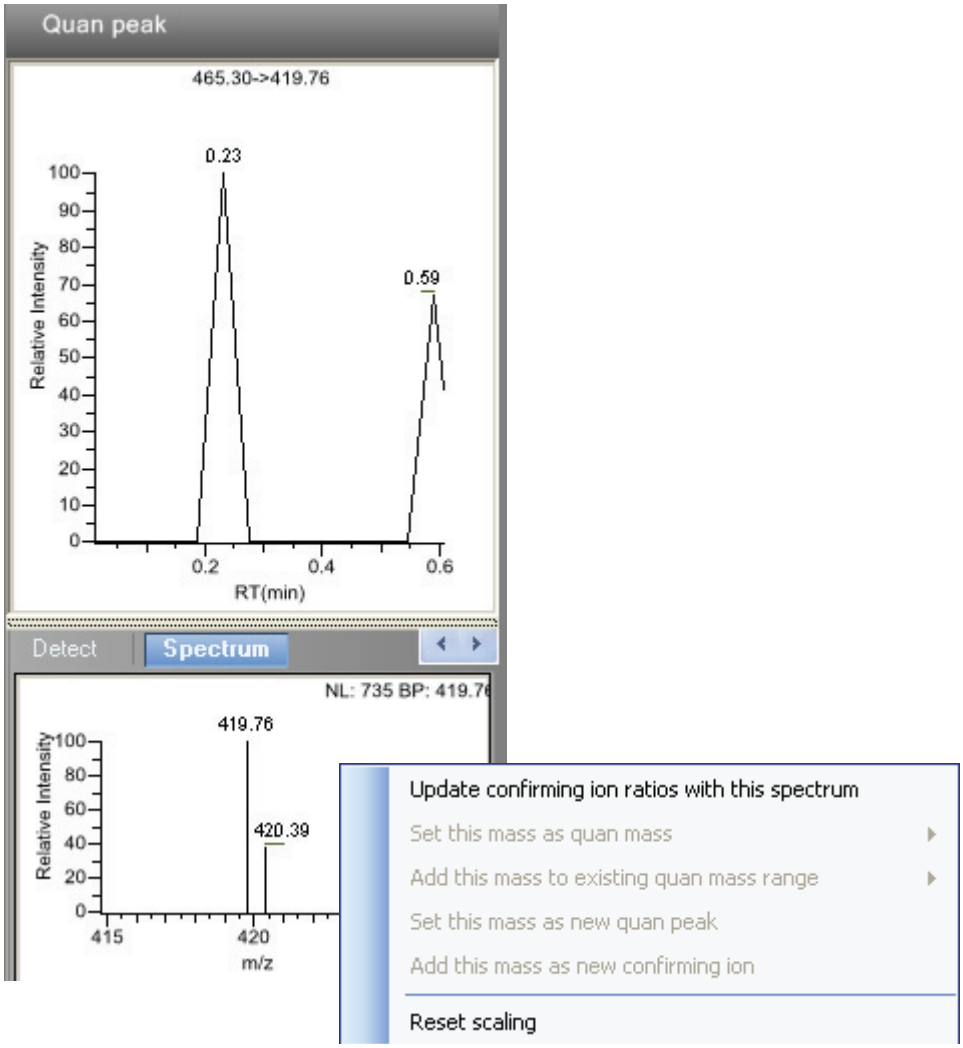


Table 12. Spectrum shortcut menu functions

Functions	Description
Update confirming ion ratios with this spectrum	Updates the confirming ion ratios using the selected peak.
Set this mass as quan mass	Adds the quan mass of the selected ion to the quantitation mass used for the quan peak.
Add this mass to existing quan mass ranges	Adds the selected mass to your existing quan mass ranges. You can then update the ion ratios to adjust the confirming ion comparisons to the new summed quan peak signal.
Set this mass as a new quan peak	Adds a new quan peak to an existing compound.
Add a mass as new confirming ion	Adds one or more confirming ions to an existing compound.
Reset scaling	Returns the chromatogram or spectrum display to its original size.

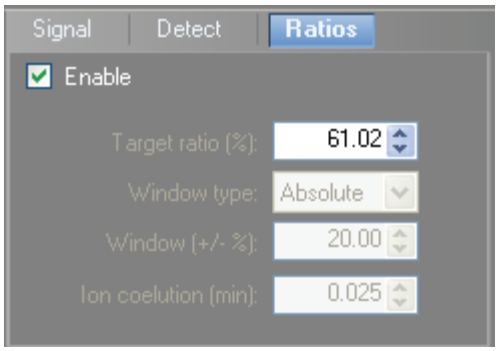
Ratios

Use the Ratios page to define the criteria for evaluating confirming or qualifying ions. the TraceFinder application detects compounds that have confirming ion values outside their acceptable window and flags them in Data Review mode and on reports.

❖ To specify ion ratio criteria

1. Enable or disable the use of the particular confirming ion.
2. In the Target ratio box, select the theoretical ratio of the confirming ion's response to the quantification ion's response.
3. In the Window type box, select **Absolute** or **Relative** as the calculation approach for determining the acceptable ion ratio range.
4. In the Window (+/-%) box, select the acceptable ion ratio range.
5. In the Ion coelution box, select the maximum difference in retention time between a confirming ion peak and the quantification ion peak

   In the following example:



   - The target ratio is expected to be 61.02% and the window is Absolute 20%, so the acceptable window for this confirming ion is 41.02% to 81.02%.
   - If, instead, the window type was Relative, the plus or minus value would be 20% of 61.02% (or 12.20%), so the acceptable window for this confirming ion would be 48.82% to 73.22%.

Ratios page

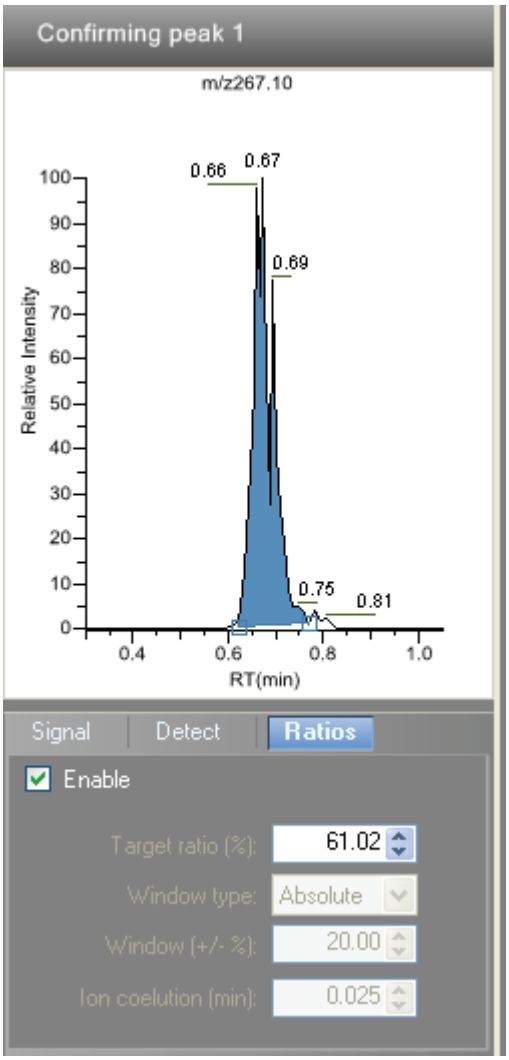


Table 13. Ratios parameters

Parameter	Description
Target ratio (%)	The theoretical ratio of the confirming ion's response to the quantification ion's response.
Window type	The absolute or relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	The acceptable ion ratio range.
Ion coelution (min)	The maximum difference in retention time between a confirming ion peak and the quantification ion peak.

Calibration

Use the Calibration page to set or edit the mathematical model used for preparing the initial calibration evaluation for one or more calibration standards.

Each target compound can have its own initial calibration settings, independent of the other compounds. You can modify the calibration approach on this page or in Data Review mode when you view the results of an actual calibration batch.

Calibration page

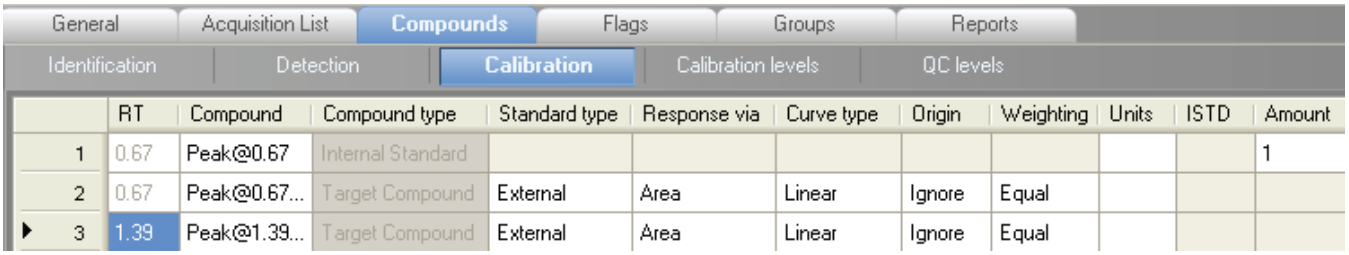


Table 14. Calibration parameters

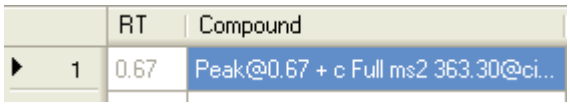
Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Compound type	Displays the compound type as an internal standard, an external standard, or a target compound.
Standard type	Specifies Internal or External standards.
Response via	The use of area or height.
Curve type	Specifies Linear, Quadratic, or AverageRF curve types.
Origin	The origin treatment as Ignore, Include, or Force. The Origin and Weighting columns are active only when you are using Linear or Quadratic curve types.
Weighting	Specifies the weighting as Equal, 1/X, 1/X^2, 1/Y, or 1/Y^2.
Units	The units to be displayed with the calculated values.
ISTD	The internal standard (ISTD) for a target compound or surrogate if the standard type is set to Internal. If you set the standard type to External, this field is inactive.
Amount	The amount of the internal standard for ISTD compounds.

Calibration Levels

On the Calibration levels page for a master method, you can define the standards for calibration. You can edit calibration levels and concentrations for master methods only. The contents of this page are read-only when you are editing a local method.

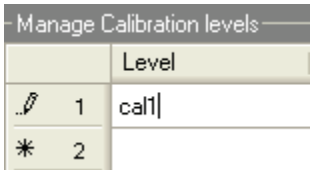
❖ To specify calibration levels and concentrations

1. Select the compound whose calibration levels and concentrations you want to define.

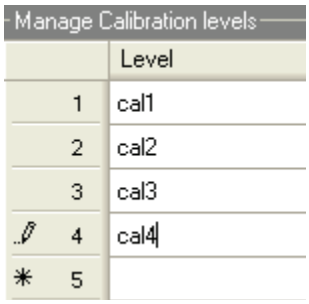


2. In the Manage Calibration levels area, type a value for the first calibration level.

   The application adds a new, empty calibration level row beneath the edited row.



3. Continue adding calibration levels.



   When you finish adding calibration levels, you can specify the concentrations for each level for each compound.

4. To enter the concentrations to the table, do the following:

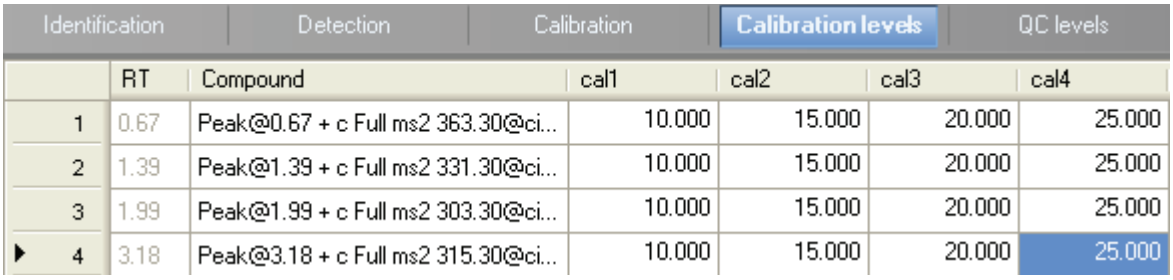
   a. Select the first calibration level table cell.

   b. Click the cell again to make it editable.

   c. Type a concentration value.

5. Repeat Step 4 for all calibration levels associated with the first compound.

6. To specify the same concentration values for all compounds, select the value you want to copy, right-click and choose **Copy down** from the shortcut menu.



Calibration levels page

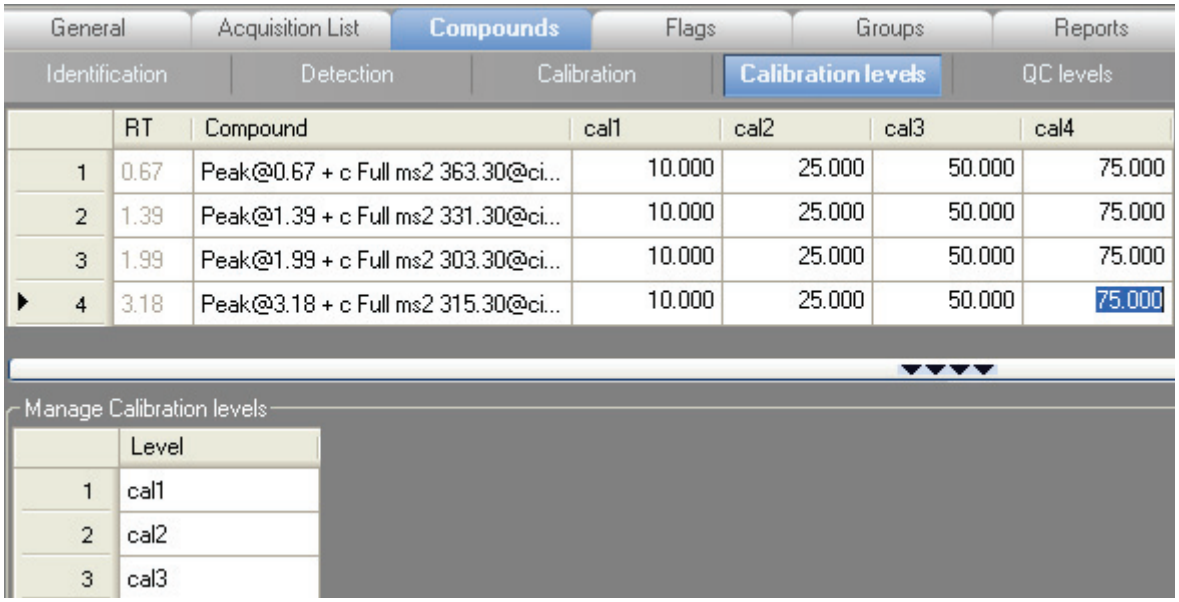


Table 15. Calibration levels parameters

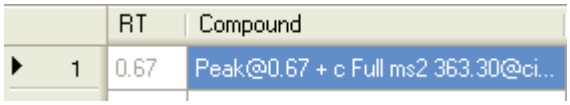
Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
cal1-cal*n*	User-defined calibration levels for the compound.
Manage Calibration levels	Defines calibration levels for the selected compound.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

QC Levels

Use the QC levels page for a master method to define the standards for QC levels. You can edit QC levels for master methods only. The contents of this page are read-only when you are editing a local method.

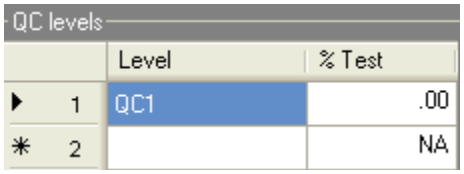
❖ To specify QC levels and concentrations

1. Select the compound whose QC levels, percentage test values, and concentrations you want to define.



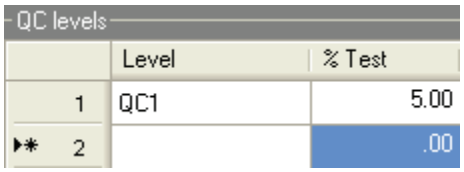
2. In the QC levels area, type a name for the first QC level.

   The application adds a new, empty QC level row beneath the edited row.

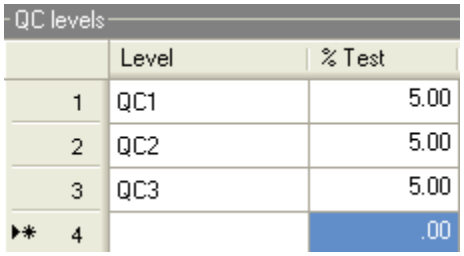


3. Type a value for the % Test.

   The % Test is the acceptable difference (as a percentage) between the known amount and the calculated (measured) amount of each QC level.



4. Continue adding QC levels and values for percentage test.



   When you finish adding QC levels, you can specify the concentrations for each level for each compound.

5. To enter the concentration values to the table, do the following:

   a. Select the first QC level table cell.

   b. Click the cell again to make it editable.

   c. Type a concentration value.

6. Repeat Step 5 for all QC levels associated with the first compound.

Identification	Detection	Calibration	Calibration levels	QC levels

	RT	Compound	QC1	QC2	QC3
1	0.67	Peak@0.67 + c Full ms2 363.30@cid40.00 [150.00-3...	10.000	15.000	25.000
2	1.39	Peak@1.39 + c Full ms2 331.30@cid40.00 [100.00-3...			

7. To specify the same concentration values for all compounds, select the value you want to copy, right-click and choose **Copy down** from the shortcut menu.

Identification	Detection	Calibration	Calibration levels	QC levels

	RT	Compound	QC1	QC2	QC3
1	0.67	Peak@0.67 + c Full ms2 363.30@cid40.00 [150.00-3...	10.000	15.000	25.000
2	1.39	Peak@1.39 + c Full ms2 331.30@cid40.00 [100.00-3...	10.000	15.000	25.000
3	1.99	Peak@1.99 + c Full ms2 303.30@cid40.00 [100.00-3...	10.000	15.000	25.000
▶ 4	3.18	Peak@3.18 + c Full ms2 315.30@cid40.00 [100.00-3...	10.000	15.000	25.000

QC levels page

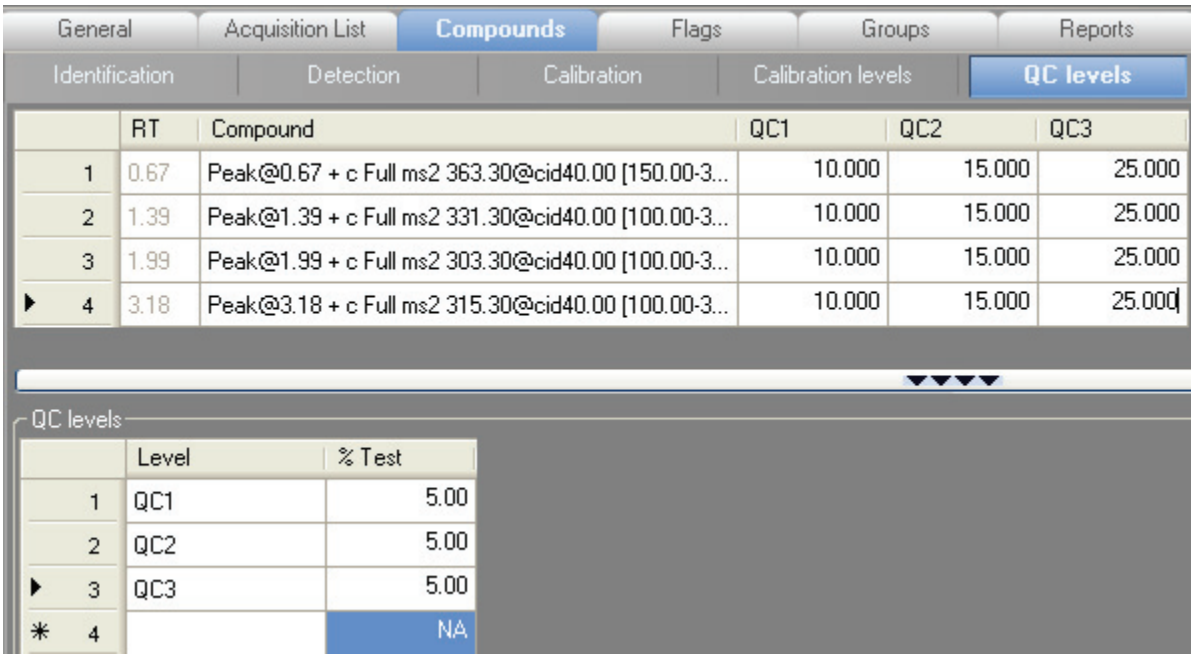


Table 16. QC levels parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
QC1-QC*n*	User-defined quality control levels for the compound.
QC levels	
Level	User-defined quality control level names.
% Test	A value for the acceptable difference (as a percentage) between the known amount and calculated (measured) amount of each QC level.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Editing the Flags Page

Use the Flags page to set limits and ranges so the TraceFinder application can review the data and results as an aid to final approval.

From the Flags page of the Master Method View, you can access these additional pages:

- Quan Flags
- Calibration Flags
- QC Check Flags
- Blank Flags
- ISTD Flags
- Solvent Blank Flags
- Surrogate Flags
- Matrix Spike Flags
- Lab Control Flags (GC only)

Quan Flags

Use the Quan page to define levels of review for quantified results. Quantified results appear on printed and electronic reports. You can also define when a quantified value is reported instead of reporting less than a particular limit.

Quan page

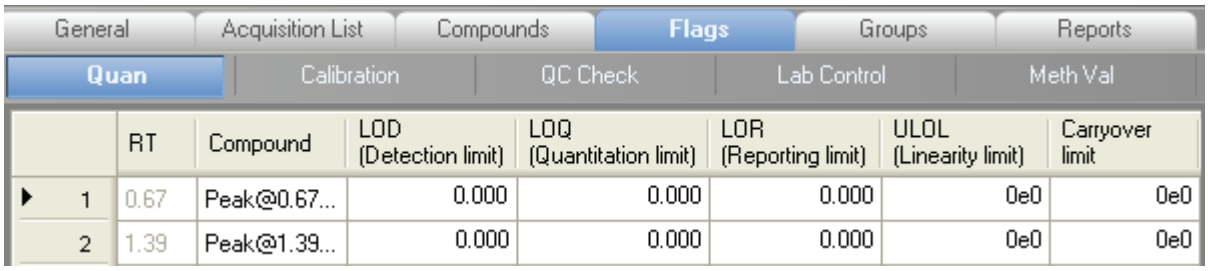


Table 17. Quan flag parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
LOD (Detection limit)	Limit of detection. The lowest amount that can be detected. Usually derived from a method detection limit (mdl) study.
LOQ (Quantitation limit)	Limit of quantitation. The lowest amount that can be confidently and accurately quantitated. This is usually the lowest calibrator amount.
LOR (Reporting limit)	Limit of reporting. Also called cutoff in some industries. This is the highest amount that can be reported, as determined by each laboratory's standard operating practices.
ULOL (Linearity limit)	Upper limit of linearity. This is usually the highest calibrator amount.
Carryover limit	The highest amount of a substance that does not leave a residual amount in the instrument. If a substance has a carry over limit of 5, amounts higher than 5 usually dirty the instrument and leave residue behind, tainting the following sample. A carryover limit of less than 5 does not leave any residual amounts of the substance.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Calibration Flags

Use the Calibration page to define acceptable criteria for initial calibration. The TraceFinder application makes the evaluation by comparing the initial calibration results for each compound found in the sample to the values defined on this page.

On the Calibration report, the application flags the calculated values for internal standard compounds that exceed these limits.

Calibration page

	RT	Compound	R^2 threshold	Max RSD (%)	Min RF	Max Amt Diff (%)
1	0.67	Peak@0.67...	0.9900	20.00	0.000	20.00
2	1.39	Peak@1.39...	0.9900	20.00	0.000	20.00
3	1.99	Peak@1.99...	0.9900	20.00	0.000	20.00
4	3.18	Peak@3.18...	0.9900	20.00	0.000	20.00

Table 18. Calibration flag parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
R^2 threshold	The minimum correlation coefficient (r^2) for an acceptable calibration (when in linear or quadratic mode).
Max RSD (%)	The maximum relative standard deviation (RSD) for an acceptable calibration (when in average RF mode).
Max Amt Diff (%)	The maximum deviation between the calculated and theoretical concentrations of the calibration curve data points (when in linear or quadratic mode).
CV Test (%)	Coefficient of Variation test. These values are added to the Data Review display.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

QC Check Flags

Use the QC Check page to review the calibration on an on-going basis. The TraceFinder application makes the evaluation by comparing the check standard results for each compound in the sample to the initial calibration using values defined on this page.

On the Check Standard report, the application flags the calculated values for internal standard compounds that exceed these limits.

For linear and quadratic modes, the maximum difference for the calculated concentration in the QC check sample versus the theoretical value is set on the QC levels page of the Compounds page.

QC Check page

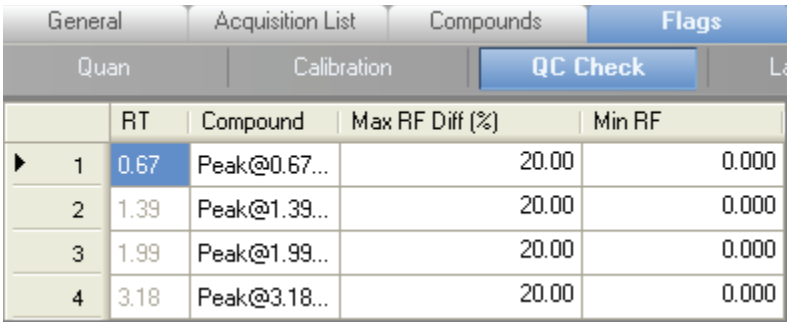


Table 19. QC Check flag parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Max RF Diff (%)	The maximum deviation between the response factor (RF) of the QC check sample and the average response factor from the calibration (when in average RF mode).
Min RF	The minimum response factor for the QC check standard (when in average RF mode).
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Lab Control Flags (GC only)

Use the Lab Control page to view and edit QC values for lab control sample and lab control sample duplicate analyses. The TraceFinder application makes the evaluation by comparing the calculated concentration for each compound in the sample to the theoretical concentration and range defined on this page.

You can prepare samples (typically known as clean matrices) as LCS or LCSD. These represent samples to which you have added known concentrations of target analytes. To define an LCS and its duplicate in a batch, select the appropriate sample type and a common sample ID.

On the Lab Control report. the application flags the calculated values for spiked compounds that exceed these limits.

Lab Control page

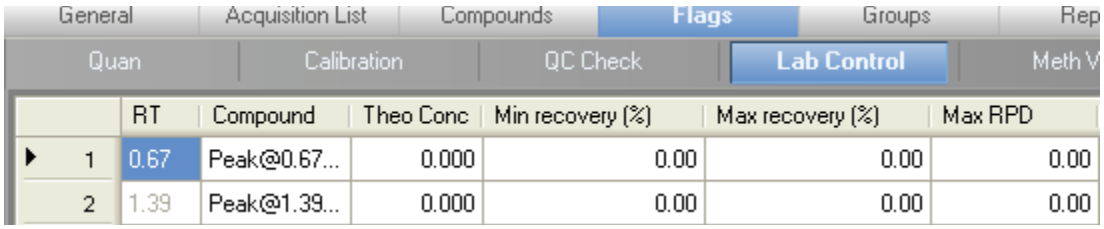


Table 20. Lab Control flag parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Theo Conc	Values for each lab control compound that represent the expected theoretical concentration of that compound in the sample.
Min recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that the application can determine by comparing the observed calculated concentration in the analysis to the expected concentration. Each LC/LCSD compound can have its own values for these fields, independent of other LC/LCSD compounds.
Max recovery (%)	
Max RPD	Specify a maximum value for relative percent difference (RPD) between two spiked samples.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Meth Val Flags (GC only)

Use the Meth Val page to view or edit QC values for method validation reporting. The application makes the evaluation by comparing the calculated concentration for each compound in the sample to the theoretical concentration and range defined on this page.

You can use these parameters to evaluate the performance of your method. For this evaluation, prepare, analyze, and evaluate a number of samples (typically 4 to 10) to document method accuracy and precision as a comprehensive whole. To define a method validation sample in the batch, select the appropriate sample type.

On the Method Validation report, the application flags the calculated values for method validation compounds that exceed these limits.

Meth Val page

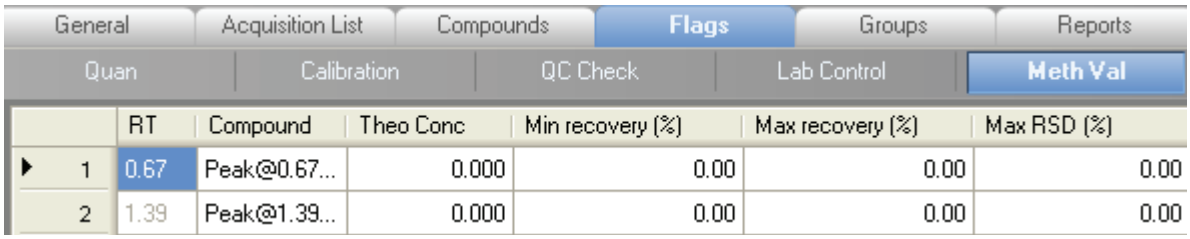


Table 21. Meth Val flag parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Theo Conc	Values for each compound that represent the expected theoretical concentration of that compound in the sample.
Min recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that the application can determine by comparing the observed calculated concentration in the analysis to the expected concentration. Each method validation compound can have its own values for these fields, independent of other method validation compounds.
Max recovery (%)	
Max RSD (%)	The maximum relative standard deviation of the set of observed concentrations for a component across the set of method validation samples.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Breakdown Flags (GC only)

Use the Breakdown page to view and edit values used for the evaluation of breakdown and degradation reporting. The TraceFinder application makes the evaluation by calculating the ratio of breakdown compounds to the native compounds.

❖ To display the list of compounds in a group

- Click anywhere in the group row.

❖ To select a group for breakdown calculation

- Select the **Active** check box in the group row.

  You can select any group in the method for breakdown calculation, but the TraceFinder application calculates and reports only those that contain breakdown and native compounds.

Breakdown page

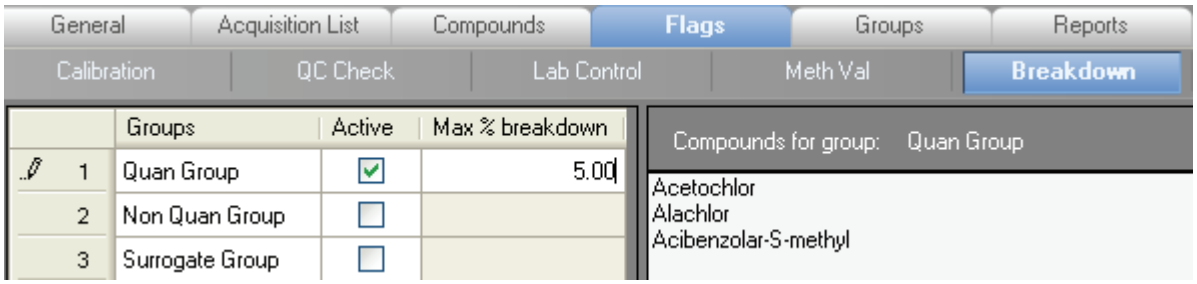


Table 22. Breakdown flag parameters

Parameter	Description
Groups	Lists all groups created on the Groups page. See "Editing the Groups Page (GC only)" on page 136.
Active	Specifies which groups are used for breakdown analysis.
Max % breakdown	The maximum allowable percentage of breakdown to native compounds. This value is calculated by summing the responses of the breakdown compounds and dividing them by the sum of the native compounds. On the Breakdown Report, the application flags the calculated values for breakdown and native compounds that exceed these limits.
Compounds for group	Lists all compounds in the selected group.

Blank Flags

Use the Blank page to define acceptable levels of target compounds in blank samples. The application makes the evaluation by comparing the calculated concentration for each compound in the sample to the maximum concentration defined on this page. You can enter the maximum concentration as a percentage of a flag value or as a specified value.

On the Blank report, the application flags the calculated values for internal standard compounds that exceed these limits.

❖ To specify the maximum concentration as a percentage

1. From the Method column list box, choose one of the following methods:
   - % of LOD
   - % of LOQ
   - % of LOR
2. In the Percentage column, type a percentage value.

❖ To specify the maximum concentration as an absolute value

1. From the Method column list box, select **Concentration**.
2. In the Max Conc column, type an absolute value.

❖ To specify no maximum concentration

- From the Method column list box, select **None**.

Blank page

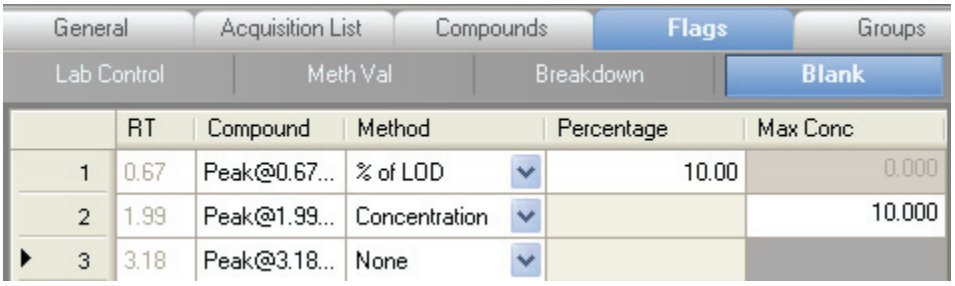


Table 23. Blank flag parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Method	The evaluation process used for comparing the calculated concentration. You can specify no maximum, a specific concentration, or a percentage of the LOR, LOD, or LOQ.

Table 23. Blank flag parameters (Sheet 2 of 2)

Parameter	Description
Percentage	The percentage of the LOR, LOD, or LOQ if you are using the percentage approach.
Max Conc	The maximum concentration if you are using an absolute value.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

ISTD Flags

Use the ISTD page to review response and retention time of internal standards (if available). The application makes the evaluation by comparing the area and retention time results for each internal standard compound in the sample to a specified range.

If all of your target compounds are set to external calibration mode or you have not identified any compounds as internal standards, this page does not show any values.

ISTD page

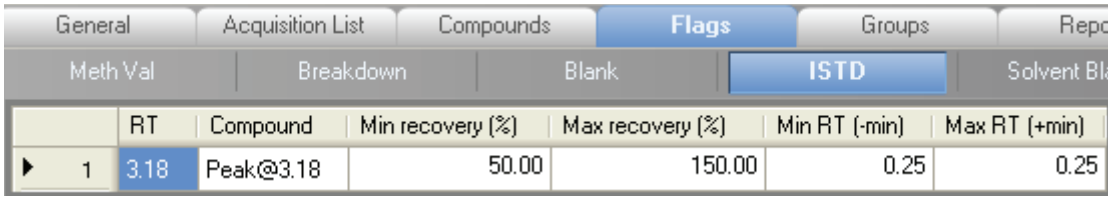


Table 24. ISTD flag parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Min recovery (%)	The minimum and maximum percent recoveries for the internal standards to define an acceptable range. For check standards, the TraceFinder application compares the response of each internal standard in each sample to a range around the average of the responses of that compound in all of the calibration standards. For all other samples, the application calculates the comparison range around the check standard responses if a check standard is available in the batch. If no check standard is available, the application tests against the initial calibration.
Max recovery (%)	

Table 24. ISTD flag parameters (Sheet 2 of 2)

Parameter	Description
Min RT (–min)	The minimum and maximum drift (in minutes) for the internal standards to define an acceptable range. For check standards, the TraceFinder application compares the retention time of each internal standard in each sample to a range around the average of the retention times of that compound in all of the calibration standards. For all other samples, the application calculates the comparison range around the check standard retention times if a check standard is available in the batch. If no check standard is available, the application tests against the initial calibration.
Max RT (+min)	
CV Test (%)	Coefficient of Variation test.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Solvent Blank Flags

Use the Solvent Blank page to view or edit QC values for solvent reporting. The evaluation is made by comparing the calculated response for each compound in the sample to the maximum response defined on this page.

On the Solvent Blank report, the application flags the calculated values for internal standard compounds that exceed these limits.

Solvent Blank page

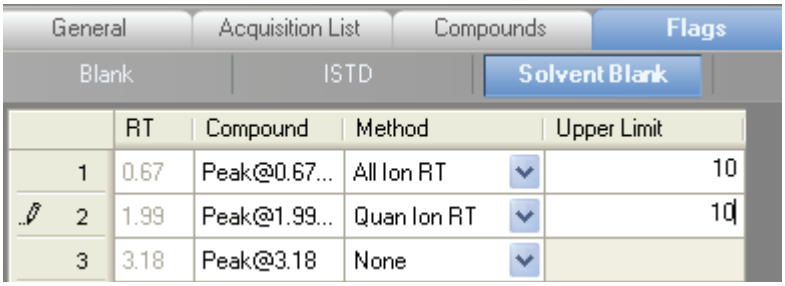


Table 25. Solvent Blank flag parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Method	The evaluation process to use a response for the quan ion only (Quan Ion RT) or a summed response for the quan ion and any confirming ions (All Ion RT). You can deactivate the solvent blank test by selecting **None**.
Upper Limit	Specifies an upper limit for each compound in the sample if an evaluation process is selected. These values are not concentrations; they are raw response values.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Surrogate Flags

Use the Surrogates page to view or edit QC values for surrogate reporting. The application makes the evaluation by comparing the calculated concentration for each surrogate compound in the sample to the range defined on this page.

On the Surrogate report, the application flags the calculated values for internal standard compounds that exceed these limits.

Surrogate page

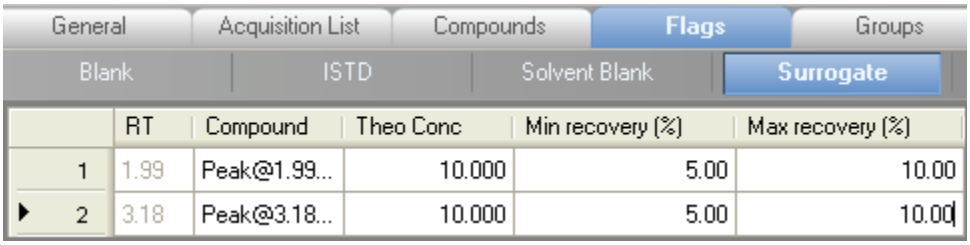


Table 26. Surrogate flag parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Theo Conc	Values for each surrogate compound that represent the expected theoretical concentration of that compound in the sample. You can apply or not apply the dilution factor for a sample to the calculated surrogate concentrations using the Correct surrogates option on the Reports page. See "Specifying Report Options" on page 142.
Min recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that can be determined by comparing the observed calculated concentration in the analysis to the expected concentration. Each surrogate can have its own values for these fields, independent of other surrogates.
Max recovery (%)	
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Matrix Spike Flags

Use the Matrix Spike page to view or edit QC values for matrix spike and matrix spike duplicate analyses. The application makes the evaluation by comparing the calculated concentration for each compound in the sample (after subtracting the original sample value) to the theoretical concentration and range defined on this page.

To evaluate matrix spike (MS) or matrix spike duplicate (MSD) compounds, prepare samples as MS or MSD. These represent samples to which you have added known concentrations of target analytes. To define a sample, its MS, and its MSD in the batch, select the appropriate Sample Type and a Sample ID.

Note Sample IDs must be unique. Duplicating Sample IDs can cause incorrect samples to be included in reports.

On the MS/MSD report, the application flags the calculated values for spiked compounds that exceed these limits.

Matrix Spike page

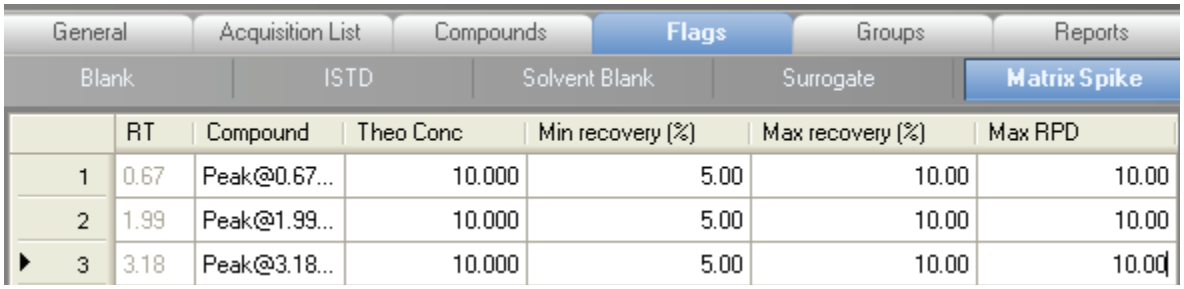


Table 27. Matrix Spike flag parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Theo Conc	Values for each surrogate compound that represent the expected theoretical concentration of that compound in the sample. You can apply or not apply the dilution factor for a sample to the calculated surrogate concentrations using the Method Options.
Min recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that can be determined by comparing the observed calculated concentration in the analysis to the expected concentration. Each surrogate can have its own values for these fields, independent of other surrogates.
Max recovery (%)	
Max RPD	Specify a maximum value for relative percent difference (RPD) between two spiked samples.

Table 27. Matrix Spike flag parameters (Sheet 2 of 2)

Parameter	Description
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT (retention time) column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Editing the Groups Page (GC only)

Use the Groups page of the Master Method View to organize compounds into functional or logical groups. You can use these groups for creating a subset of target compounds for quantitative processing or a list of non-quantitative compounds for breakdown processing. See "Groups page" on page 137.

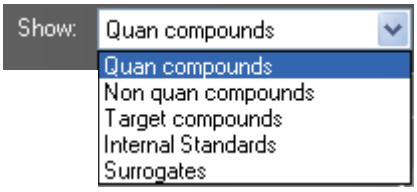
For quantitative processing, the TraceFinder application processes all compounds in the method and stores the complete result set, but only those in the selected group are visible in Data Review mode. Limiting the displayed compounds to those in the selected group can be useful when working with a master method containing a large list of compounds, only some of which are required for analysis in certain samples. In that case, the application requires only a single method and can reduce the results. To display only those compounds to be used in quantitative processing, select **Quan compounds** from the Show list box.

For non-quantitative processing, you can select the Breakdown and Native compounds that the TraceFinder application uses for breakdown reporting. To view only those compounds to be used in non-quantitative processing, select **Non-quan compounds** from the Show list box.

You can create as many quantitative and non-quantitative groups as you want and the same compound can be in multiple groups.

❖ To create a group

1. From the Show list box, select the type of compounds you want to view.



2. At the bottom of the Groups area, click **Add Group**.

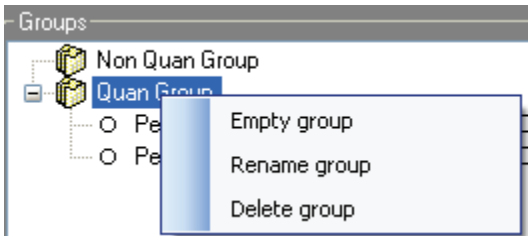
   The Add a new Group dialog box opens.

3. Type a name for the new group and click **OK**.

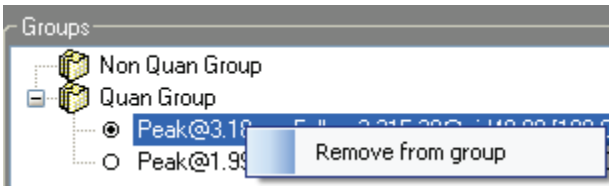
   The new group appears in the Groups area.

4. Drag a compound from the Compounds area onto a group name (as if you were moving files into a folder).

5. To remove all the compounds from a group, rename the group, or delete it, right-click the group name and choose from the shortcut menu.



6. To remove a single compound, click the compound name in the group, right-click. and choose **Remove from group** from the shortcut menu.



Groups page

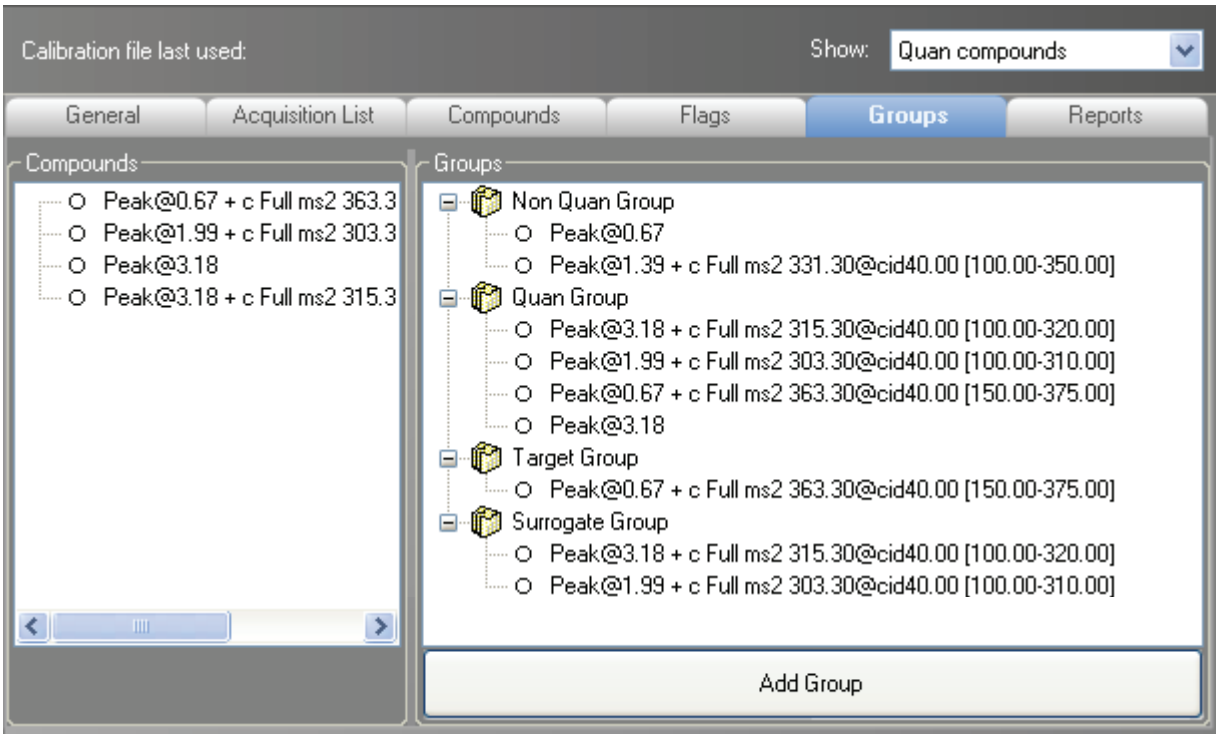


Table 28. Groups parameters

Parameter	Description
Compounds	Lists all available compounds.
Groups	Lists all available groups.
Add Group	Opens the Add a new Group dialog box where you can create a new group.
Shortcut menu	
Empty group	Removes all compounds from the selected group.
Rename group	Changes the name of the selected group.
Delete group	Removes the selected group and all the compounds in it.
Remove from group	Removes the selected compound from its group.

Editing the Reports Page

Use the Reports and Custom Reports pages to specify how you want to save or print your reports.

For the Quantitation Report type, you can modify quan report, user interface, quan flag, and surrogate correction options in the Report Options pane.

This section includes instructions for the following tasks:

- Specifying Report Formats
- Specifying Report Options

Specifying Report Formats

For each standard report you generate, you can create a hardcopy printout, a PDF (.pdf) file, or an XML (.xml) file. In addition to the report type, you can specify a report title for each of your reports. The default report title is the report name.

For each custom report you generate, you can create a hardcopy printout or an XLS (.xlsm) file. You cannot specify a report title for a custom report.

Use the following procedures:

- To specify standard reports types and output formats
- To view an example standard report
- To specify custom report types and output formats

❖ To specify standard reports types and output formats

1. Click the **Reports** tab.

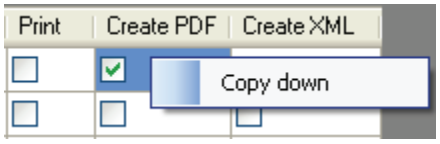
   The Reports page displays the Report Name, Report Title, and the options to create a hardcopy, a PDF file, or an XML file. See "Reports page" on page 140.

2. To edit the Report Title, double-click the name and type your new name.

   The TraceFinder application uses this name for all reports that use this master method. You cannot edit the Report Title from other report views.

3. To specify the type of report output to create for each report type, select the check box in the appropriate column.

4. To duplicate the output type for all reports, click the cell to select it, then right-click and choose **Copy down** from the shortcut menu.



All check boxes in the column below the selected cell duplicate the selected or cleared state of the selected cell.

By default, all report types are cleared.

❖ To view an example standard report

1. Click the magnifying button, , to view an example PDF of the report type.

   The right pane of the view displays an example PDF report with typical PDF viewer controls.

2. To minimize the PDF viewer, click the minimize icon, .

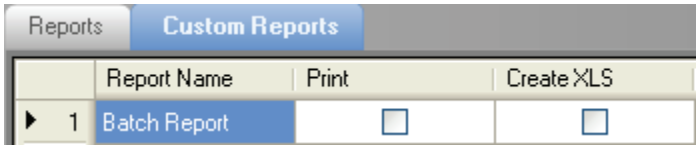
❖ To specify custom report types and output formats

1. Click the **Custom Reports** tab.

   The Custom Reports page lists all the reports that are saved in the following folder:

   `..\Thermo\TraceFinder\Templates\Reports`

   The Custom Reports page displays the Report Name and the options to create a hardcopy printout or XLS file. See "Custom Reports page" on page 141.



2. To specify the type of report output to create for each report type, select the check box in the appropriate column.

3. To duplicate the output type for all reports, right-click the cell and choose **Copy down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell.

Reports page

	Example	Report Name	Report Title	Print	Create PDF	Create XML
1		Batch Report	Batch Report	☐	☐	☐
2		Blank Report	Blank Report	☐	☐	☐
3		Breakdown Report	Breakdown Report	☐	☐	☐
4		Calibration Density Report	Calibration Density Report	☐	☐	☐
5		Calibration Report	Calibration Report	☐	☐	☐
6		Check Standard Report	Check Standard Report	☐	☐	☐
7		Chromatogram Report	Chromatogram Report	☐	☐	☐
8		Compound Calibration Report	Compound Calibration Report	☐	☐	☐
9		Confirmation Report	Confirmation Report	☐	☐	☐
10		Confirmation Report 2	Confirmation Report 2	☐	☐	☐
11		High Density Internal Standard Report	High Density Internal Standard Report	☐	☐	☐
12		High Density Internal Standard Report Long	High Density Internal Standard Report Long	☐	☐	☐
13		High Density Sample Report 1	High Density Sample Report 1	☐	☐	☐
14		High Density Sample Report 1 Long	High Density Sample Report 1 Long	☐	☐	☐
15		High Density Sample Report 2	High Density Sample Report 2	☐	☐	☐
16		High Density Sample Report 2 Long	High Density Sample Report 2 Long	☐	☐	☐
17		High Density Sample Report 3	High Density Sample Report 3	☐	☐	☐
18		High Density Sample Report 3 Long	High Density Sample Report 3 Long	☐	☐	☐
19		Internal Standard Summary Report	Internal Standard Summary Report	☐	☐	☐
20		Ion Ratio Failure Report	Ion Ratio Failure Report	☐	☐	☐
21		LCSLCSD Report	LCSLCSD Report	☐	☐	☐
22		Manual Integration Report	Manual Integration Report	☐	☐	☐
23		Method Detection Limit Report	Method Detection Limit Report	☐	☐	☐
24		Method Report	Method Report	☐	☐	☐
25		Method Validation Report	Method Validation Report	☐	☐	☐
26		MSMSD Report	MSMSD Report	☐	☐	☐
27		Solvent Blank Report	Solvent Blank Report	☐	☐	☐
28		Surrogate Recovery Report	Surrogate Recovery Report	☐	☐	☐

Table 29. Reports parameters

Parameter	Description
Example	Displays a sample of the report type.
Report Name	The name of a report.
Report Title	The user-defined title to be used on a report.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files.
Create XML	Reports to be exported in XML format.

Custom Reports page

	Report Name	Print	Create XLS
1	AltCalibrationReport	☑	☐
2	Alternate BatchReport	☐	☐
3	Alternate CalibrationReport	☐	☐
4	Alternate ConfirmationReport	☐	☐
5	Alternate MatrixSpikeReport	☐	☐
6	Alternate SampleReport	☐	☐
7	Alternate SummaryReport	☐	☐
8	BatchReport	☐	☐
9	BlankReport	☐	☐
10	CalibrationDensityReport	☐	☐
11	CalibrationReport	☐	☐
12	CheckStandardReport	☐	☐
13	CompoundCalibrationReport	☐	☐
14	ConfirmationReport	☐	☐
15	ConfirmationReport2	☐	☐
16	HighDensitySampleReport1Long	☐	☐
17	HighDensitySampleReport2Long	☐	☐
18	HighDensitySampleReport3Long	☐	☐
19	QuantitationReport	☐	☐

Table 30. Custom Reports parameters

Parameter	Description
Report Name	The name of a report.
Print	Reports to be sent to the printer.
Create XLS	Reports to be exported in Excel spreadsheet (.xlsm) format.

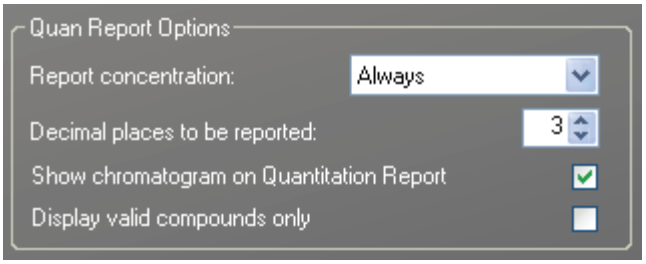
Specifying Report Options

Use the report options to choose display features for standard report types.

Use the following procedures:

- To specify quantitation report options
- To specify user interface options
- To specify quantitation flag options
- To correct surrogates

❖ To specify quantitation report options

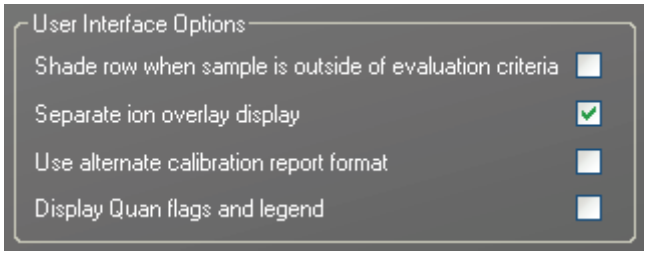


1. To report the calculated concentration at all times or only when the quantified value exceeds LOD, LOQ, or LOR, choose the appropriate value from the **Report concentration** list box.

   These limits are defined in "Quan Flags" on page 123.

2. To select the number of decimal places to report for calculated concentrations, set the value in the Decimal places to be reported box.
3. To include a chromatogram of the sample in the report, select the **Show chromatogram on Quantitation Report** check box.
4. To display only valid compounds, select the **Display valid compounds only** check box.

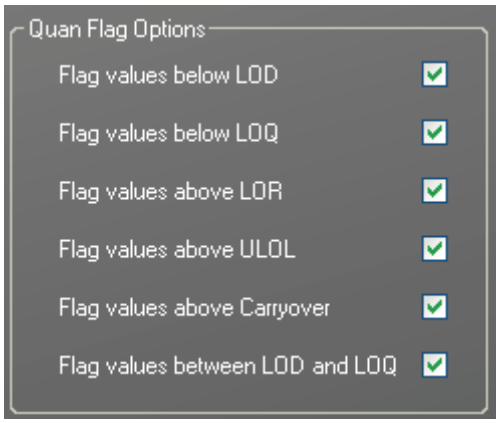
❖ To specify user interface options



1. To shade a compound row on any of the reports if a value fails one of the criteria used for evaluation, select the **Shade row when sample is outside of evaluation criteria** check box.

2. To separate the ion overlay pane from the confirming ion plots, select the **Separate ion overlay display** check box.
3. To use an alternate format for the Calibration Report designed to print more concisely and limit the report to a maximum of 7 calibration standards, select the **Use alternate calibration report format** check box.
4. To display flags and a legend on high density reports, select the **Display Quan flags and legend** check box.

❖ To specify quantitation flag options

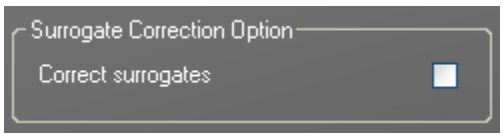


- Select the values you want to display in the report.

  Values are above or below the limits defined on the Quan page.

  These flags appear on a variety of reports and are defined in the Report options parameters table.

❖ To correct surrogates



- To apply the conversion factor (specified in the sample row in the batch) to the sample's calculated concentrations for surrogates as the conversion factor is applied to target compounds, select the **Correct surrogates** check box.

Report options

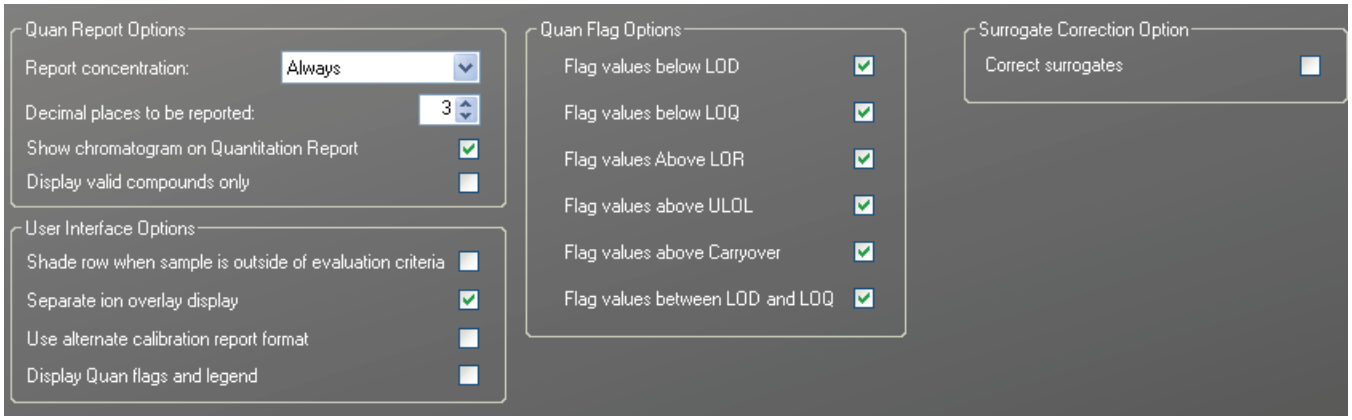


Table 31. Report options parameters (Sheet 1 of 2)

Parameter	Description
Quan Report Options	
Report concentration	Report the concentration at all times or only when the quantified value exceeds either the limit of detection (LOD), the limit of quantitation (LOQ), or the limit of reporting (LOR). Report concentration: Always, >LOD, >LOQ, or >LOR.
Decimal places to be reported	Number of decimal places to be included in the report. Maximum value is 6.
Show chromatogram on Quantitation Report	Displays a chromatogram (TIC trace) of the sample on the quantitation report.
Display valid compounds only	Prints only the positive compounds in a sample. If a compound is valid within a sample and is above the specified Quan Flag Options limits, the application reports the compound.
User Interface Options	
Shade row when sample is outside of evaluation criteria	Shades a compound row on any of the reports if a value fails one of the criteria used for evaluation.
Separate ion overlay display	Separates the ion overlay pane from the confirming ion plots in data review.
Use alternate calibration report format	Uses an alternate format for the Calibration Report that is designed to print more concisely (this report is limited to a maximum of 7 calibration standards).
Display Quan flags and legend	Displays manual flags, confirming manual flags, quan flags, and a legend on high density reports.
Quan Flag Options	Values that are above or below limits defined on the Quan flags page. These flags appear on a variety of reports.

Table 31. Report options parameters (Sheet 2 of 2)

Parameter	Description
Flag values below LOD	Flags values below the limit of detection (LOD).
Flag values below LOQ	Flags values below the limit of quantitation (LOQ).
Flag values above LOR	Flags values above the limit of reporting (LOR).
Flag values above ULOL	Flags values above the upper limit of linearity (ULOL).
Flag values above Carryover	Flags values above the carryover limit.
Flag values between LOD and LOQ	Flags values between the limit of detection and the limit of quantitation.
Surrogate Correction Option	
Correct surrogates	Applies the conversion factor (specified in the sample row in the batch) to the sample's calculated concentrations for surrogates as the conversion factor is applied to target compounds. For example, if you added surrogates to the sample as part of sample preparation and you require a dilution for analysis, the application dilutes the surrogates and target compounds and it can apply a dilution correction to correct for this dilution. However, if you added surrogates after a dilution has occurred, then you can leave the option cleared, so that while the target compounds are corrected for the dilution, the surrogates are reported 'as is.'

Using the Acquisition Mode

This chapter describes the tasks associated with the TraceFinder Acquisition mode.

Contents

When you plan to work with multiple samples or use similarly designed batches, use the Acquisition mode to reduce the amount of data you must enter.

Because the nature and types of batches are often similar (in some cases specified by laboratory standard practices), a user in the role of Lab Director or Supervisor can define a batch template that supplies the basic structure of a batch.

If you have a master method, you can create a batch and run the samples. Batches represent one or more samples that are to be acquired, processed, reviewed, and reported as a set. After you create a batch of samples, you can submit the batch and review the results in the Data Review mode or you can go directly to viewing and printing reports.

You can also set up a calibration batch with known concentrations of the target compounds to compare the sample against the calibration in future batches.

Working with Batches

This section includes instructions for the following tasks:

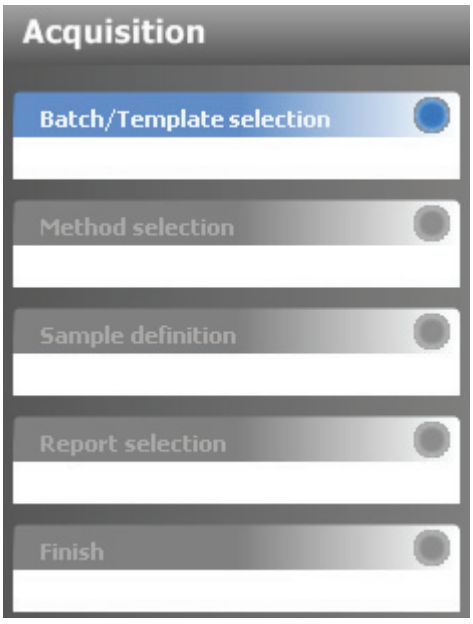
- Opening and Navigating the Acquisition Mode
- Creating Batches

Opening and Navigating the Acquisition Mode

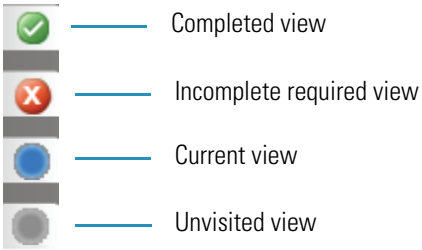
To open the Acquisition mode, click **Acquisition** in the navigation pane or from the dashboard.

The TraceFinder application does not use the navigation pane in the Acquisition mode in the same way it uses the navigation pane in other modes. In the Acquisition mode, this pane keeps track of your progress as you move through the views to create and submit a batch or a batch template.

Figure 2. Task pane when you enter Acquisition mode

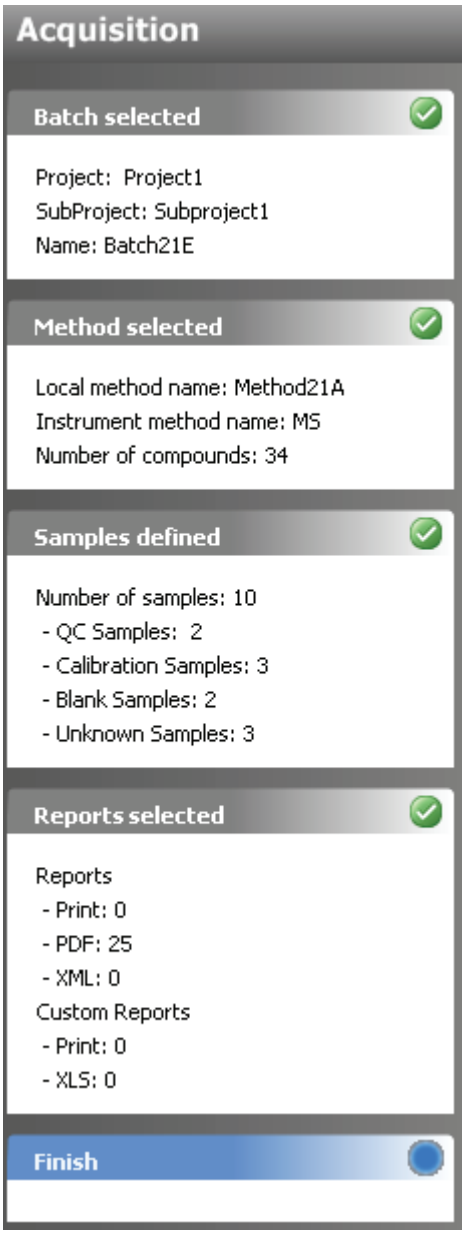


The status of each view in the Acquisition mode shows you which tasks are completed and which tasks are not.



As you complete each view, the task panes display the parameters you specified for your batch.

Figure 3. Example task pane when you have completed Acquisition mode



Creating Batches

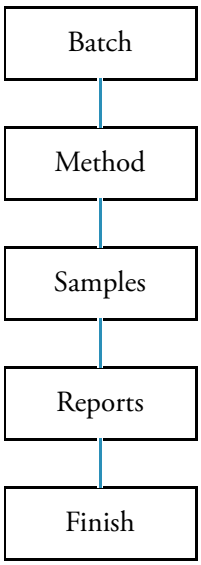
These are the major steps you use in Acquisition mode to create a batch:

- Selecting a Batch
- Selecting a Method
- Defining the Sample List
- Selecting and Reviewing Reports
- Submitting the Batch

Workflows

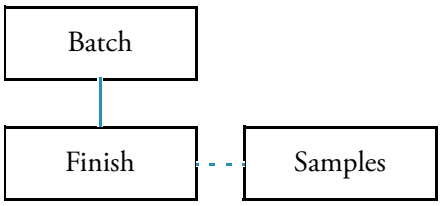
Depending on how you create your batch, you use different views in the Acquisition mode. The following workflows show the Acquisition views required for each batch creation approach. Depending on the approach you use to create a batch, you will use one of these specific workflows.

❖ **Creating an original batch**



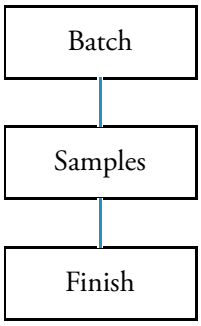
To create an original batch, start with the instructions "To start a new batch" on page 152.

❖ Acquiring a previously saved (.tbr) batch



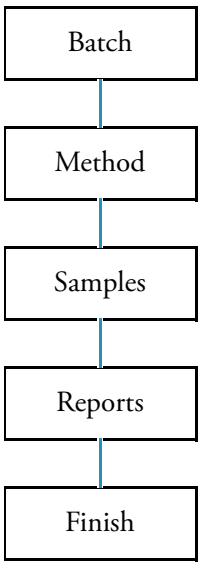
To acquire a previously saved batch, start with the instructions "To select a ready-to-acquire batch" on page 153.

❖ Editing and processing a previously acquired batch



To process a previously acquired batch, start with the instructions "To select a previously acquired batch" on page 154.

❖ Creating a batch template



This workflow is available only to users in the role of Lab Director or Supervisor.

To create batch template, start with the instructions "To create a batch template" on page 155.

Selecting a Batch

In Batch/Template Selection view of the Acquisition mode, you can choose to create a new batch in any of your current projects/subprojects.

Use the following procedures:

- To start a new batch
- To select a template for the new batch
- To select a ready-to-acquire batch
- To select a previously acquired batch
- To create a batch template

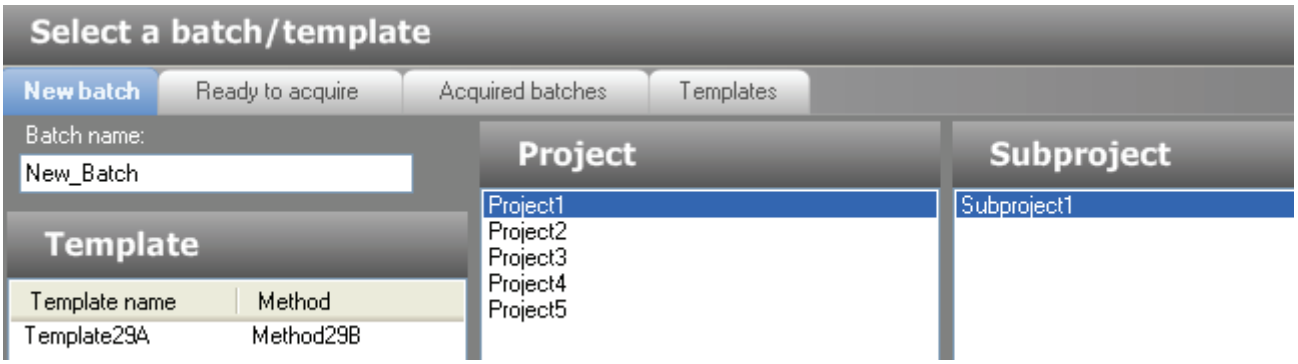
❖ To start a new batch

1. Click the **New batch** tab.

   From this page, you can create a new batch.

2. Type a name for the new batch in the Batch name box.

3. Select the project and subproject where you want to create the new batch.



4. To continue to the next view, click **Next**.

   The Method selection view of the Acquisition mode opens. See "Selecting a Method" on page 156.

> **Tip** If the Next button is not enabled, the batch name you gave already exists. Type a new name or add a numerical character to the end of the name. The Next button is enabled as soon as you change the batch name to a unique name.

❖ To select a template for the new batch

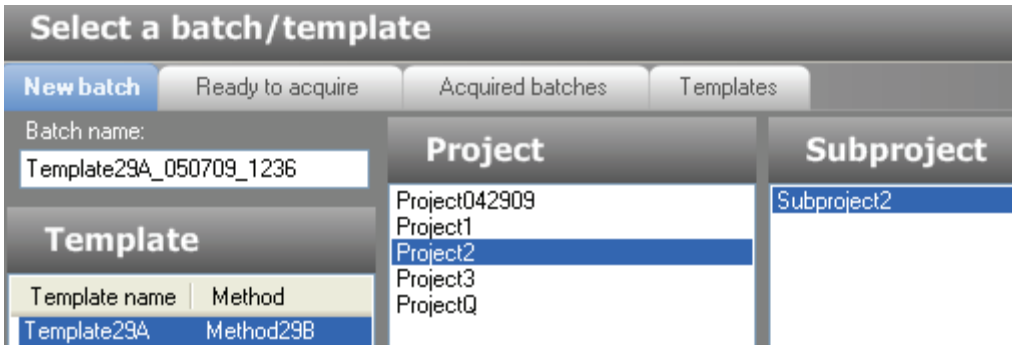
1. Click the **New batch** tab.

   From this page, you can create a new batch using a batch template.

2. Select the template and method combination you want to use.

   The system creates a Batch name with the selected template name and the date/time stamp. The default project and subproject associated with this template are selected, but you can change them.

3. (Optional) Select a different project and subproject where you want to create the new batch.



4. To continue to the next view, click **Next**.

   The Sample definition view of the Acquisition mode opens. See "Defining the Sample List" on page 157.

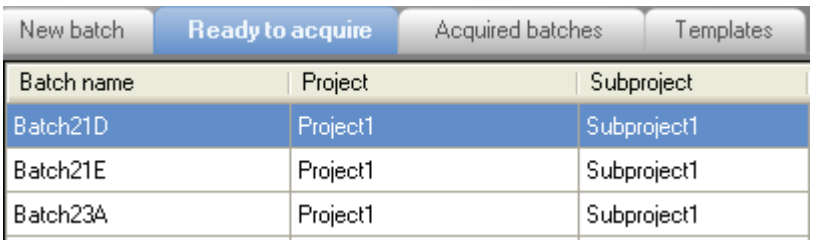
❖ To select a ready-to-acquire batch

1. Click the **Ready to acquire** tab.

   All your unacquired, saved batches are displayed with the file extension .tbr (to be run). All .tbr batches are stored in the following folder:

   `..\Tracefinder\Projects\`*`projectname`*`\`*`subprojectname`*`\Batches`

2. Select the batch you want to acquire.



3. To continue to the next view, click **Next**.

   The Finish view of the Acquisition mode opens. From the Finish view, you can save the batch, submit the batch for acquisition, or go to the Sample definition view to edit the samples list for this batch.

4. Do one of the following:

   - To prepare the batch for acquisition, click **Acquire**.

     For detailed instructions, see "Submitting the Batch" on page 168.

     –Or–

   - To edit the samples list, click **Previous**.

     For detailed instructions on editing a samples list, see "Defining the Sample List" on page 157.

     –Or–

   - To save the batch to the Ready to acquire list, click **Save**.

     The TraceFinder application saves your batch as a to-be-run (.tbr) file, closes the Acquisition mode, and returns you to the application dashboard.

     Batches are saved to the following folder with the file extension .tbr:

     `..\TraceFinder\Projects\`*`projectname`*`\`*`subprojectname`*`\Batches`

❖ To select a previously acquired batch

1. Click the **Acquired batches** tab.

   From this page, you can resubmit a previously acquired batch, edit the batch, or save it to be acquired later.

2. In the Project pane, select a project name.

   All subprojects included in the selected project are displayed in the Subproject pane.

3. In the Subproject pane, select a subproject name.

   All previously acquired batches included in the selected subproject are displayed in the Batch pane.

4. In the Batch pane, select the batch you want to reacquire.

5. To continue to the next view, click **Next**.

   The Sample definition view of the Acquisition mode opens. See "Defining the Sample List" on page 157.

❖ To create a batch template

1. Click the **Templates** tab.

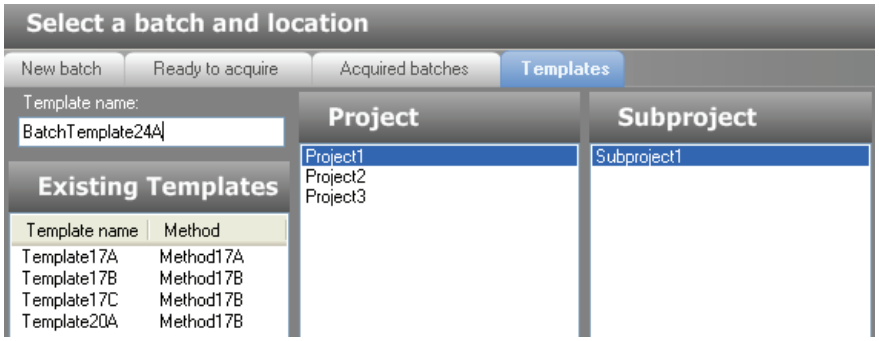
   From this page, you can create a new batch template.

   Note This page is available only to users in the role of Lab Director or Supervisor.

2. In the Template name box, type a name for your new batch template.
3. Select a project name in the Project pane.

   The Subproject pane displays all subprojects included in the selected project.

4. Select a subproject name in the Subproject pane.



5. To continue to the next view, click **Next**.

   The Method selection view of the Acquisition mode opens. See "Selecting a Method" on page 156.

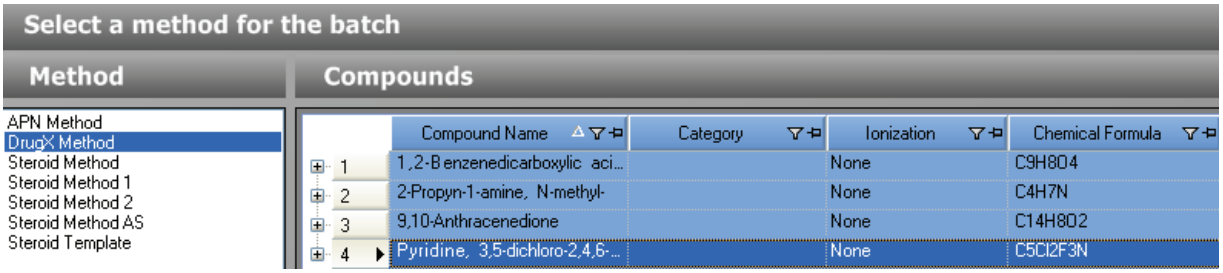
Selecting a Method

On the Method selection view of the Acquisition mode, select a method to use for the batch or batch template you are creating.

❖ To specify a method

1. Select a method from the Method list.

   The Compounds pane displays the compounds in the method. You cannot edit the compounds list from the Acquisition mode.



2. On the Method selection view, click **Next**.

   The Sample definition view opens. See "Defining the Sample List" on page 157.

Defining the Sample List

On the Sample definition view of the Acquisition mode, you can create a list of samples for the batch. You can add samples, insert samples, import a sample list, or remove samples from the list.

As you enter sample values, you can use the Copy down and Fill down commands to enter column values. For detailed instructions on using Copy down and Fill down to enter column values, see Appendix B, "Using Copy Down and Fill Down."

Use the following procedures:

- To add samples to the list
- To insert samples into the list
- To import samples into the list
- To remove samples from the list

When you have finished defining the list of samples, click **Next.**

- If you are creating a batch from scratch, creating a batch from a template, or editing a batch template, the Report selection view opens. See "Selecting and Reviewing Reports" on page 163.
- If you are editing a previously acquired a batch or a .tbr batch, the Finish selection view opens. See "Submitting the Batch" on page 168.

❖ To add samples to the list

1. Select the number of sample rows to add and click **Add**.

> **Tip** To add a single sample row, you can use the **Add** button or you can right-click and choose **Add sample** from the shortcut menu.

2. Type a file name in the Filename column for each sample.
3. Select a sample type from the Sample type list box for each sample.

Available sample types			
LC and GC			
Matrix Blank	Chk Std	MS	Unknown
Cal Std	MDL	MSD	Solvent
GC only			
LCS	LCSD	Meth Val	Breakdown

For a detailed description of sample types, see "Sample Types" on page 179.

4. For each Cal Std or Chk Std sample, select a level from the Sample level list.

   The sample levels are defined in the master method. If there are no levels to select from the Sample level list, ask a user with Supervisor or Lab Director permissions to edit the method and specify the levels.

   For detailed instructions about defining sample levels, see Chapter 4, "Using the Method Development Mode."

5. Type a vial position in the Vial position column for each sample.

   Tip Use the Fill down command to make entering vial positions easier.

6. Type a volume in the Injection volume column for each sample.

7. (Optional) Type or edit the values for the remaining columns.

   Note When you use the horizontal scroll bar at the bottom of the samples list, the Status and Filename columns stay fixed while the other columns scroll right and left.

❖ To insert samples into the list

1. Select the sample above which you want to insert new, unknown samples.

   You cannot use the Insert command to create the first sample row.

2. Select the number of samples to insert and click **Insert**.

   The application inserts the unknown samples above the selected sample.

Inserted samples

Samples

	Status	Filename	Sample type	Sample level	Sample ID
1		cal_std_5	Cal Std	10	cal std = 5 ng/uL
2			Unknown		
3			Unknown		
4		cal_std_10	Cal Std	10	cal std = 10 ng/uL

3. Type a file name in the Filename column for each sample.

4. Select a sample type from the Sample type list box for each sample.

Available sample types			
LC and GC			
Matrix Blank	Chk Std	MS	Unknown
Cal Std	MDL	MSD	Solvent
GC only			
LCS	LCSD	Meth Val	Breakdown

For a detailed description of sample types, see "Sample Types" on page 179.

5. For each Cal Std or Chk Std sample, select a level from the Sample level list.

   The sample levels are defined in the master method. If there are no levels to select from the Sample level list, ask a user with Supervisor or Lab Director permissions to edit the method and specify the levels.

   For detailed instructions about defining sample levels, see Chapter 4, "Using the Method Development Mode."

6. Type a vial position in the Vial position column for each sample.

   Tip Use the Fill down command to make entering vial positions easier.

7. Type a volume in the Injection volume column for each sample.

8. (Optional) Type or edit the values for the remaining columns.

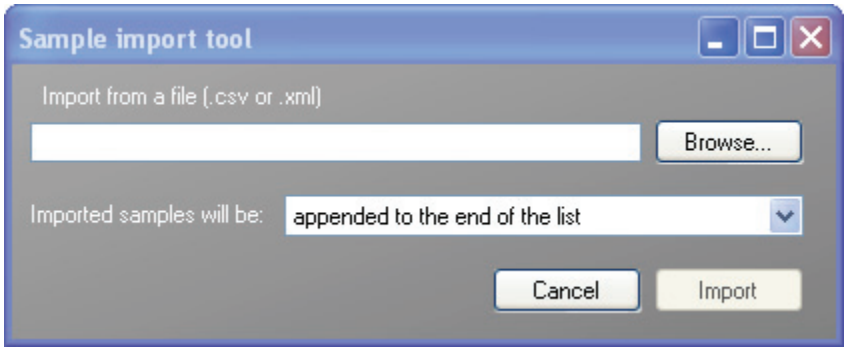
   Note When you use the horizontal scroll bar at the bottom of the samples list, the Status and Filename columns stay fixed while the other columns scroll right and left.

❖ To import samples into the list

1. Click **Import**.

   The Sample import tool dialog box opens.

   From this dialog box, you can import a sample list from a .csv file or .xml file.

2. Click **Browse** and select a .csv or .xml file that contains the sample definitions you want to import.

   Note The .csv or .xml file format must match the TraceFinder file format.

3. From the Imported samples will be list, select either **appended to the end of the list** or **inserted at the selected row**.

4. Click **Import**.

   The Sample import tool dialog box closes, and the specified samples are added to the Samples list.

5. For each Cal Std or Chk Std sample, select a level from the Sample level list.

   The sample levels are defined in the master method. If there are no levels to select from the Sample level list, ask a user with Supervisor or Lab Director permissions to edit the method and specify the levels.

   For detailed instructions on defining sample levels, see Chapter 4, "Using the Method Development Mode."

6. Type a vial position in the Vial position column for each sample.

   Tip Use the Fill down command to make entering vial positions easier.

7. Type a volume in the Injection volume column for each sample.

8. (Optional) Enter or edit the values for the remaining columns.

   Note When you use the horizontal scroll bar at the bottom of the samples list, the Status and Filename columns stay fixed while the other columns scroll right and left.

❖ To remove samples from the list

1. Select the samples you want to remove.

   Tip Use the CTRL or SHIFT keys to select multiple samples.

2. Right-click and choose **Remove selected samples** from the shortcut menu.

Sample definition view

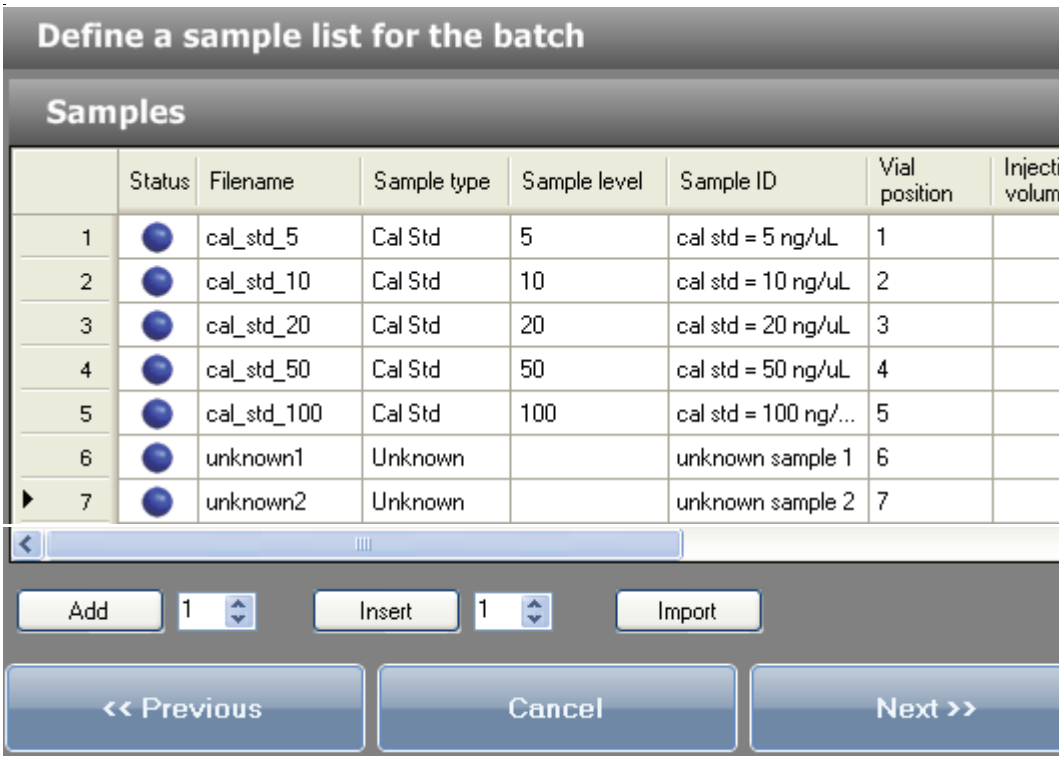


Table 32. Sample definition view parameters (Sheet 1 of 2)

Parameter	Definition
Add	Adds the specified number of empty rows to the sample grid.
Insert	Inserts the specified number of empty rows above the selected row.
Import	Opens the Sample import tool where you can import samples defined in a .csv file or an .xml file.
Previous	Returns you to the previous Acquisition mode view.
Cancel	Confirms that you want to exit the Acquisition mode. When you cancel out of the Acquisition mode, your edits are not saved.
Next	Takes you to the next Acquisition mode view.
Shortcut menu	
Add sample	Adds a single empty row to the sample grid.
Insert sample	Inserts a single empty row to the sample grid above the selected row.
Insert copy sample	Copies the currently selected row and inserts a copy above the row.
Remove selected samples	Removes selected samples from the sample grid.

Table 32. Sample definition view parameters (Sheet 2 of 2)

Parameter	Definition
Copy down	Copies the value in the selected row to all rows below it. For detailed instructions about using the Copy down command, see Appendix B, "Using Copy Down and Fill Down."
Fill down	Enters sequential values in the column starting with the value in the selected row and ending with the last row in the column. For detailed instructions about using the Fill down command, see Appendix B, "Using Copy Down and Fill Down."
Status color codes	 Sample is acquired but not processed.  Sample is acquired and processed.  Sample is not acquired.

Selecting and Reviewing Reports

On the Report selection view, you can specify the types of reports you want to create. For a complete list of report types and examples of output files, see Appendix A, "Reports."

For each standard report you generate, you can create a hardcopy printout, a PDF (.pdf) file, or an XML (.xml) file. In addition to the report type, you can specify a report title for each of your reports.

For each custom report you generate, you can create a hardcopy printout or an XLS (.xlsm) file. You cannot specify a report title for a custom report.

When you have finished specifying your report options, click **Next**. to go to the Finish view. See "Submitting the Batch" on page 168.

The resulting output files for your reports are written to the following folder:

`..\projectname\subprojectname\Batches\batchname\Reports`

Use the following procedures:

- To edit a standard report title
- To preview a standard report
- To specify a standard report in print, PDF, or XML format
- To specify a custom report in print or XLS format
- To export standard or custom reports to a specific folder

❖ To edit a standard report title

1. Click the **Reports** tab.

   The Reports page lists all the available standard reports. The Reports page displays the report name, report title, and the options to create printed, PDF, or XML output. See "Standard Reports page" on page 166.

2. Click the Report Title column and edit the default title.

   The default report title is the same as the report name. The TraceFinder application lists reports in alphabetical order by Report Title. When you change a report title and refresh the view, it rearranges the reports accordingly.

❖ To preview a standard report

1. Click the **Reports** tab.

   The Reports page lists all the available standard reports. The Reports page displays the report name, report title, and the options to create printed, PDF, or XML output. See "Standard Reports page" on page 166.

2. Click the magnifying icon, , to view an example of the report type as a PDF file.

   The right pane of the view displays an example PDF report with typical PDF viewer controls.

3. To minimize the PDF viewer, click the minimize icon, .

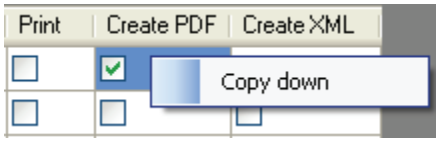
❖ To specify a standard report in print, PDF, or XML format

1. Click the **Reports** tab.

   The Reports page lists all the available standard reports. The Reports page displays the report name, report title, and the options to create printed, PDF, or XML output. See "Standard Reports page" on page 166.

2. For each type of report you want to create, select the check box in the Print, Create PDF, or Create XML columns.

3. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.



   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell.

❖ To specify a custom report in print or XLS format

1. Click the **Custom Reports** tab.

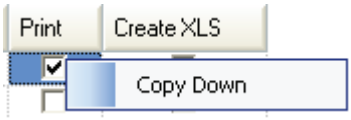
   The Custom Reports page lists all the reports that are saved in the following folder:

   `..\Thermo\TraceFinder\Templates\Reports`

   The Custom Reports page displays the Report Name and the options to create printed or XLS output. See "Custom Reports page" on page 167.

2. For each report you want to create, select the check box in the Print or Create XLS columns.

3. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.



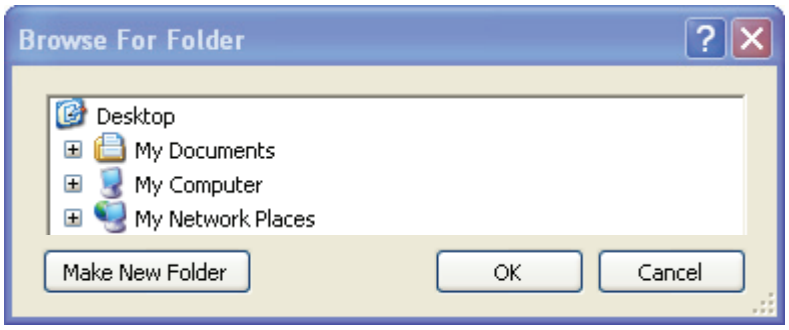
   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell.

❖ To export standard or custom reports to a specific folder

1. Select the **Export Results** check box at the bottom of the view.

   The Browse For Folder dialog box opens.

2. Locate and select the folder where you want to save the reports.
3. To create a new reports folder within the selected folder, click **Make New Folder** and type the new folder name.
4. Click **OK**.

   All standard and custom reports are written to the specified folder in addition to the batch Reports folder.

Standard Reports page

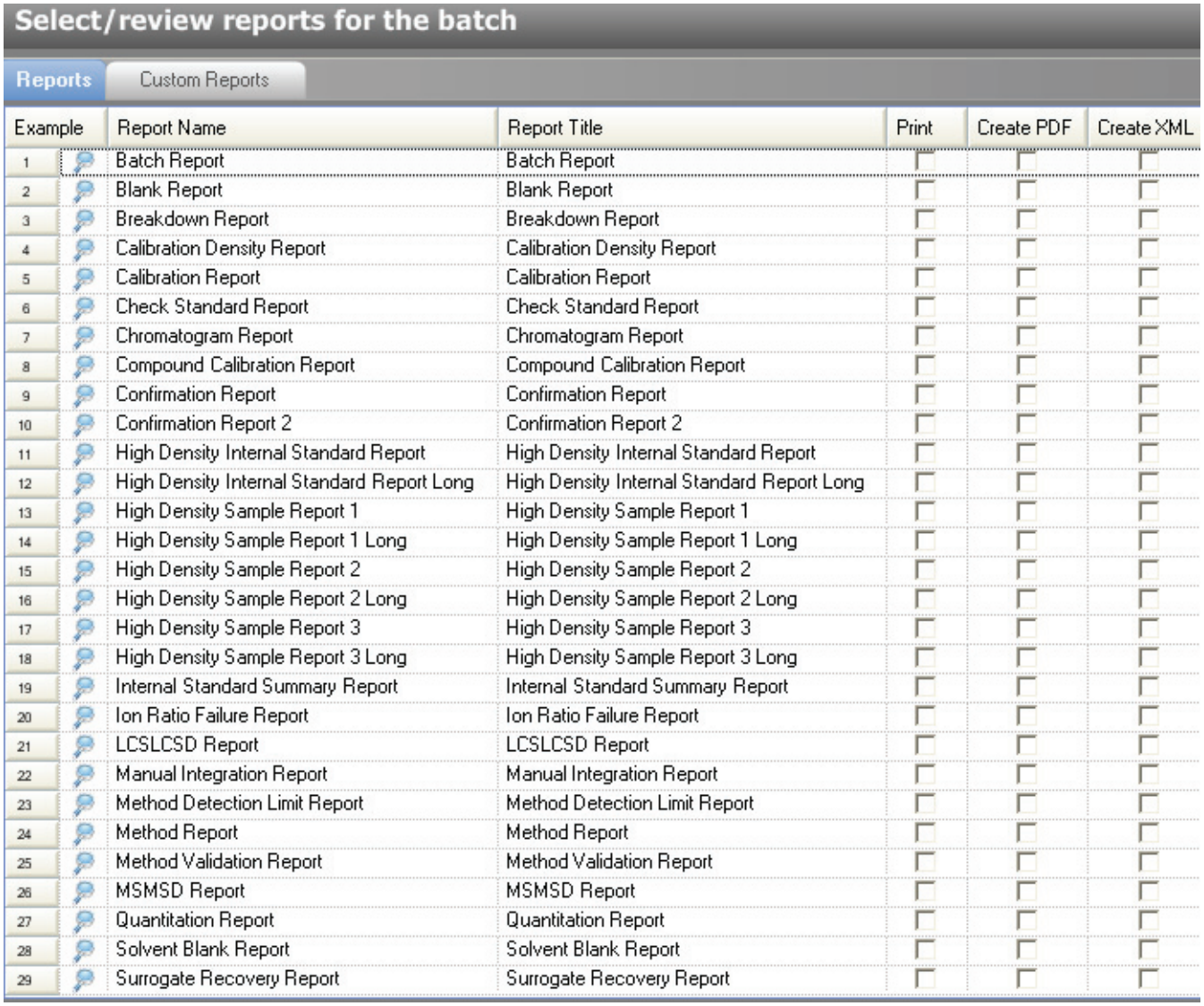


Table 33. Standard reports parameters (Sheet 1 of 2)

Parameter	Description
Example	Displays an example PDF for the report type. This example provides a model of the report type only; it does not reflect your data.
Report Name	The name of a report.
Report Title	User-editable title to be used on a report.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files.

Table 33. Standard reports parameters (Sheet 2 of 2)

Parameter	Description
Create XML	Reports to be exported in XML format.
Shortcut menu: Copy Down	Copies the selected or cleared state to all subsequent reports in the column.

Custom Reports page

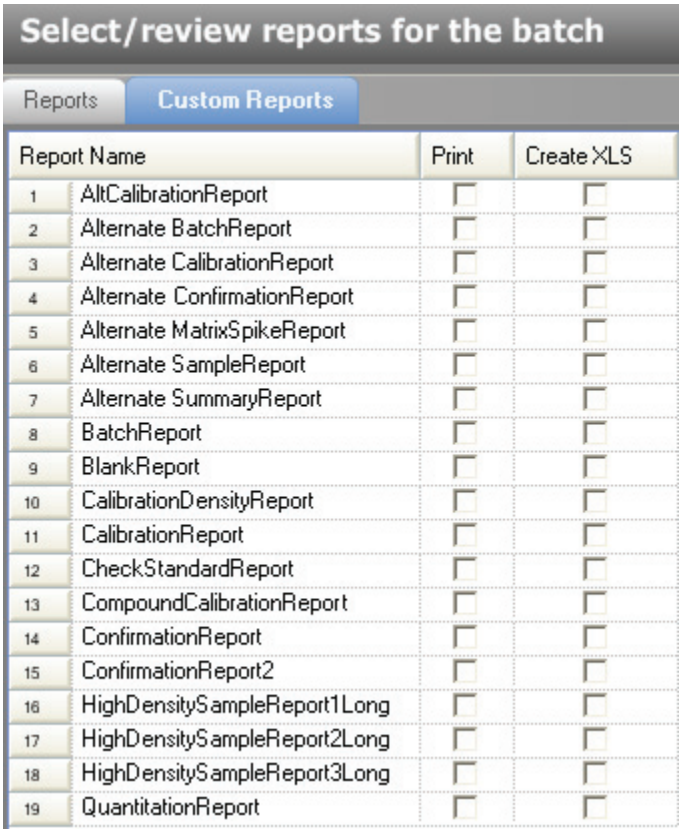


Table 34. Custom Reports parameters

Parameter	Description
Report Name	The name of a report.
Print	Reports to be sent to the printer.
Create XLS	Reports to be exported in Excel Macro-Enabled Workbook file (.xlsm) format.
Shortcut menu: Copy Down	Copies the selected or cleared state to all subsequent reports in the column.

Submitting the Batch

On the Finish view of the Acquisition mode, you can specify a startup method, a shutdown method, or a calibration batch. You can save the batch to be acquired later or you can choose to acquire data, process data, or create reports. See "Finish view" on page 174.

Note If you are working with a batch template, the only available function is Save.

Use the following procedures:

- To specify startup or shutdown methods
- To specify a calibration batch
- To specify device states
- To save a batch for later acquisition
- To start an acquisition
- To view the output files

❖ To specify startup or shutdown methods

1. (Optional) Select a method from the System Startup Method list.

   The TraceFinder application runs this method before running the batch. No autosampler injection takes place. This feature is not available for all instruments.

2. (Optional) Select a method from the System Shutdown Method list.

   The TraceFinder application runs this method after running the batch. No autosampler injection takes place. This feature is not available for all instruments.

❖ To specify a calibration batch

1. In the Calibration area, select a calibration (.calx) file from the list.

2. Do one of the following:

   - To use the selected calibration file to process the current data, select the **Use calibration** option.

     The method must be the same for the calibration batch and the current batch.

     –Or–

   - To add calibration data from the current batch to the selected calibration file, select the **Extend calibration** option.

❖ To specify device states

- In the System Status area, select the name of the device, right-click, and then choose a device state from the shortcut menu.

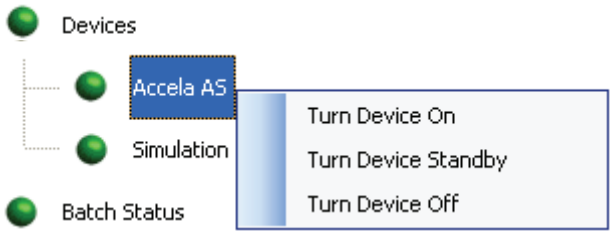


Table 35. Instrument states

Instrument state	Description
Turn Device On	Keeps the system in the On state when the current run is completed, so you can begin another run without waiting. All power and flows are maintained at operational levels. Default: On
Turn Device Standby	Keeps the system in the Standby state when the current run is completed, so you can begin another run with only a short delay between runs. Some devices do not have a Standby feature. For devices with this feature, the device enters a power-saving or consumable-saving mode, and you can switch the device back on in approximately 15 minutes. Depending on the instrument, this state turns gas and liquid flows off but maintains heaters and other subsystems in an On state so that there is no warm-up time required when you change from Standby to On.
Turn Device Off	Keeps the system in the Off state when the current run is completed. The Off state indicates that all power to the instrument, which can be controlled by the TraceFinder application, is turned off. This includes power to all heaters and subassemblies, but in some cases not all subassemblies. Some devices do not have an Off feature. For devices that do have this feature, the device enters a power-saving or consumable-saving mode, and you can switch the device back on. When several runs are queued, the application uses the system power scheme of the last submitted run.

❖ To save a batch for later acquisition

- From the Finish view, click **Save**.

  The TraceFinder application saves your batch as a to-be-run (.tbr) file, closes the Acquisition mode, and returns you to the application dashboard.

❖ To start an acquisition

1. Click **Acquire**.

   The Submit Options dialog box opens. See "Submit Options" on page 172.

2. Select the tasks you want to perform: acquire data, process data, or create reports.
3. Select the **Use** check box for the device that you want to use for this acquisition.
4. (Optional) Select the **Start Device** check box to indicate the device that is used to initiate the communication with the other instruments.

   This is usually the autosampler.

5. (Optional) Select the **Start when ready** check box to tell the application to start all instruments together when they are all ready.

   When this is cleared, individual instruments can start at different times and then have to wait for the last instrument to be ready.

6. (Optional) Select the **Priority** check box to move this batch to the top of the queue (after any currently acquiring batch).
7. (Optional) Click **Cancel** to exit the Acquisition mode without performing any tasks.
8. To start the selected processes, click **OK**.

   The selected processes begin, and the TraceFinder application returns you to the dashboard and shows the real-time display at the bottom of the dashboard.

   The real-time display is visible from the dashboard and all modes. You can begin another batch in the Acquisition mode while you watch the real-time display of the currently acquiring batch.

Figure 4. Submit Options

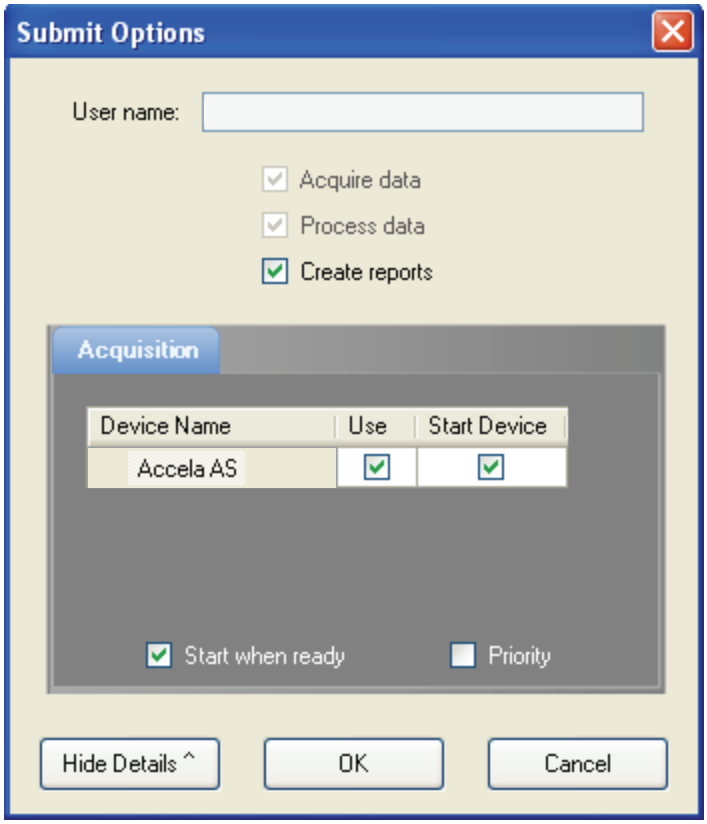


Table 36. Submit Options parameters (Sheet 1 of 2)

Parameter	Description
User name	Name of the current user.
Acquire data	Submits the current batch to acquisition.
Process data	Processes the data for the current batch.
Create reports	Creates reports for the current batch.
Acquisition pane	
Device Name	Lists all configured instruments. If the instrument you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the TraceFinder application. You cannot configure an instrument while the TraceFinder application is running.
Use	Specifies the instruments used for this acquisition.
Start Device	Specifies the instrument that is used to initiate the communication with the other instruments. This is usually the autosampler.

Table 36. Submit Options parameters (Sheet 2 of 2)

Parameter	Description
Start when ready	Tells the TraceFinder application to start the specified device when all the instruments are ready to acquire data. When this is cleared, individual instruments can start at different times and then have to wait for the last instrument to be ready.
Priority	When there are batches in the queue, moves this batch to the top of the queue, after the currently acquiring batch.
Hide/Show Details	Collapses or expands the acquisition details of the Submit Options dialog box.
OK	Begins the selected processes.
Cancel	Closes the Submit Options dialog box without submitting any tasks.

❖ To view the output files

- The TraceFinder application writes saved batches to the Batches folder with the file extension .tbr (to be run):

  `..\TraceFinder\Projects\`*`projectname`*`\`*`subprojectname`*`\Batches`

- For each acquired sample, the application writes an RSX file to the Data folder:

  `..\`*`projectname`*`\`*`subprojectname`*`\Batches\`*`batchname`*`\Data`

- The application saves method information to the Methods folder:

  `..\`*`projectname`*`\`*`subprojectname`*`\Batches\`*`batchname`*`\Methods\`*`methodname`*

- The application writes the reports to the Reports folder:

  `..\`*`projectname`*`\`*`subprojectname`*`\Batches\`*`batchname`*`\Reports`

Finish view

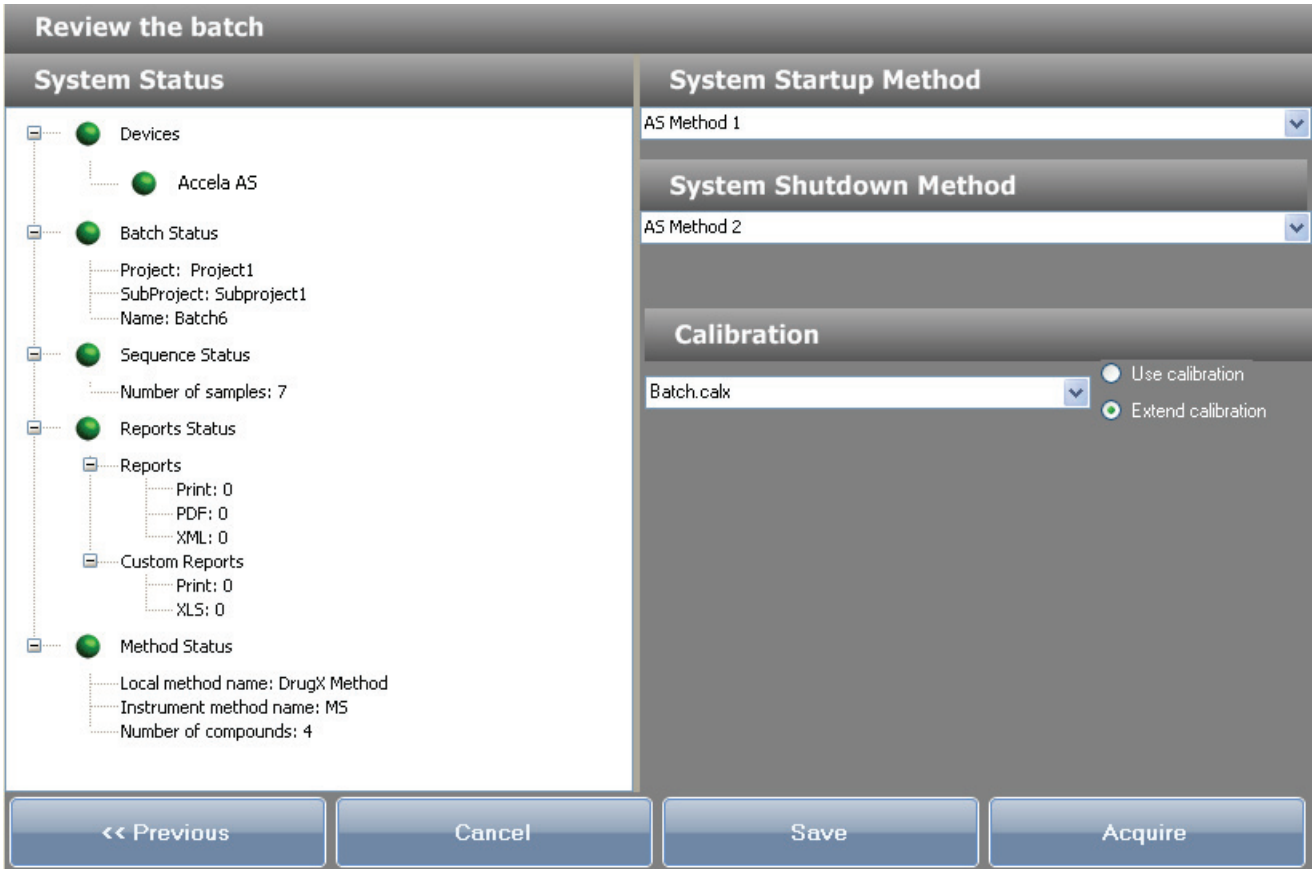


Table 37. Finish view parameters (Sheet 1 of 2)

Parameter	Description
System Status	The System Status pane displays the following: • The devices used for the acquisition • The project, subproject, and name of the batch • The number of samples in the batch • The number of standard and custom reports to be printed and saved as PDF, XML, or XLS files • The local method and instrument method used for the batch • The number of compounds in the method
System Startup Method	The instrument method that runs before the batch. No autosampler injection takes place. This feature is not available for all instruments.
System Shutdown Method	The instrument method that runs after the batch. No autosampler injection takes place. This feature is not available for all instruments.

Table 37. Finish view parameters (Sheet 2 of 2)

Parameter	Description
Calibration	• Use calibration: Uses the selected calibration file to process the current data. • Extend calibration: Adds calibration data from the current batch to the selected calibration file.
Save	Saves the current batch as a to-be-run (.tbr) file.
Acquire	Opens the Submit Options dialog box where you can specify options for acquisition, processing, and generating reports.

Real-time Display

You can access the real-time display from the dashboard and from any mode in the TraceFinder application.

❖ **To access the real-time display from the dashboard**

- Click **Real Time Status**.

The real-time status displays at the bottom of the dashboard.

❖ **To access the real-time display from all modes**

- Click **Real time status**.

The real-time status displays at the bottom of the current view.

The real-time status display has four additional pages of information:

- Acquisition page
- Instrument page
- Devices page
- Queues page

Figure 5. Acquisition page

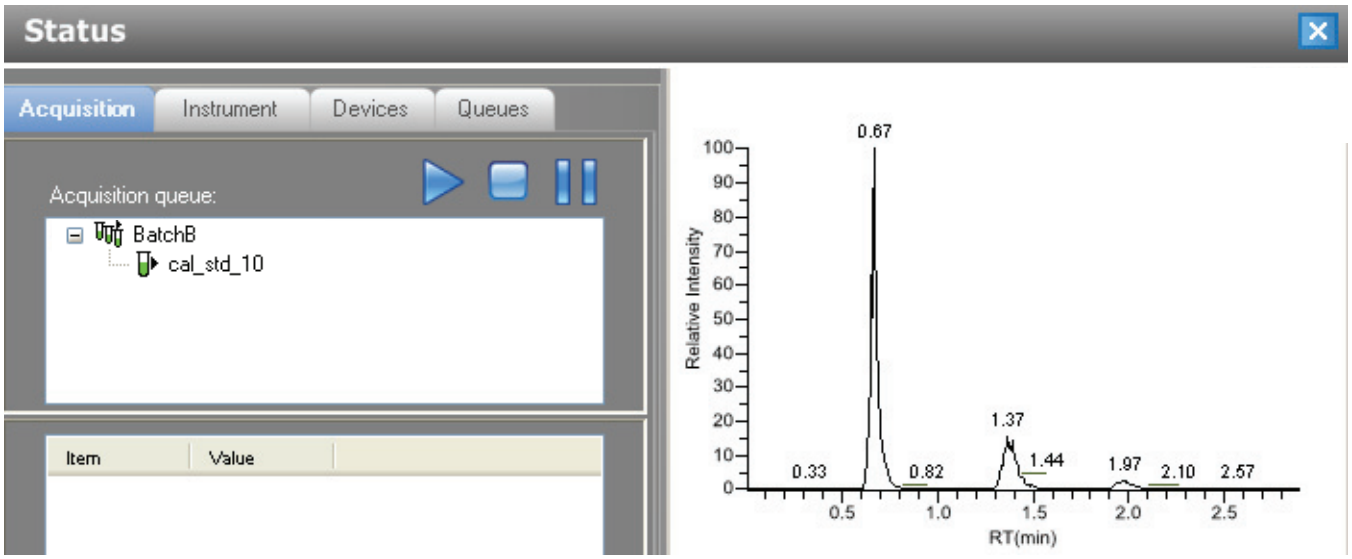


Figure 6. Instrument page

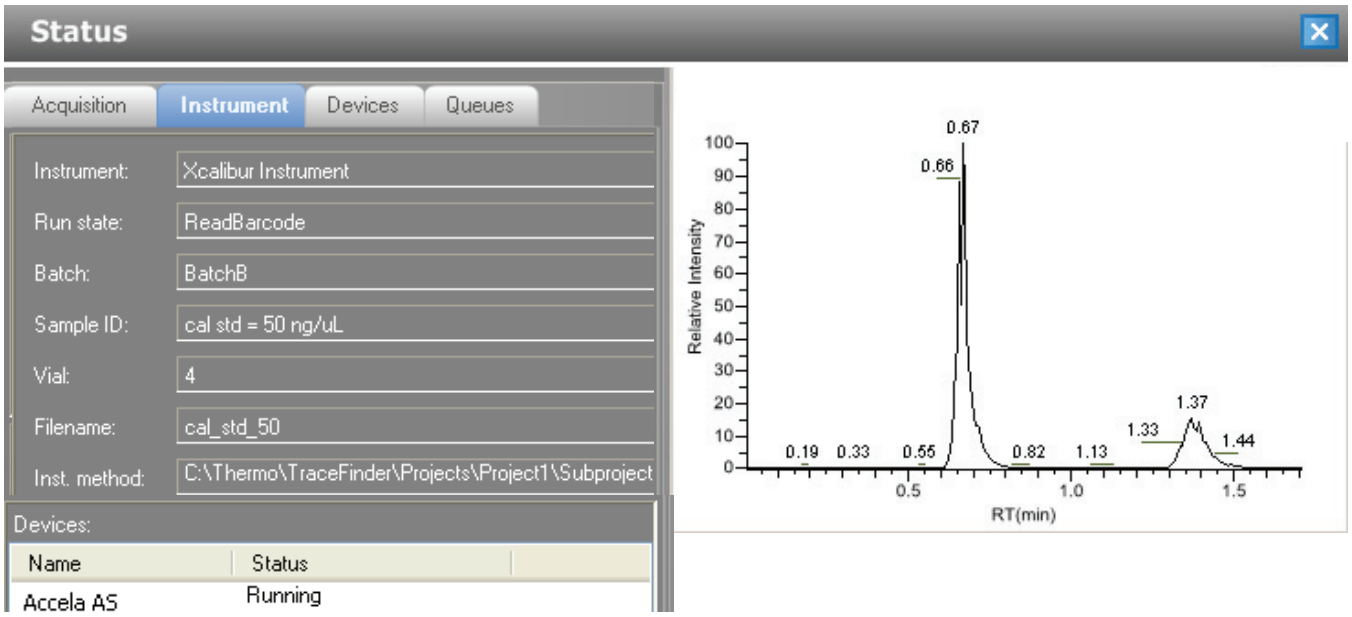


Figure 7. Devices page

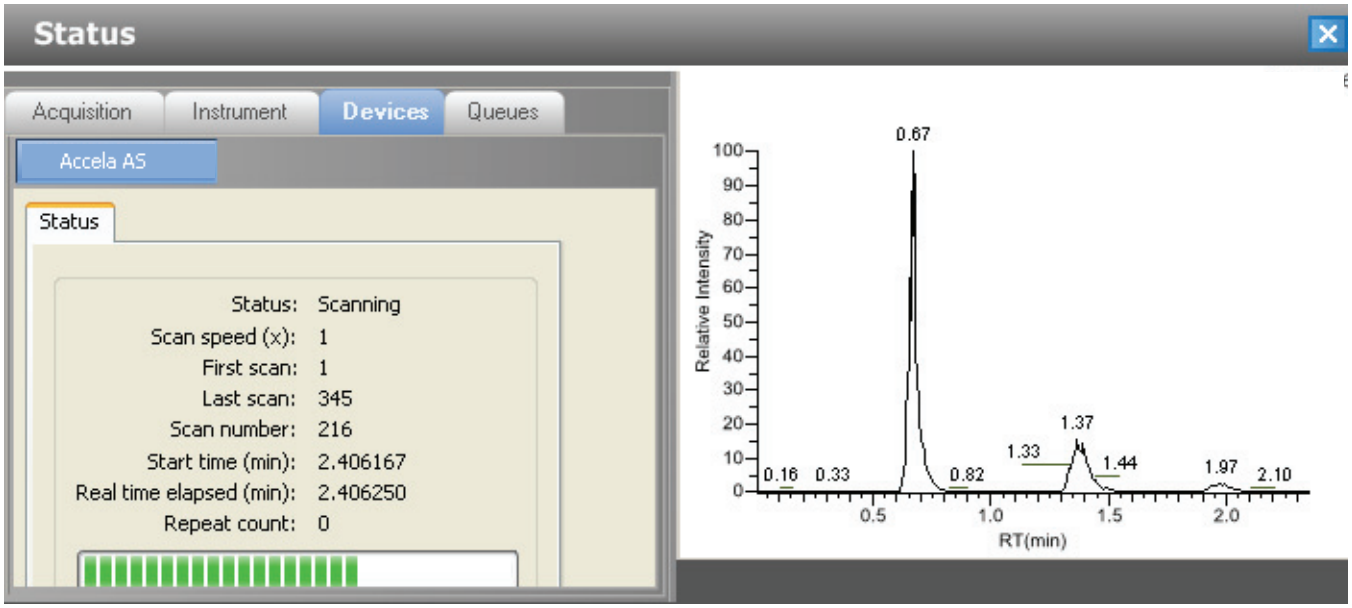
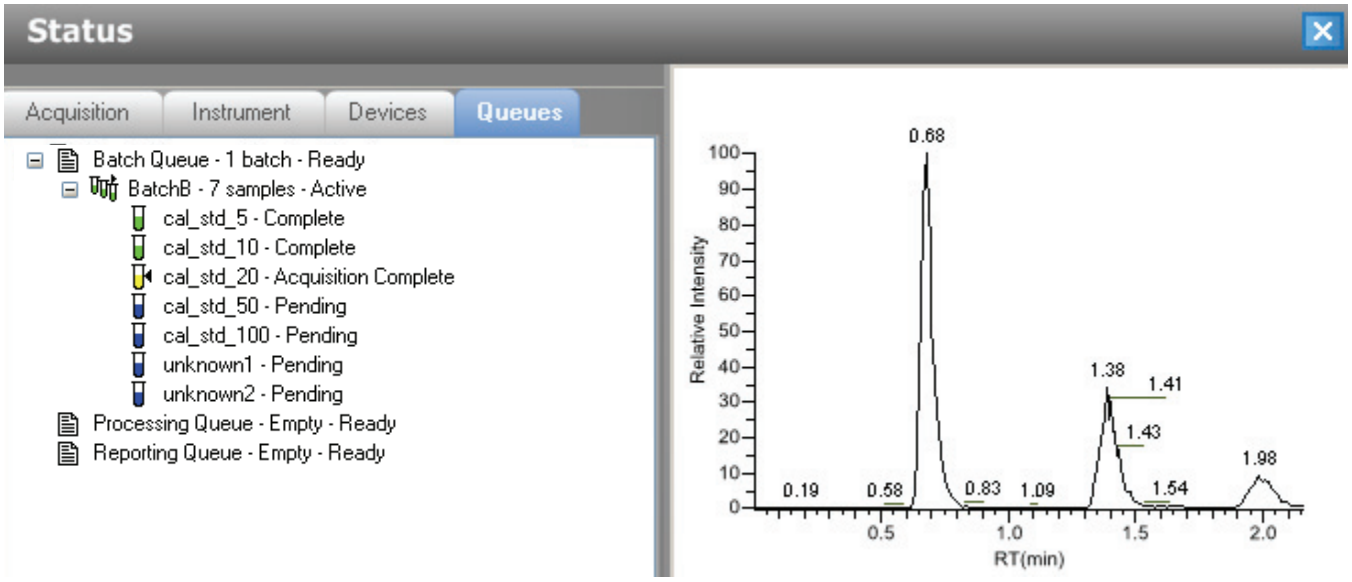


Figure 8. Queues page



Sample Types

The TraceFinder application uses the following sample types in all sample definitions and reports.

To view example standard reports specific to a sample type, see Appendix A, "Reports."

Table 38. Sample type definitions

Sample type	Definition
Matrix Blank	Contains no target compounds but might contain an ISTD when you use the internal standard quantitative analysis technique. By analyzing a blank sample, you can confirm that there are no residual compounds in the solvent system that can cause erroneous results.
Cal Std	(Calibration standard) Contains known amounts of all target compounds. The purpose of a standard is to measure the response of the instrument to the target compounds so that the processing software can generate a calibration curve for each compound.
Chk Std	(Check standard) Contains a known amount of one or more specific target compounds. The application places check standard samples in the sequence so that it can test quantitative analysis results for quality assurance purposes. After the application analyzes the check standard sample, it compares the measured quantity with the expected value and an acceptability range. The quantitative analysis of a check standard sample is classified as *passed* if the difference between the observed and expected quantities is within the user-defined tolerance. A check standard sample is classified as *failed* if the difference between the observed and expected quantities is outside the user-defined tolerance.
LCS (GC only)	Lab control sample.
LCSD (GC only)	Lab control sample duplicate.
MDL	Method detection limits sample.
Meth Val (GC only)	Method validation sample.
MS	Matrix spike sample.
MSD	Matrix spike duplicate sample.
Breakdown (GC only)	Used in gas chromatography for breakdown methods.
Solvent	Contains only solvent.

Using the Data Review Mode

This chapter includes instructions for using the features of the Data Review mode.

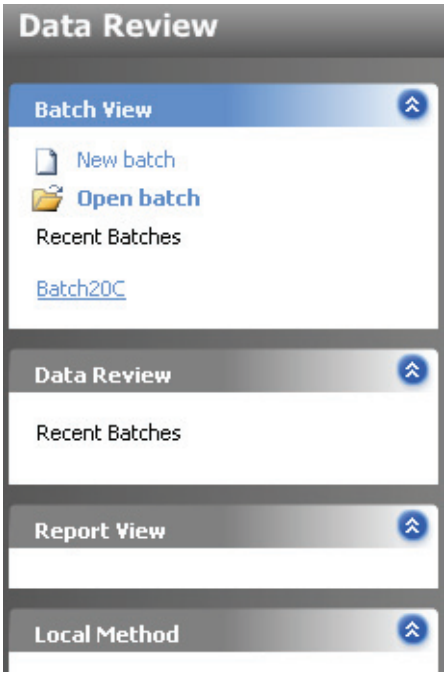
Contents

In the Data Review mode, you can review batches, batch data, reports, and local methods.

❖ To access the Data Review mode

- Click **Data Review** from the dashboard or the navigation pane.

The Data Review navigation pane opens.



Working in Batch View

In the Batch view, you can manually create and edit a new batch or open and edit a previously saved batch. When you submit a batch, you can acquire, process, or create reports for the submitted samples.

This section contains information about the following:

- Creating a New Batch
- Editing a Batch
- Submitting a Batch

Creating a New Batch

In Batch view, you can create a new batch.

Use the following procedures:

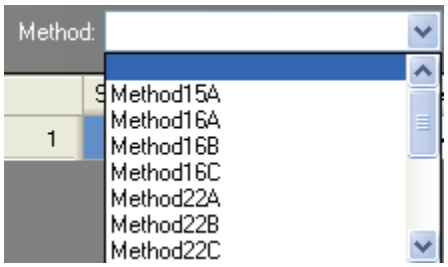
- To create a batch
- To add samples to the list
- To insert samples into the list
- To import samples into the list
- To copy a sample
- To re-inject a sample
- To edit sample values
- To rearrange the columns
- To remove samples from the list

❖ To create a batch

1. Choose **New batch** in the Batch View task pane or choose **File > New > Batch**.

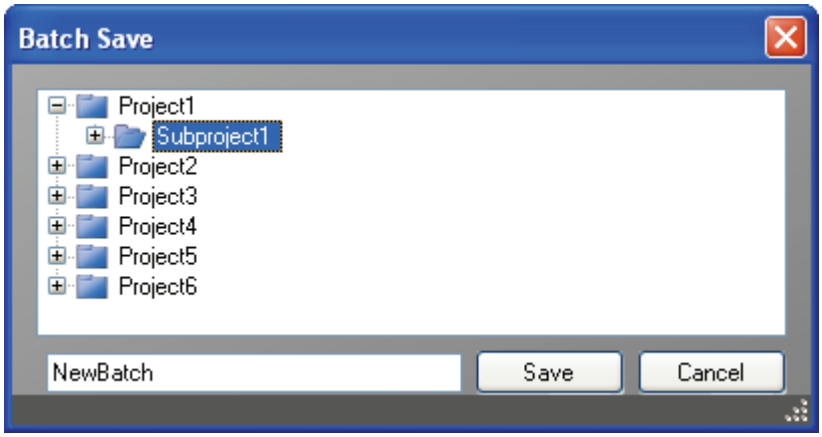
   A new, unnamed batch opens with one Unknown sample. You must choose a master method before you can save your new batch.

2. Choose a master method from the Method list.



3. Choose **File > Save > Batch**.

   The Batch Save dialog box opens.



4. Select a project and a subproject and enter a name for your new batch.

   Tip To enable the Save button, you must select a subproject and enter a unique batch name. If the Save button is not enabled, either you have entered a name that is already used or you have not selected a subproject.

5. Click **Save**.

❖ To add samples to the list

- Right-click the sample list pane and choose **Add sample** from the shortcut menu, or use the **Add Sample** icon to add multiple sample rows.

The application adds the specified number of new, empty samples to the end of the sample list.

❖ To insert samples into the list

1. Select the sample above which you want to insert empty samples.
2. Right-click the sample list pane and choose **Insert sample** from the shortcut menu, or use the Insert Sample icon to insert multiple sample rows.

The new, unknown samples are inserted above the selected sample.

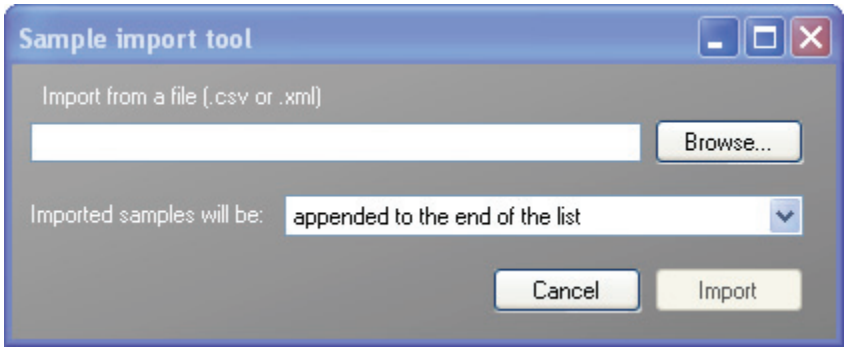
Samples

	Status	Filename	Sample type	Sample level	Sample ID
1		cal_std_5	Cal Std	10	cal std = 5 ng/uL
2			Unknown		
3			Unknown		
4		cal_std_10	Cal Std	10	cal std = 10 ng/uL
5		cal_std_20	Cal Std	15	cal std = 20 ng/uL

❖ To import samples into the list

1. Click **Import**.

The Sample import tool dialog box opens.



From this dialog box, you can import samples from a .csv file or .xml file.

2. Click **Browse** and select a .csv or .xml file that contains the samples you want to import.
3. From the Imported samples will be list, select **appended to the end of the list** or **inserted at the selected row**.
4. Click **Import**.

The Sample import tool dialog box closes and the application adds the specified samples to the Samples list.

❖ To copy a sample

1. Select the sample you want to copy.
2. Right-click and choose **Insert copy sample** from the shortcut menu.

   TraceFinder inserts the copy above the selected sample.

❖ To re-inject a sample

1. In the sample list, select the sample you want to re-inject.
2. Right-click and choose **Reinject this sample** from the shortcut menu.

   The TraceFinder application creates a copy of the selected sample and appends INJ001 to the file name. Additional re-injections of the same sample are numbered INJ002, INJ003, and so forth.

   The TraceFinder application copies all parameter values from the original sample.

❖ To edit sample values

1. For each sample, double-click the Filename column (or right-click and choose **Browse in raw file** from the shortcut menu) and locate the raw data file to use for the sample.
2. For each added sample, click the Sample type column and select a sample type from the list.

Available sample types			
LC and GC			
Matrix Blank	Chk Std	MS	Unknown
Cal Std	MDL	MSD	Solvent
GC only			
LCS	LCSD	Meth Val	Breakdown

3. For each Cal Std or Chk Std sample, click in the Sample level cell and select a level from the list.

   The sample levels were defined in the master method. If there is nothing to select in the Sample level list, do the following:

   a. Return to the Method Development mode.
   b. Open the method.
   c. Click the **Calibration levels** tab.
   d. Add the levels.
   e. Save the method.
   f. Return to the Data Review mode, and begin this batch again.

   You must close your original batch without saving and start a new batch. For detailed instructions, see Chapter 4, “Using the Method Development Mode.”

4. Enter or edit the values for the remaining columns.

   When you use the scroll bar at the bottom of the samples list, the Status and Filename columns remains fixed and only the other columns scroll right and left.

   For instructions to automatically copy or fill values in these columns, see Appendix B, "Using Copy Down and Fill Down."

❖ To rearrange the columns

1. To resize a column, drag the header separator on the right side of the column.
2. To move a column, drag the column header.

   The Status and Filename columns can be swapped with each other, but they cannot be moved to any other location in the table.

   When you close the application, it saves the new column order and width.

❖ To remove samples from the list

1. Select the samples you want to remove.

   Make sure the first column indicates that the samples are selected.

2. Right-click and choose **Remove selected samples** from the shortcut menu.

Editing a Batch

In Batch view, you can open a saved batch and edit the samples list. You can add samples, edit samples, or remove samples. If the batch has already been acquired, you can select specific samples for re-injection. If the batch has unacquired samples when you complete your edits, you can save it as a .tbr (to be run) batch.

Use the following procedures:

- To open a saved batch
- To edit samples in a batch
- To re-inject a sample from a previously acquired batch
- To submit all samples in the batch
- To submit selected samples

❖ To open a saved batch

- Do one of the following:
  - From the Batch View task pane, click **Open Batch.**

    –Or–
  - Click a batch name in the Recent Batches list. Do not double-click.

  The selected batch opens in the Batch View.

❖ To edit samples in a batch

- Use the commands described in "Working in Batch View" on page 182.

  You can edit samples, add new samples, re-inject acquired samples, or delete samples.

❖ To re-inject a sample from a previously acquired batch

1. In the sample list, select the sample you want to re-inject.
2. Right-click and choose **Reinject this sample** from the shortcut menu.

   The TraceFinder application creates a copy of the selected sample and appends INJ001 to the file name. Additional re-injections of the same sample are numbered INJ002, INJ003, and so forth.

   The TraceFinder application copies all parameter values from the original sample.

Previously acquired samples are indicated with a green status indicator (acquired and processed) and are grayed out. Samples created for re-injection are indicated with a blue status indicator (not acquired).

	cal_std_50_INJ001	Cal Std	10
	cal_std_50_INJ002	Cal Std	10
	cal_std_50	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

3. To save this batch with the new samples for re-injection, choose **File > Save > Batch** from the main menu.

   The batch is saved as a .tbr batch. You can open this batch from the Ready to acquire page in the Acquisition mode and acquire the re-injection samples.

Submitting a Batch

In Batch view, you can submit an entire batch or only selected samples in the batch. When you submit a batch, you can choose to acquire, process, or create reports for the submitted samples.

❖ To submit all samples in the batch

1. Do one of the following:
   - Right-click and choose **Submit batch** from the shortcut menu.

     –Or–
   - Click the **Submit batch** icon,  .
2. In the Submit Options dialog box, select if you want to process data and create reports in addition to acquiring the samples.
   - You can choose to process samples that have already been acquired.
   - You can choose to acquire and process unacquired samples (including re-injections).
   - You can choose to create reports for all submitted samples.
3. Click **OK**.

❖ To submit selected samples

1. Select the samples you want to submit.
2. Do one of the following:
   - Right-click and choose **Submit selected samples** from the shortcut menu.

     –Or–
   - Click the **Submit selected samples** icon,  .
3. In the Submit Options dialog box, select if you want to process data and create reports in addition to acquiring the samples.
   - You can choose to process samples that have already been acquired.
   - You can choose to acquire and process unacquired samples (including re-injections).
   - You can choose to create reports for all submitted samples.
4. Click **OK**.

Batch view

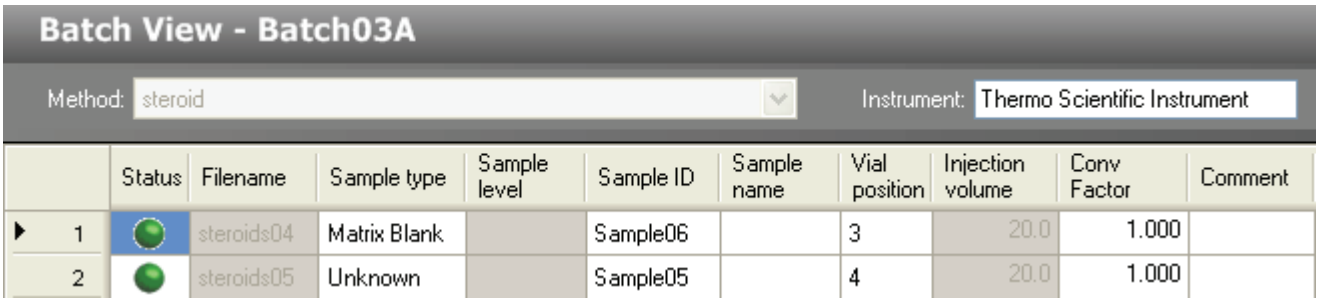


Table 39. Batch View shortcut menu

Command	Description
Add sample	Adds a single empty row to the sample grid.
Insert sample	Inserts a single empty row to the sample grid above the selected row.
Insert copy sample	Copies the currently selected row and inserts a copy above the row.
Reinject this sample	Creates a copy of the selected sample and appends INJ001 to the file name. Additional re-injections of the same sample are numbered INJ002, INJ003, and so forth.
Remove selected samples	Removes selected samples from the sample grid.
Import samples	Opens the Sample Import Tool. See "To import samples into the list" on page 184.
Submit selected samples	Submits all selected samples to be acquired or processed.
Submit batch	Submits all samples in the batch to be acquired or processed.
Browse in raw file	Opens a dialog box where you can select a rawfile to use for the sample row.

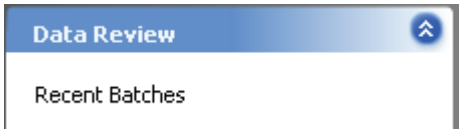
Working in Data Review

In the Data Review view, you can view the data generated by the master method. Use the Data Review view to verify the data for a sample-specific compound before you generate reports. You can use the functions in the Data Review view to investigate and edit the quantification values in a batch.

❖ To open the Data Review view

1. Do one of the following (to open Data Review mode):
   - From the dashboard, click **Data Review**.

     –Or–
   - Click **Data Review** in the navigation pane of the current mode.
2. In the Data Review navigation pane, click **Data Review** (to open the Data Review view).



The Data Review view for the currently selected batch opens.

Data Review Panes

The Data Review view is divided into four panes:

- Use the Quantitative data pane to select a particular sample. Status indicators for each sample indicate if the sample is unacquired, acquiring, or completed. See "Quantitative Data" on page 192.
- Use the Compounds pane to select a particular compound within that sample's result set. When you select a file and compound, the values displayed in the data grid reflect the quantification data for that unique combination. See "Compounds" on page 199.
- The Quantification peak pane and Qualification pane provide graphical information to complement the textual information displayed in the upper panes. See "Quantification Peak" on page 200 and "Qualification" on page 205.

Tip To resize the panes, drag the separators that divide the panes.

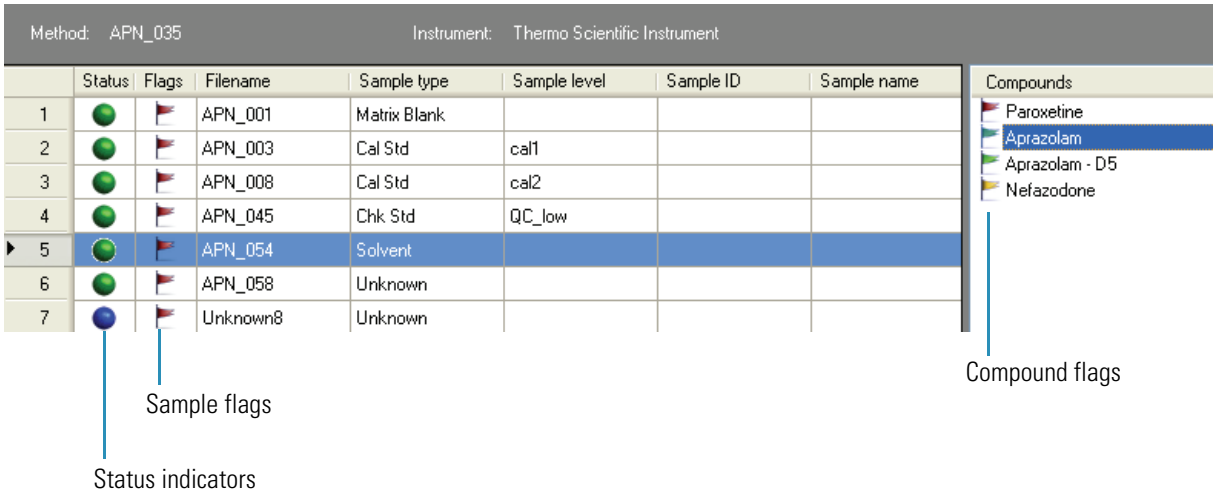
Quantitative Data

The Quantitative data pane displays all the quantitative data for the samples of a batch. The list of compounds that are available for a specific method is displayed in the Compounds pane.

The currently active compound is highlighted in the Compounds pane. You can then select it by clicking the name. The Compounds pane works with the Quantitative data pane to select a unique sample and compound combination, which then has its textual and graphical values displayed throughout the rest of the Data Review window.

In the Quantitative data pane, you can make a compound active or inactive. Switching a compound to inactive status does not remove its data and calculated values from the result set; instead, the TraceFinder application masks off the appearance of that compound for that particular sample and grays the compounds in the Compounds list. For a calibration standard, the application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. It is no longer part of the result set.

The Flags column in the Quantitative data pane displays a red flag if there is a problem with the results of the sample.



When your cursor pauses over a flag, a Tooltip displays the specific problems with the sample or compound.

Status Indicators

Status indicators show the current status of each sample during the acquisition and processing:

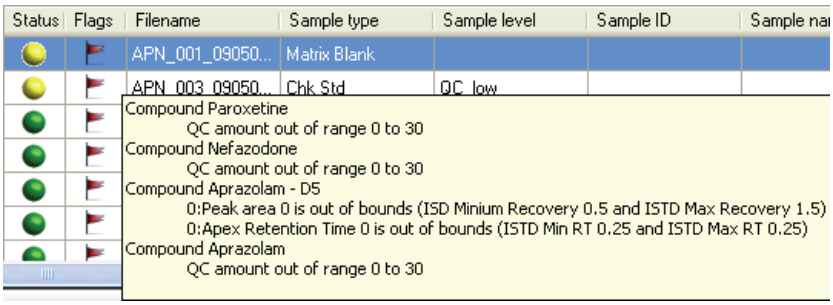
- Yellow for samples that have not been acquired
- Orange for samples that are currently acquiring
- Blue for samples that have been acquired but not processed
- Green for samples that have been acquired and processed

Sample Flags

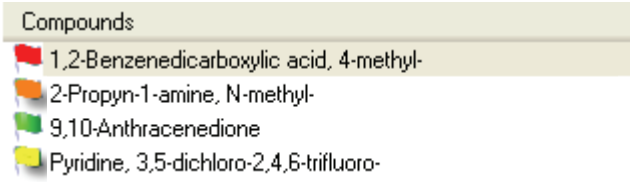
Sample flags are displayed when compounds within the samples have an error. Sample flags are always red.

- Sample flags remain static when you switch between compounds for chromatogram review until a change is completed, for example, when a compound is manually integrated and no longer falls outside the accepted criteria.

- Sample flags list a summary of all compound indicator messages within the sample when your cursor pauses over the flag.



Compound flags



Flags are displayed in these situations:

- When a compound has violated (or is activated by) any of the values set in the method. See "Editing the Flags Page" on page 122.
- For compounds that are not found in Cal Std, Chk Std, and Surrogate sample types.
- For compounds that are outside the specified ion ratio range.
- For compounds that are not found.

These criteria do not apply to Matrix Blank sample types when the compound is an internal standard.

The compounds list is sorted first by flag indicators, and then by compound names. Compound flags indicate the following:

- Red flags for compounds that have ion ratio failures or method validation failures.
- Orange flags for compounds that are below the LOQ, below the LOD, or between the LOD and LOQ values specified in the method.
- Green flags for compounds that are over the LOR amount specified in the method.
- Yellow flags for compounds that are below the LOR amount specified in the method.
- No flag for compounds that have no errors or there were no report options selected.

Use the following procedures:

- To make a compound active or inactive
- To exclude a calibration point

❖ To make a compound active or inactive

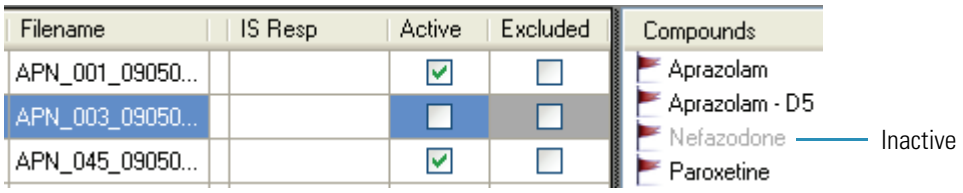
1. Select the sample in the Quantitative data pane.

   All compounds in that sample are displayed in the Compounds pane. The status of a compound in a sample is determined by the Component Active Status pane in the Batch View for the batch. Inactive compounds are grayed out.

2. In the Compounds pane, select the compound you want to make inactive.

3. In the Quantitative data pane, select or clear the **Active** check box.

   Use the horizontal scroll bar at the bottom of the table to scroll to the Active column.



❖ To exclude a calibration point

- In the Quantitative data pane, select the **Excluded** check box for the sample.

  When a value is no longer used for calibration, it remains part of the calibration dataset and is displayed in the graphical view of the calibration curve.

Quantitative data pane

Method: Batch1680B_Steroid Method Instrument: Thermo Scientific Instrument

	Status	Flags	Filename	Sample type	Sample level	Sample ID	Sample name	Comment	Vial position	Injection volume
1			steroids02...	Unknown		Sample02			1	20.0
2			steroids03	Unknown		Sample03			2	20.0
3			steroids04	Unknown		Sample04			3	20.0
4			steroids05	Unknown		Sample05			4	20.0

Integration mode	Height	*Area	Actual RT	Expected RT	Calc Amt	Theo Amt	Resp ratio	IS Amt	IS Resp
Method	312402	2958671	3.16	3.19	N/A		4.372	0.600	676792
Method	152082	1590374	3.17	3.19	N/A		2.361	0.600	673528
Method	71110	766235	3.15	3.19	N/A		0.992	0.600	772347
Method	583384	6056721	3.11	3.19	N/A		9.472	0.600	639426

Active	Excluded	% Diff	% RSD	% CV
☑	☐	N/A	N/A	N/A
☑	☐	N/A	N/A	N/A
☑	☐	N/A	N/A	N/A
☑	☐	N/A	N/A	N/A

Cells in the Quantitative data pane that should not have a value, such as theoretical concentration for an unknown, are shaded and empty. Cells that should have a value, but none exists, report N/A (not available). Results for compounds that are not detected display N/F (not found).

Table 40. Quantitative data parameters (Sheet 1 of 3)

Parameter	Description
Status	• Yellow for samples that have not been acquired • Orange for samples that are currently acquiring • Blue for samples that have been acquired but not processed • Green for samples that have been acquired and processed
Flags	Displayed only when a compound within the sample has an error. Sample flags are always red.
Filename	Name of the raw data file that contains the sample data.

Table 40. Quantitative data parameters (Sheet 2 of 3)

Parameter	Description
Sample type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: LC and GC: Matrix Blank, MDL, Solvent, Cal Std, MSD, Unknown, Chk Std, or MS GC only: LCS, LCSD, Meth Val, or Breakdown
Sample level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined alphanumeric string that identifies a sample.
Sample name	A user-defined name that identifies a sample.
Comment	A user-defined comment for the sample.
Vial Position	The tray vial number used for the autosampler acquisition.
Injection volume	The injection volume in microliters of sample to be injected. When you are using an autosampler, you can set the default injection volume in the Autosampler dialog box in the Instrument View. The minimum and maximum injection volumes that you can use depend on the Autosampler you configure. The usable range depends on the injection mode and might be smaller than the range displayed.
Integration mode	Indicates whether the peaks have been manually integrated or integrated from the original method.
Height	The distance from the peak maximum to the peak base, measured perpendicular to the ordinate. When the Resp ratio is specified as Height, this column is indicated with an asterisk (*Height).
Area	The area obtained by integrating peak intensities from the start to the end of the peak. When the Resp ratio is specified as Area, this column is indicated with an asterisk (*Area).
Actual RT	Actual retention time for the compound. Retention time is the time after injection at which a compound elutes and the total time that the compound is retained on the chromatograph column.
Expected RT	Expected retention time for the compound.
Calc Amt	The amount present in the sample, as determined using the calibration curve and the response ratio.
Theo Amt	Theoretical amount of the compound expected in the sample.

Table 40. Quantitative data parameters (Sheet 3 of 3)

Parameter	Description
Resp ratio	The ratio of the Response value to the IS Response value. If the Response is specified as Area in the processing method, the units of both Response and IS Response are counts-sec. If the Response is specified as Height in the processing method, the units of both Response and IS Response are counts.
IS Amt	Amount of internal standard.
IS Resp	Response of the internal standard.
Active	Displays or hides a compound for a particular sample. When a calibration standard is marked inactive, the application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. It is no longer part of the result set.
Excluded	Turns a compound on or off in the Calibration curve of the Qualification pane.
%Diff	The calculated amount minus the expected amount, divided by the expected amount, and then multiplied by 100.
%RSD	Standard deviation of the multiple samples of one level, multiplied by 100, and divided by the average of the multiple samples of that level. This calculation is based on the calculated amounts.
%CV	Coefficient of Variation. Standard deviation of the multiple samples of one level, multiplied by 100, and divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.

Compounds

The Compounds pane works with the Quantitative data pane to display textual and graphical values for a unique file and compound combination.

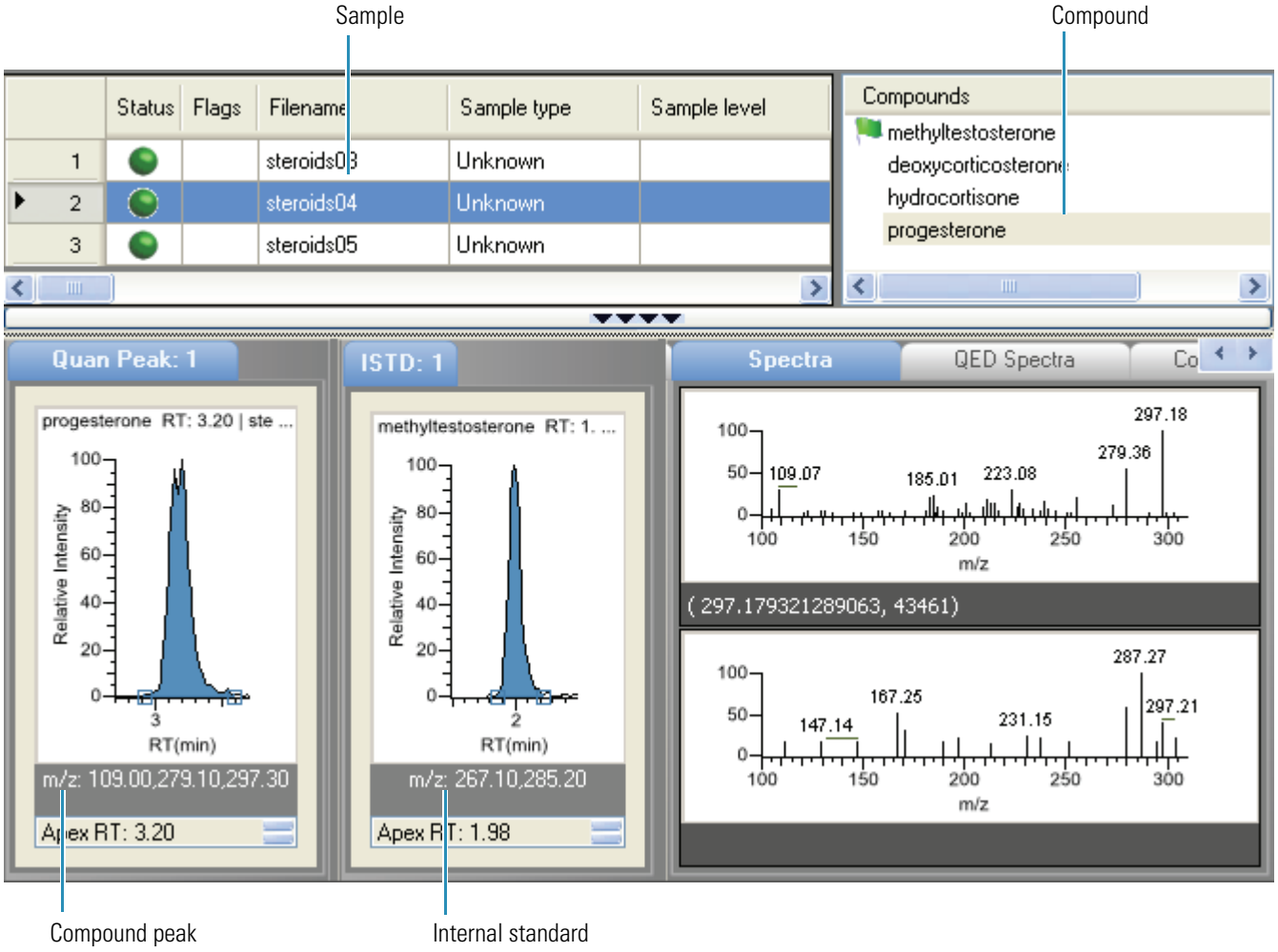
❖ To display peaks for a specific compound

1. In the Quantitative data pane, select the sample.

   The Compounds pane lists all compounds specified in the method.

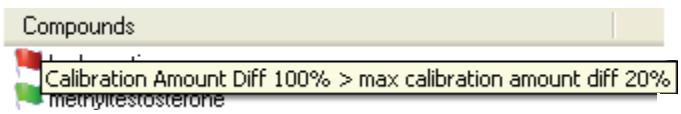
2. In the Compounds pane, select the compound in the sample.

   The Quan peak pane displays the peaks for the selected compound and its internal standard.



❖ To display specific problems with a compound

- Pause the cursor over the flag to display the problems with the compound.



Quantification Peak

The Quantification pane displays the compound selected in the Quantitative data and Compounds panes. You can store two peak value sets (method and manual integration settings) with each compound in each file. These settings can result in a different set of stored values. The method values were originally calculated based on the processing method parameters. The manual values are a result of what has been viewed or altered.

When the sample contains an internal standard, the chromatogram shows both the analyte and the internal standard in side-by-side panes.

Use the following procedures:

- To zoom in on a peak
- To manually integrate a quantification or qualification ion
- To manually add a peak
- To remove a manually created peak
- To switch between method and manual Integration modes
- To change the displayed information for detected peaks
- To modify the peak detection settings

❖ To zoom in on a peak

1. In the chromatogram plot, drag your cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view to help you examine the peak limits for enhanced review and confirmation.

2. To restore the default view, right-click the chromatogram plot and choose **Reset scaling** from the shortcut menu.

❖ To manually integrate a quantification or qualification ion

1. Place your cursor over one of the two peak delimiter tags in the Quantification peak pane.

   When the tag can be selected, the cursor changes to a crosshair style cursor. You can zoom in on the baseline to make it easier to select the tag.

2. Drag the tag to another location, and release your cursor to place the peak delimiter tag at its new location and automatically update the peak values (area, height, and so forth) into the result set.

   Both the Quantification peak pane and the Integration mode column in the Quantification data pane reflect the change between method and manual modes. The generated reports for these data identify the manual modifications.

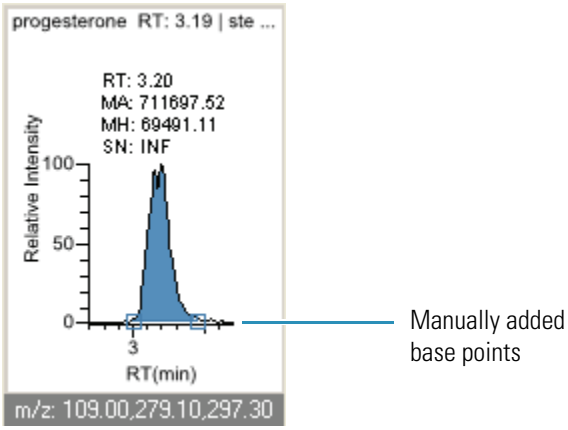
❖ To manually add a peak

1. Right-click anywhere in the Quantification peal pane, and choose **Add peak** from the shortcut menu.

   If a peak is already detected, the Add peak command is not enabled.

2. Click to indicate the left and right base points for the peak.

   The application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



❖ To remove a manually created peak

- Right-click the chromatogram plot, and choose **Remove peak** from the shortcut menu.

  The application removes the manually added peak.

❖ To switch between method and manual Integration modes

- Right-click the chromatogram view and choose **Method integration settings** or **Manual integration settings** from the shortcut menu.

  Initially, the method and manual integration settings that are stored for a compound and file are identical and when you select one mode it does not affect the saved result set. However, when manual data are available, the chromatogram plots and the result set update as you switch between method and manual modes.

  As you switch between modes, the changes are reflected in each pane. The generated reports for this data identify the manual modifications.

❖ To change the displayed information for detected peaks

1. Right-click the quantification chromatogram plot and pause the cursor over **Peak labels**.
2. Choose to display labels for the peak retention time, peak height, peak area, or signal to noise.

   The label types in the list are selected for displayed labels and cleared for labels that are not displayed.

3. To remove a label, select the label type again and clear it.

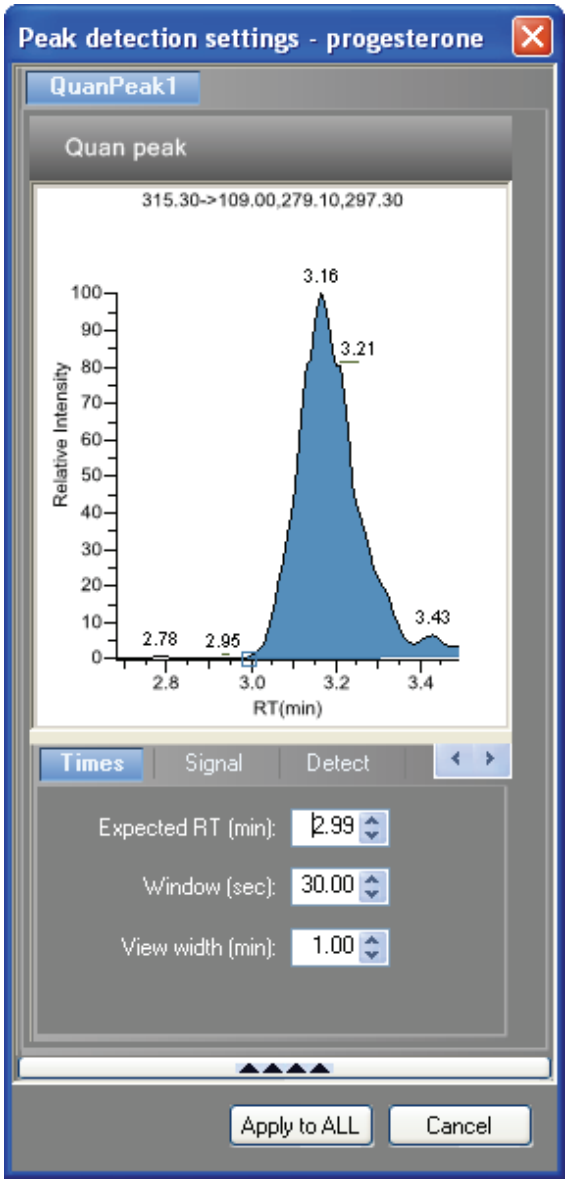
   Label settings are globally applied to quan peaks, confirming peaks, and internal standard peaks.

> **Note** The labels do not always update on all peak displays. To update all labels, select a different compound, and then reselect the compound whose labels you changed.

❖ To modify the peak detection settings

1. Right-click the chromatogram view and choose **Peak detection settings** from the shortcut menu.

   The Peak detection setting dialog box opens. This dialog box contains the detection settings defined in the method.

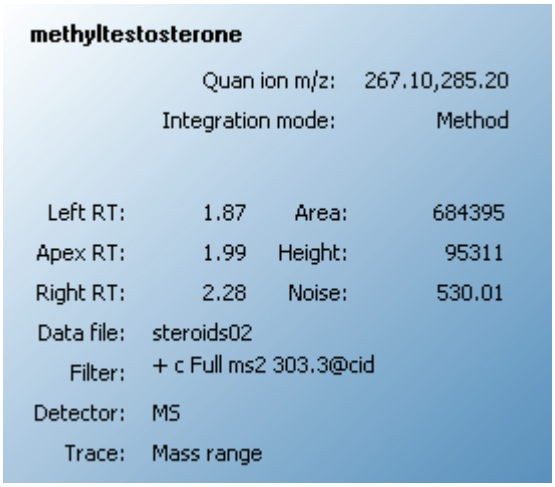


2. Edit any of the detection settings.

   For detailed descriptions of all detection settings, see "Detection" on page 97.

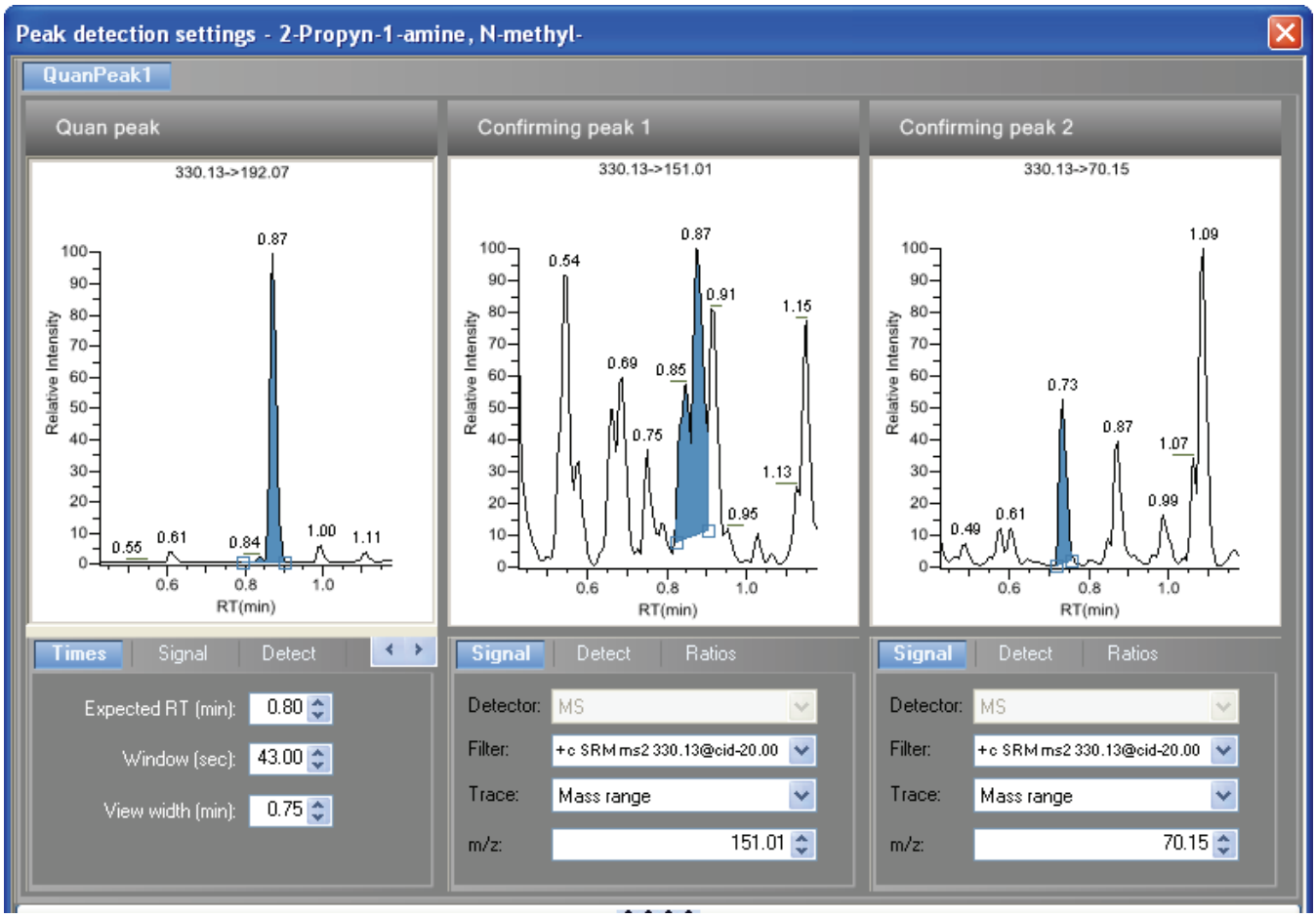
3. To save your changes to this compound in all samples in this batch, click **Apply to All**.

Quantification peak shortcut menu

Command	Description
Method integration settings	Displays method integration settings.
Manual integration settings	Displays manual integration settings.
Add peak - Remove peak - Cancel add peak	Adds a peak, removes a peak, or cancels an add peak operation in progress.
Confirming ion list	Select the confirming ions to be viewed.
Peak labels	Displays or hides the peak labels (Label area, Label retention time, Label height, or Label signal to noise).
Show peak info	Displays peak information for the selected compound. For example: 
Reset scaling	Resets the original scaling after a zoom operation.
Peak detection settings	Opens the Peak detection settings dialog box for the selected compound.

Peak Detection Settings

Use the Peak detection settings dialog box to adjust detection settings that were specified in the method.



For detailed descriptions of all detection settings, see "Detection" on page 97.

Qualification

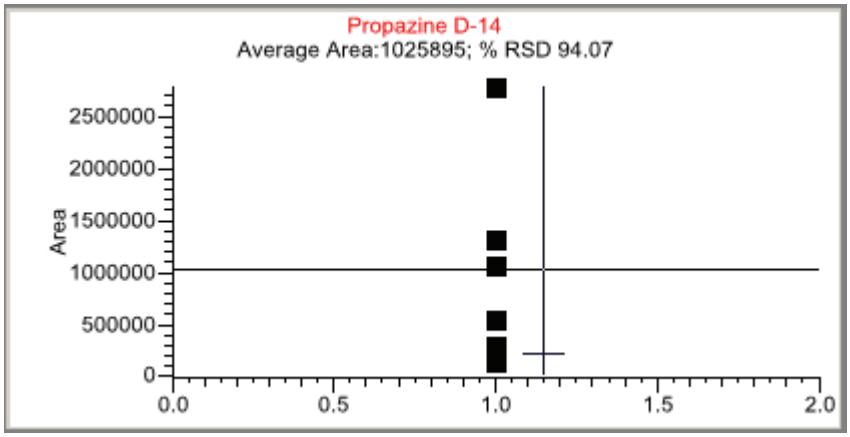
The Qualification pane displays the compound selected in the Quantification data pane and Compounds pane.

The Qualification pane consists of five pages:

- Calibration Curve
- Spectra
- QED Spectra
- Confirming Ions
- Ion Overlay

Calibration Curve

The Calibration curve page displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration.



❖ To manually exclude a calibration point

- In the Quantitative data pane, select the **Excluded** check box for the sample.

❖ To zoom in on an area

1. In the Calibration curve plot, drag your cursor to delineate a rectangle around an area.

   The delineated area expands to fill the view.

2. To restore the method default view, right-click the calibration curve plot and choose **Reset scaling** from the shortcut menu.

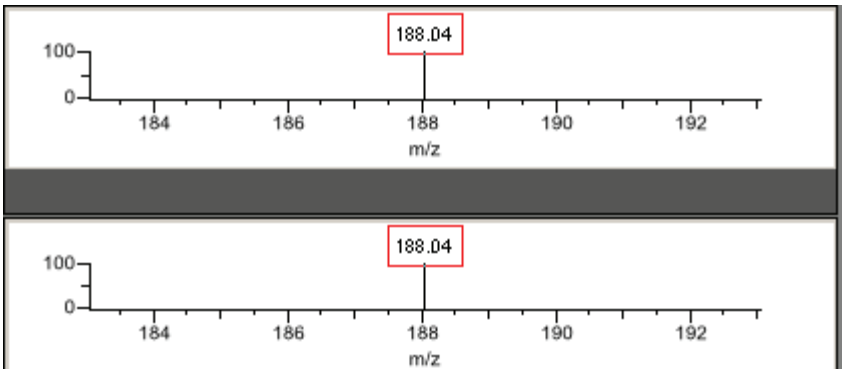
   Changes to the calibration settings are immediately applied to the entire results set, but they are saved only when you save the batch.

Calibration curve shortcut menu

Command	Description
Standard type	Sets the standard type to External or Internal.
Calibration curve type	Sets the calibration curve type to Linear, Quadratic, or Average RF. • Linear: Allows all settings with this exception: When Origin is set to Include, all Weighting values are grayed out and Weighting is set to Equal. • Quadratic: Allows all settings with this exception: When Origin is set to Include, all Weighting values are grayed out and Weighting is set to Equal. • Average RF: Allows no Weighting or Origin selections. All Weighting and Origin values are grayed out. Weighting is set to Equal, and Origin is set to Ignore.
Response via	Sets the response via to Area or Height.
Weighting	Sets the weighting to equal, 1/X, 1/X^2, 1/Y, or 1/Y^2.
Origin	Sets the origin to Ignore, Force, or Include.
Units	Sets the units.
Done with settings	
Reset scaling	Resets the original scale in the calibration curve pane.

Spectra

The Spectra page displays a comparison of the spectra found in the data and the method reference.



❖ To zoom in on an area

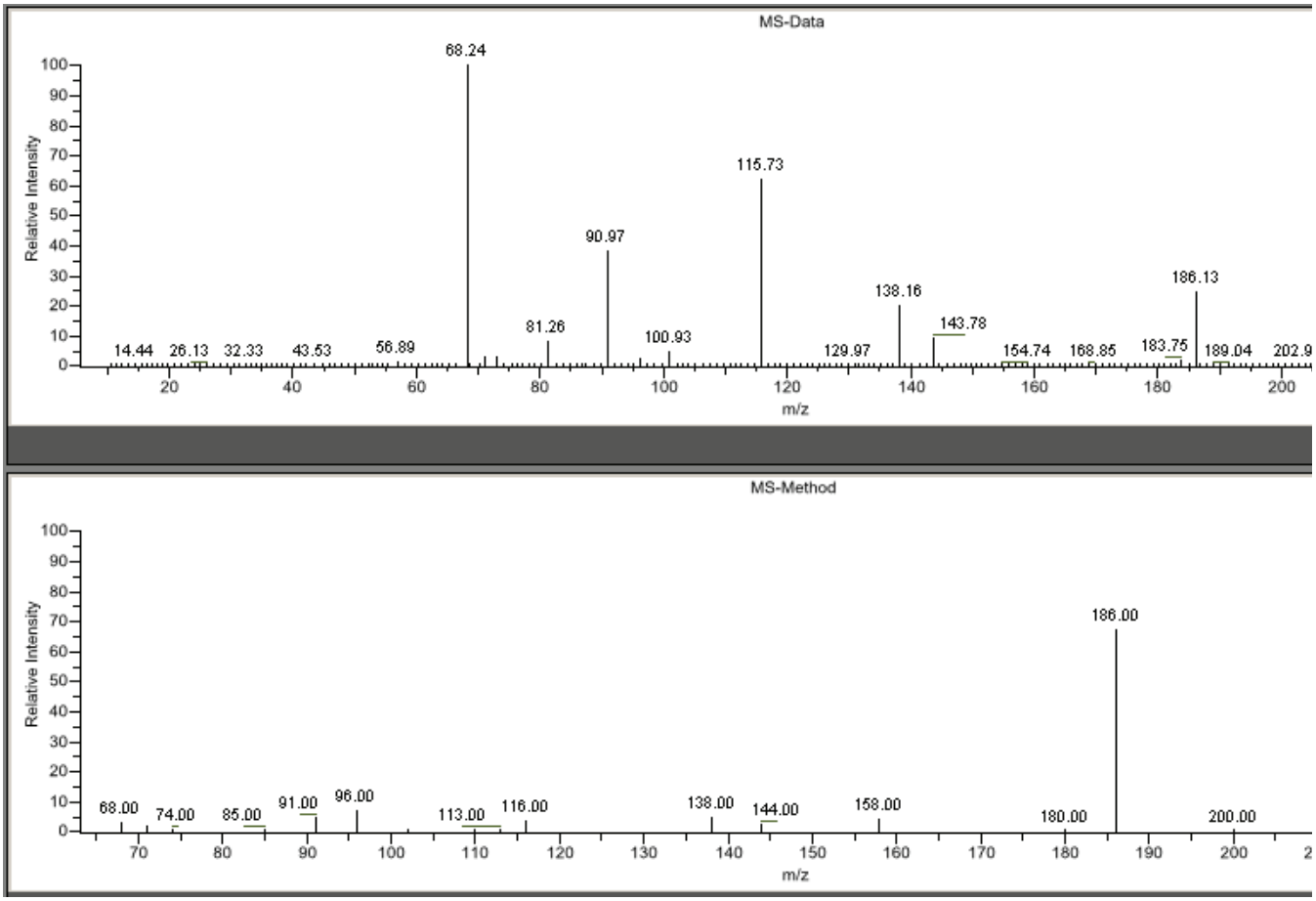
1. Drag your cursor to delineate a rectangle around an area.

   The delineated area expands to fill the view.

2. To restore the method default view, right-click the spectra plot and choose **Reset scaling** from the shortcut menu.

QED Spectra

The QED spectra displays the averaged QED spectra from the rawfile and the datastore match. If the sample contains no QED data, the page is blank.



❖ To zoom in on an area

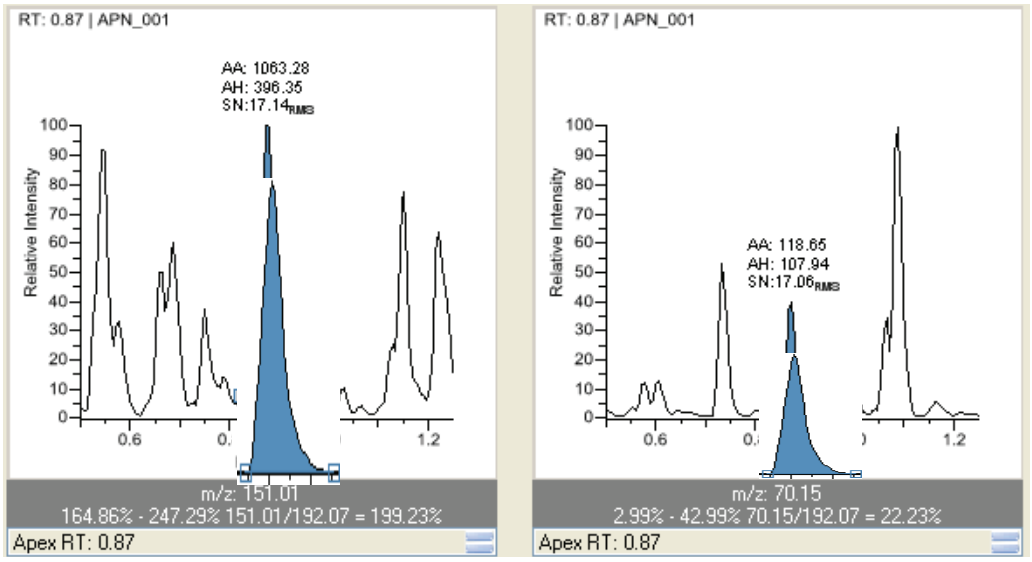
1. Drag your cursor to delineate a rectangle around an area.

   The delineated area expands to fill the view.

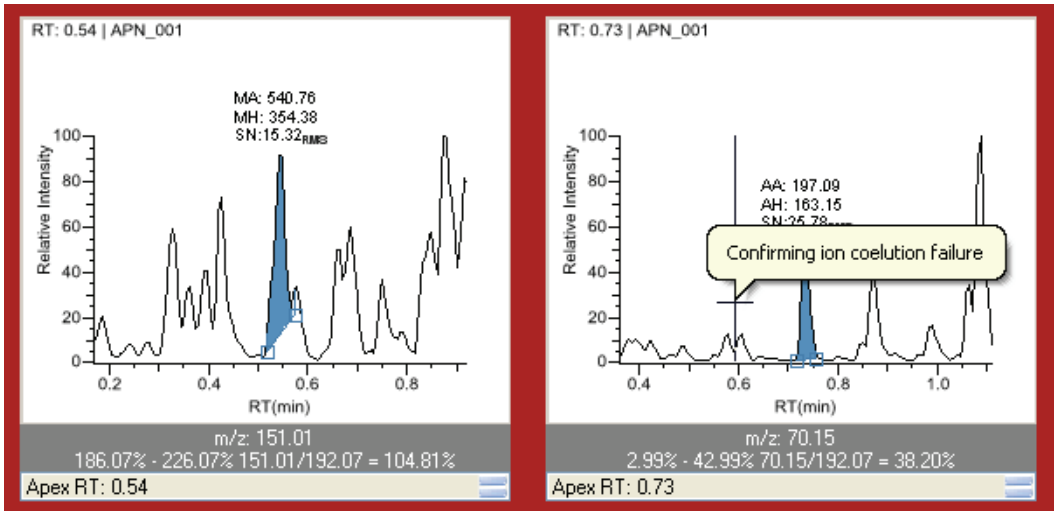
2. To restore the method default view, right-click the spectra plot and choose **Reset scaling** from the shortcut menu.

Confirming Ions

The Confirming Ions page displays a graphical view of all qualifying/confirming ions for the selected sample and compound and displays calculated ion ratios and ion ratio acceptance windows. A red border indicates that an ion ratio is outside of its window. Depending on the method option settings, another ion view is available on the Ion Overlay page. See "Ion Overlay" on page 212.



A red border indicates that an ion ratio is outside of its window.



Use the following procedures:

- To manually add a peak
- To remove a manually created peak
- To zoom in on a peak
- To change the displayed information for detected peaks
- To display the peak information window

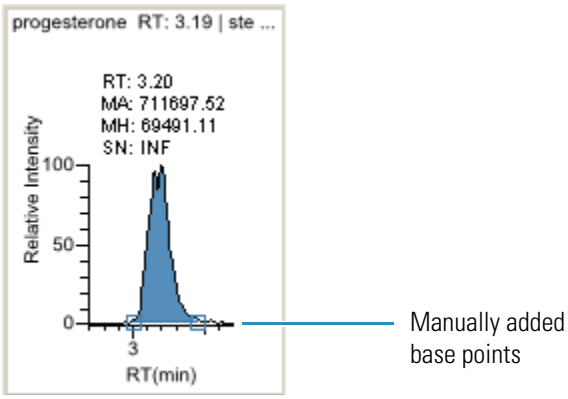
❖ To manually add a peak

1. Right-click the chromatogram plot and select **Add peak** from the shortcut menu.

   If a peak is already detected, the Add peak command is not enabled.

2. Click to indicate the left and right base points for the peak.

   The application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



❖ To remove a manually created peak

- Right-click the chromatogram plot, and choose **Remove peak** from the shortcut menu.

  The application removes the manually added peak.

❖ To zoom in on a peak

1. In the chromatogram plot, drag your cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view to help you examine the peak limits for enhanced review and confirmation.

2. To restore the method default view, right-click the chromatogram plot and choose **Reset scaling** from the shortcut menu.

❖ To change the displayed information for detected peaks

1. Right-click the chromatogram plot and pause the cursor over **Peak labels**.
2. Choose to display labels for the peak retention time, peak height, peak area, or signal to noise.

   The label types in the list are selected for displayed labels and cleared for labels that are not displayed.

3. To remove a label, select the label type again and clear it.

   Label settings are globally applied to quan peaks, confirming peaks, and internal standard peaks.

Note The labels do not always update on all peak displays. To update all labels, select a different compound, then reselect the compound whose labels you changed.

❖ To display the peak information window

1. Right-click the quantification and confirming ion chromatogram plots.
2. Choose **Show Peak Info** from the shortcut menu.

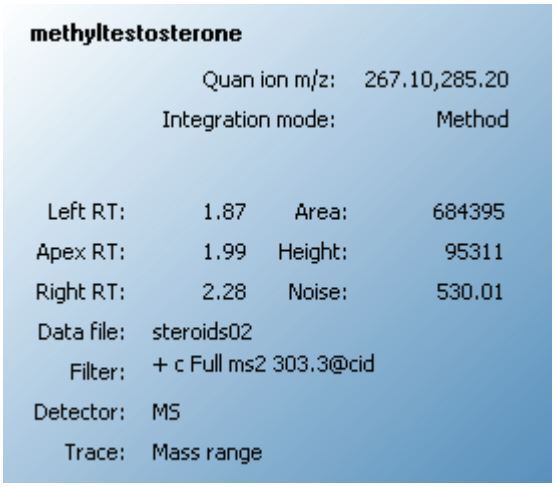
   Information in this window includes the data stream processed for this ion, consisting of a particular detector, filter (if applicable), and trace. For example, an MS detector might show a filter of "+ c Full ms [35.00-500.00]" and a Mass Range trace.

   This window also shows the peak area and height, along with the retention times of the peak integration and the peak apex.

Confirming ions shortcut menu (Sheet 1 of 2)

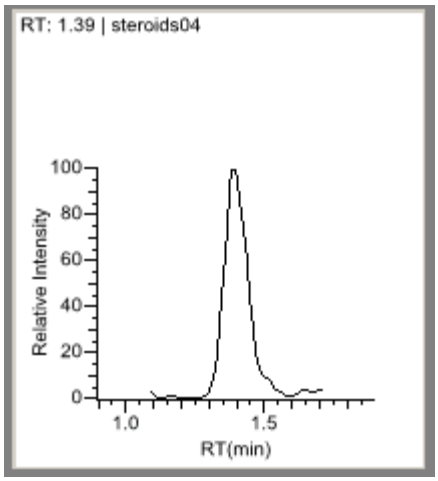
Command	Description
Method integration settings	Displays method integration settings.
Manual integration settings	Displays manual integration settings.
Add peak - Remove peak - Cancel add peak	Adds a peak, removes a manually added peak, or cancels an add peak operation in progress.
Range Calc method: Manual	Selects the method used to calculate the ion ratio range windows: Manual, Average, Weighted average, or Level
Range calc level	Range based on the calibration level
Target ratio:	Specifies the theoretical ratio of the confirming ion's response to the quantification ion's response.
Window type:	Specifies the Absolute or Relative calculation approach for determining the acceptable ion ratio range.
Window: %	Specifies the acceptable ion ratio range.
Peak labels	Displays or hides the peak labels (Label area, Label retention time, Label height, or Label signal to noise).

Confirming ions shortcut menu (Sheet 2 of 2)

Command	Description
Show peak info	Displays peak information for the selected compound. For example: 
Reset scaling	Resets the original scaling after a zoom operation.
Peak detection settings	Opens the Peak detection settings dialog box for the selected compound. See "Peak Detection Settings" on page 204.

Ion Overlay

The Ion Overlay page represents an overlay of the entire ion set—quantification and qualifying/confirming—for the selected sample and compound. Use this page to graphically review the peak apex alignment and co-eluting peak profiles.



❖ To zoom in on a peak

1. Drag your cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the method default view, right-click the chromatogram plot and choose **Reset scaling** from the shortcut menu.

Working in Report View

Use the Report View to view the reports for the currently selected batch in the Data Review view.

❖ To open the Report View

1. Do one of the following:
   - From the dashboard, click **Data Review**.

     –Or–

   - Click **Data Review** in the navigation pane.
2. In the Data Review navigation pane, click **Report View**.

   The Report View for the currently selected batch opens.

❖ To display a report

1. Select a report type from the Select a report list.

   Only the report types created for the current batch are displayed in the list.
2. (Optional) When the report type includes separate reports for each sample, select a sample file.

❖ To print a report

1. Select the report you want to print from the Select a report list.
2. Do one of the following:
   a. Click the **Print Report** icon,  .

      The Print dialog box for your default printer opens.

   b. Follow the typical procedure to print from your printer.

      Landscape reports are automatically rotated to fit the paper.

   –Or–

   - Choose **File > Print Batch** from the main menu.

   All reports for the batch are sent to your default printer. There is no dialog box or confirmation message.

❖ To export a report

1. Select the report you want to print from the Select a report list.
2. Click the **Export Report** icon,  .

   The Export Report dialog box opens.
3. Locate the folder where you want to write the report file and click **Save**.

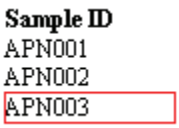
   The TraceFinder application writes the Crystal Reports (.rpt) or custom reports file to the specified folder.

❖ To search for text

1. Select a report from the Select a report list.
2. Click the **Find Text** icon,  .

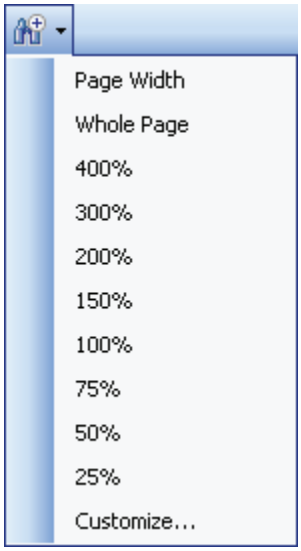
   The Find Text dialog box opens.
3. Enter your text and click **Find Next**.

   When the TraceFinder application locates the text, it encloses the text in a red box.



❖ To enlarge the report text

1. Select a report from the Select a report list.
2. Click the **Zoom** icon,  , and select a zoom scale.



Working in the Local Method View

A local method is a copy of a master method associated with a batch.

❖ To open the Local Method View

1. Do one of the following:
   - From the dashboard, click **Data Review**.

     –Or–

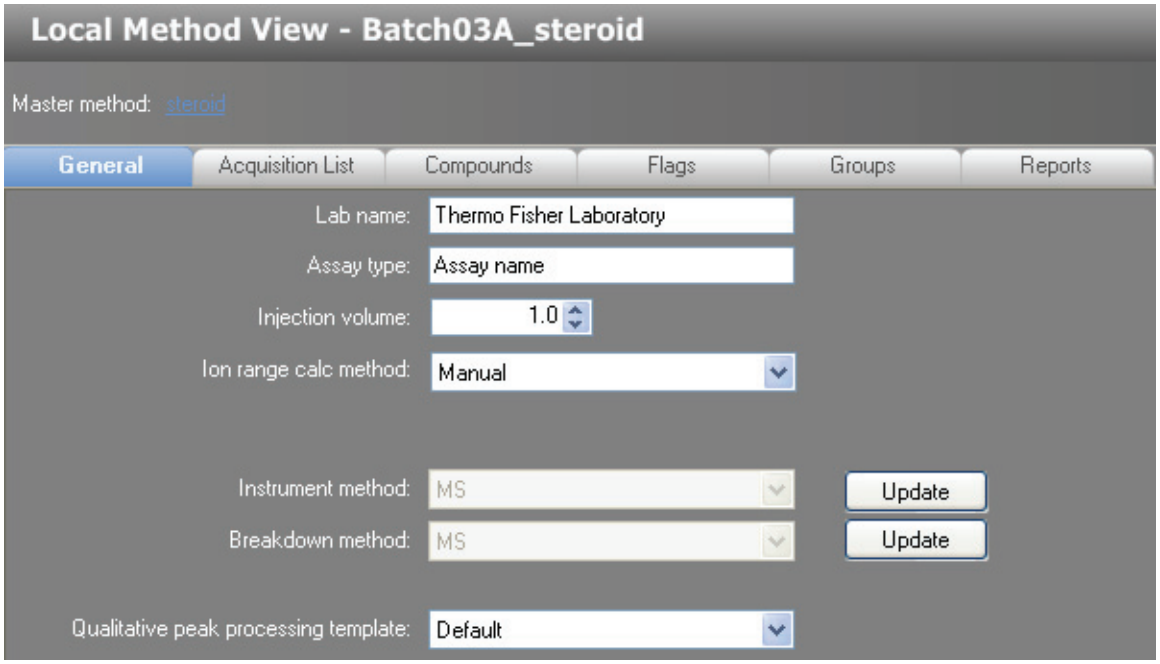
   - Click **Data Review** in the navigation pane.
2. In the Data Review navigation pane, click **Local Method**.

   The Local Method View for the currently selected batch opens. Local methods are named *BatchName_MasterMethodName*.

   You can edit many of the method parameters in a local method.

   For detailed descriptions of method parameters, see "Working with Master Methods" on page 62.
3. Enter any local changes to the method.
4. Choose **File > Save**.
5. To process the batch or create new reports with the edited local method, return to the Batch View and submit the batch.



Reports

This appendix contains information about standard and custom reports.

Contents

The report engine can generate several different types of reports designed to meet the needs of the laboratory, the laboratory's customers, and key regulatory agencies that might review the results. The following types of reports meet the requirements of various methods and worldwide regulatory agencies and are designed to help track the performance of the system and method. The TraceFinder application can produce both standard reports and custom reports.

Specifying Reports

As an IT Administrator or Lab Director, you can configure a list of reports that are available for Method Development or Acquisition modes.

For detailed information about configuring reports, see "Specifying the Reports Configuration" on page 40.

For detailed information about specifying reports when you create a method, see "Editing the Reports Page" on page 138.

For detailed information about specifying reports when you create a batch in Acquisition mode, see "Selecting and Reviewing Reports" on page 163.

Standard Reports

For each standard report you generate, you can create a hardcopy print, a PDF (.pdf), or an XML (.xml) output format. In addition to the report type, you can specify a report title for each of your reports. The default report title is the report name.

TraceFinder can generate the following types of standard reports:

- Batch Report
- Blank Report
- Breakdown Report
- Calibration Density Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Confirmation Report
- Confirmation Report 2
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report
- Solvent Blank Report
- Surrogate Recovery Report

To view an example of each type of standard reports, see "Sample Reports" on page 221.

Custom Reports

For each custom report you generate, you can create a hardcopy printout or an XLS (.xlsm) output file. The default report title is the report name.

A user in the role of IT Administrator or Lab Director can configure custom reports to generate a single report for an entire batch or to create separate reports for each sample. Rather than creating separate reports for each sample, this method uses data from only the last sample to create a single report for the entire batch.

The TraceFinder application includes the following custom reports:

- AltCalibrationReport
- Alternate BatchReport
- Alternate CalibrationReport
- Alternate ConfirmationReport
- Alternate MatrixSpikeReport
- Alternate SampleReport
- Alternate SummaryReport
- BatchReport
- BlankReport
- CalibrationDensityReport
- CalibrationReport
- CheckStandardReport
- CompoundCalibrationReport
- ConfirmationReport
- ConfirmationReport2
- HighDensitySampleReport1Long
- HighDensitySampleReport2Long
- HighDensitySampleReport3Long
- QuantitationReport

Report Flags

When generating or viewing a report, you might see one of the following quantification or calibration flags listed on the page.

Table 41. Quantification flags

Flag	Definition
b	Compound was observed at a concentration in a matrix blank sample above the specified limit.
s	Compound was observed at a response in a solvent blank sample above the specified limit.
J	Compound was observed at a concentration above the limit of detection, but below the limit of quantitation.
I or *	Confirming/qualifying ion ratio for a compound was observed outside the target ratio range or the coelution between quantification and confirming/qualifying ion was larger than acceptable limit.
C	Compound was observed at a concentration above the specified carryover limit.
?	Compound was observed at a concentration above the specified linearity limit.
D	Compound was observed at a concentration below the specified limit of detection.
Q	Compound was observed at a concentration below the specified limit of quantitation.
POS	Compound was observed at a concentration above the specified cutoff.

Table 42. Calibration flags

Flag	Definition
D	Calibration for this compound exceeded the specified maximum percent relative standard deviation (%RSD).
F	Response factor for this compound was below the specified minimum response factor (Min RF).
R	Calibration for this compound was below the specified minimum correlation coefficient (r^2).
A	Back calculation of the calibration points for this compound exceeded the specified maximum percent difference (Max %D).
X	Calibration point for this compound was excluded from the overall calibration by manual selection.
X(ISNF)	Calibration point for this compound was excluded from the overall calibration because its associated internal standard was not found.

A QA/QC failure is identified by an asterisk (*), a shaded row, or the word Fail.

Values on a report that are the result of a manual integration will use an uppercase M to signify a manually integrated quantification ion and a lowercase m to signify a manually integrated qualifying/confirming ion. On alternative reports, manual integration are signified by a black box around the value.

Sample Reports

This section shows samples of the following standard report types:

- Batch Report
- Blank Report
- Breakdown Report
- Calibration Density Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Confirmation Report
- Confirmation Report 2
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- High Density Internal Standard Report
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- QC Standard Report
- Quantitation Report
- Solvent Blank Report
- Surrogate Recovery Report

Tip To easily view reports in landscape format, choose **View > Rotate View > Clockwise** from the Adobe Acrobat viewer menu.

Batch Report

Batch Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Filename	Date/time	Sample ID	Sample name	Level	Sample type	Pos	Inj vol	Conv Factor	Comment
FreshBlankWednesday	6/27/2007 4:38:40 PM	SampleID-14	D-14	N/A	Solvent	Tray1:1	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
5ppb-001	6/27/2007 12:54:35 AM	SampleID008	D008	N/A	Unknown	Tray1:15	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
5ppb-002	6/27/2007 1:25:44 AM	SampleID002	D008	N/A	Unknown	Tray1:16	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
5ppb-003	6/27/2007 1:56:52 AM	SampleID003	D003	N/A	Unknown	Tray1:17	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
5ppb-004	6/27/2007 2:28:00 AM	SampleID004	D004	N/A	Unknown	Tray1:18	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
5ppb-005	6/27/2007 2:59:10 AM	SampleID005	D005	N/A	Unknown	Tray1:19	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
5ppb-006	6/27/2007 3:30:18 AM	SampleID006	D006	N/A	Unknown	Tray1:20	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
500ppt-001	6/26/2007 9:16:35 PM	SampleID008	D008	QC	Chk Std	Tray1:8	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
500ppt-002	6/26/2007 9:47:43 PM	SampleID002	D002	QC	Chk Std	Tray1:9	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
500ppt-003	6/26/2007 10:18:49 PM	SampleID003	D003	N/A	Unknown	Tray1:10	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
500ppt-004	6/26/2007 10:49:57 PM	SampleID004	D004	N/A	Unknown	Tray1:11	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
500ppt-005	6/26/2007 11:21:05 PM	SampleID005	D005	N/A	Unknown	Tray1:12	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
500ppt-006	6/26/2007 11:52:16 PM	SampleID006	D006	N/A	Unknown	Tray1:13	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
500ppt-007	6/27/2007 12:23:23 AM	SampleID007	D007	N/A	Unknown	Tray1:14	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
blank	6/26/2007 5:07:26 PM	SampleID-14	D-14	N/A	Matrix Blank	Tray1:1	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
blank_070627103703	6/27/2007 10:37:03 AM	SampleID-14	D-14	N/A	Matrix Blank	Tray1:1	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
blank_070627110817	6/27/2007 11:08:17 AM	SampleID-14	D-14	N/A	Matrix Blank	Tray1:1	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
blank_070627145523	6/27/2007 2:55:23 PM	SampleID-14	D-14	N/A	Matrix Blank	Tray1:1	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
Cal001	6/26/2007 5:38:40 PM	SampleID-13	D-13	c1	Cal Std	Tray1:2	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
Cal002	6/26/2007 6:09:47 PM	SampleID002	D002	c2	Cal Std	Tray1:3	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
Cal003	6/26/2007 6:40:58 PM	SampleID003	D003	c3	Cal Std	Tray1:4	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
Cal004	6/26/2007 7:12:06 PM	SampleID004	D004	c4	Cal Std	Tray1:5	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
Cal005	6/26/2007 7:43:12 PM	SampleID005	D005	c5	Cal Std	Tray1:6	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
Cal006	6/26/2007 8:14:20 PM	SampleID006	D006	c6	Cal Std	Tray1:7	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC

Batch Report

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	**Method:**	Preview2_EPA536-Triazines
User:	AMER\jamie.humphries		EPA536-Triazines
Batch:	Preview2	**Cali File:**	Preview2.calx

Cal007	6/26/2007 8:45:28 PM	SampleID007	D007	N/A	MDL	Tray1:1	100.000	1.0	New Dilutions 6/26/2007 Hypersil Gold 100x2.1 3u CTC
DACTTest001	6/27/2007 11:42:07 AM	SampleID021	D021	N/A	MS	Tray1:1	100.000	1.0	New dilution of DACT

Blank Report

Blank Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:1	SampleID-14	blank_070627145523	N/A	D-14	6/27/2007 2:55:23 PM	New Dilutions 6/26/2007 Hypersil Gold 100x2

Internal Standards	RT	QIon	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
DIA D-5	N/F	137.00	N/F	N/F	N/F	1.000	ng/ml	1.000	ng/ml
DEA D-7	16.00	147.10	499	Linear	0.000	1.000	ng/ml	1.000	ng/ml
Cyanazine D-5	17.09	219.10	1045	Linear	0.000	1.000	ng/ml	1.000	ng/ml
Simazine D-10	N/F	137.00	N/F	N/F	N/F	1.000	ng/ml	1.000	ng/ml
Atrazine D-5	18.18	179.00	1499	Linear	0.000	1.000	ng/ml	1.000	ng/ml
Propazine D-14	18.88	188.04	137	Linear	0.000	1.000	ng/ml	1.000	ng/ml

Target Compounds	RT	QIon	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units	Max Conc	
DIA	14.20	132.09	4866	Linear	0.000	-0.124	ng/ml	-0.124	ng/ml	0.200	**Pass**
DEA	15.94	146.06	399	Linear	0.800	4.062	ng/ml	4.062	ng/ml	0.200	**Fail**
Cyanazine	17.12	214.03	16779	Linear	16.062	61.101	ng/ml	61.101	ng/ml	0.200	**Fail**
Simazine	17.24	124.17	414	Linear	0.000	0.161	ng/ml	0.161	ng/ml	0.200	**Pass**
Atrazine	18.36	174.06	89	Linear	0.059	0.249	ng/ml	0.249	ng/ml	0.200	**Fail**
Propazine	19.22	196.00	78	Linear	0.570	3.957	ng/ml	3.957	ng/ml	0.200	**Fail**

Manually integrated ☐

Breakdown Report

Breakdown Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: DGT4K5D1\Beena
Batch: 2
Method: 2_bkdn1
bkdn1
Cali File: 2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	level 2 = 10 ng/uL	level2	N/A		2/22/2008 9:37:36 AM	

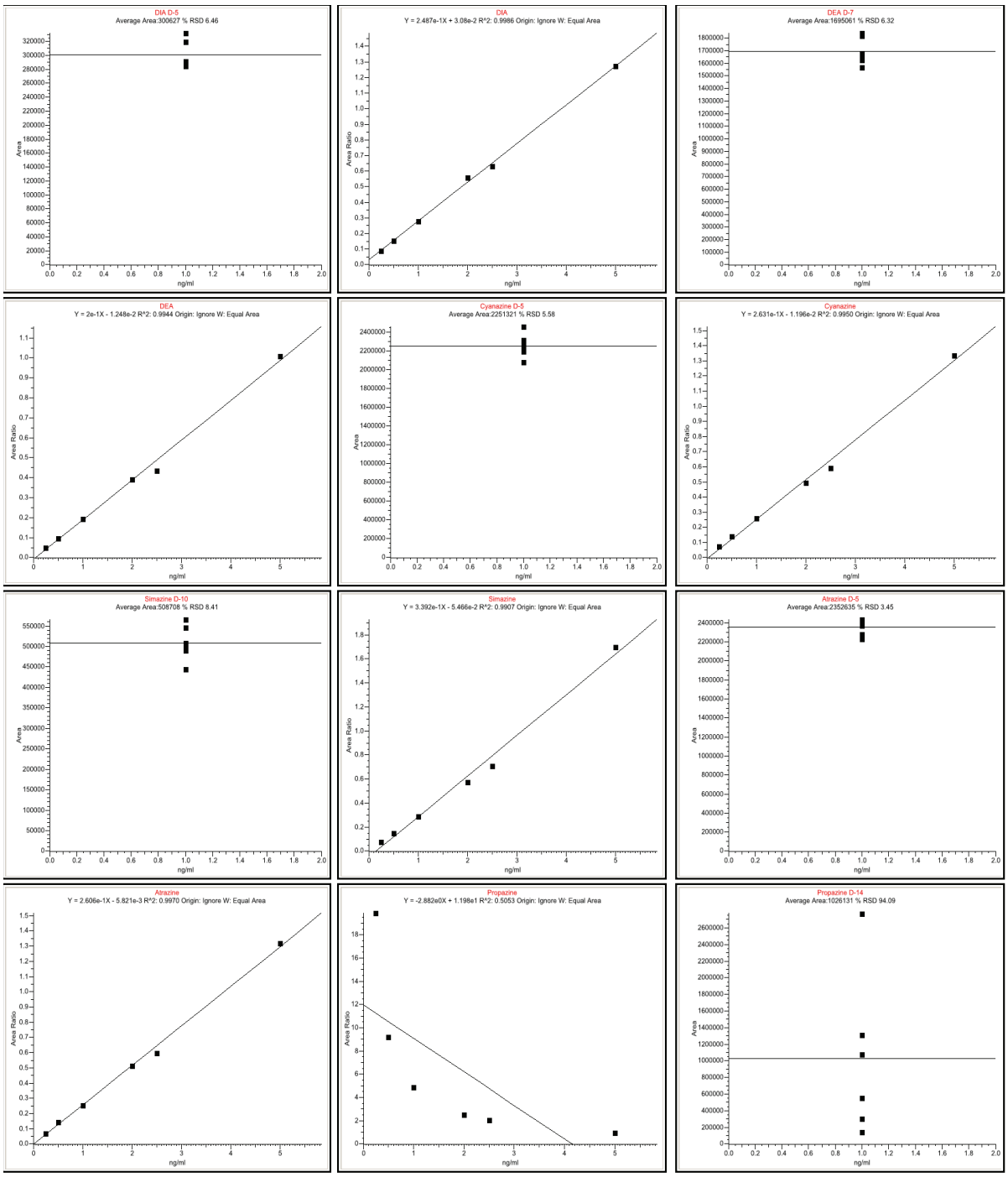
Group name	Type	Response	% Breakdown	Max % Breakdown	Results
grp1			94.81%	80.00%	Fail
Peak@6.07	Native	5070111			
Peak@4.44	Breakdown	23600215			
Peak@4.99	Breakdown	13048952			
Peak@5.96	Breakdown	55935361			

Group name	Type	Response	% Breakdown	Max % Breakdown	Results
grp2			73.95%	20.00%	Fail
Peak@6.07	Native	5070111			
Peak@6.78	Breakdown	9920308			
Peak@6.98	Breakdown	4475695			

Calibration Density Report

Calibration Density Report

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	**Method:**	Preview2_EPA536-Triazines
User:	AMER\jamie.humphries		EPA536-Triazines
Batch:	Preview2	**Cali File:**	Preview2.calx



Calibration Report

Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Calibration summary

Compound	Manually integrated	Curve type	A0 y-Intercept Mean RF	A1 Slope	A2	R^2 R^2 %RSD	Flag
DIA D-5		I	300627			6.46	
DIA		L	3.08e-2	2.487e-1		0.9986	
DEA D-7		I	1695061			6.32	
DEA		L	-1.248e-2	2e-1		0.9944	A
Cyanazine D-5		I	2251321			5.58	
Cyanazine		L	-1.196e-2	2.631e-1		0.9950	A
Simazine D-10		I	508708			8.41	
Simazine		L	-5.466e-2	3.392e-1		0.9907	A
Atrazine D-5		I	2352635			3.45	
Atrazine		L	-5.821e-3	2.606e-1		0.9970	
Propazine		L	1.198e1	-2.882e0		0.5053	RA
Propazine D-14		I	1026131			94.09	
					Average %RSD:	36.45	

Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Calibration data points

Compound	Curve type	c1	c2	c3	c4	c5	c6
DIA D-5	I	318793	331167	290167	284217	287980	291439
DIA	L	0.090	0.152	0.277	0.558	0.632	1.274
DEA D-7	I	1835531	1814511	1625976	1645818	1679937	1568595
DEA	L	0.050	0.097	0.192	0.390	0.436	1.010
Cyanazine D-5	I	2315307	2452747	2208963	2194598	2255487	2080823
Cyanazine	L	0.074	0.137	0.258	0.493	0.590	1.336
Simazine D-10	I	564878	545558	489931	508415	499551	443913
Simazine	L	0.073	0.148	0.290	0.573	0.705	1.700
Atrazine D-5	I	2430347	2429903	2377500	2279499	2367556	2231004
Atrazine	L	0.069	0.143	0.253	0.515	0.598	1.319
Propazine	L	19.840	9.206	4.859	2.513	2.062	0.947
Propazine D-14	I	141663	306171	550388	1072853	1313475	2772239

Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:2	SampleID-13	Cal001	c1	D-13	6/26/2007 5:38:40 PM	New Dilutions 6/26/2007 Hypers
Tray1:3	SampleID002	Cal002	c2	D002	6/26/2007 6:09:47 PM	New Dilutions 6/26/2007 Hypers
Tray1:4	SampleID003	Cal003	c3	D003	6/26/2007 6:40:58 PM	New Dilutions 6/26/2007 Hypers
Tray1:5	SampleID004	Cal004	c4	D004	6/26/2007 7:12:06 PM	New Dilutions 6/26/2007 Hypers
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hypers
Tray1:7	SampleID006	Cal006	c6	D006	6/26/2007 8:14:20 PM	New Dilutions 6/26/2007 Hypers

Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard
Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.
Manually integrated

Check Standard Report

Check Standard Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:8	SampleID008	500ppt-001	QC	D008	6/26/2007 9:16:35 PM	New Dilutions 6/26/2007 Hy

Compound	Curve Type	Daily RF	Mean RF	Min RF	RF %D	Max RF % D	QC amt	Calc amt	Amt %D	Max Amt %D	Flag
DIA	L	0.322		10.000			0.500	0.523	4.55	20.00	Pass
DEA	L	0.194		10.000			0.500	0.546	9.29	20.00	Pass
Cyanazine	L	0.277		10.000			0.500	0.573	14.50	20.00	Pass
Simazine	L	0.289		10.000			0.500	0.587	17.49	20.00	Pass
Atrazine	L	0.275		10.000			0.500	0.55	9.96	20.00	Pass
Propazine	L	18.060		10.000			0.500	1.022	104.39 *	20.00	Fail

Internal standard summary:

Compound	Std Response	Min	Max	Sample Response	
DIA D-5	300627	150314(50.00%)	450941(150.00%)	303819	
DEA D-7	1695061	847531(50.00%)	2542592(150.00%)	1668978	
Cyanazine D-5	2251321	1125660(50.00%)	3376981(150.00%)	2124617	
Simazine D-10	508708	254354(50.00%)	763062(150.00%)	474250	
Atrazine D-5	2352635	1176317(50.00%)	3528952(150.00%)	2220242	
Propazine D-14	1026131	513066(50.00%)	1539197(150.00%)	288218	*
	Std RT	**Min**	**Max**	**Sample RT**	
DIA D-5	14.22	13.97(-0.25)	14.47(+0.25)	14.23	
DEA D-7	15.90	15.65(-0.25)	16.15(+0.25)	15.89	
Cyanazine D-5	17.15	16.90(-0.25)	17.40(+0.25)	17.15	
Simazine D-10	17.29	17.04(-0.25)	17.54(+0.25)	17.30	
Atrazine D-5	18.27	18.02(-0.25)	18.52(+0.25)	18.29	
Propazine D-14	19.07	18.82(-0.25)	19.32(+0.25)	19.08	

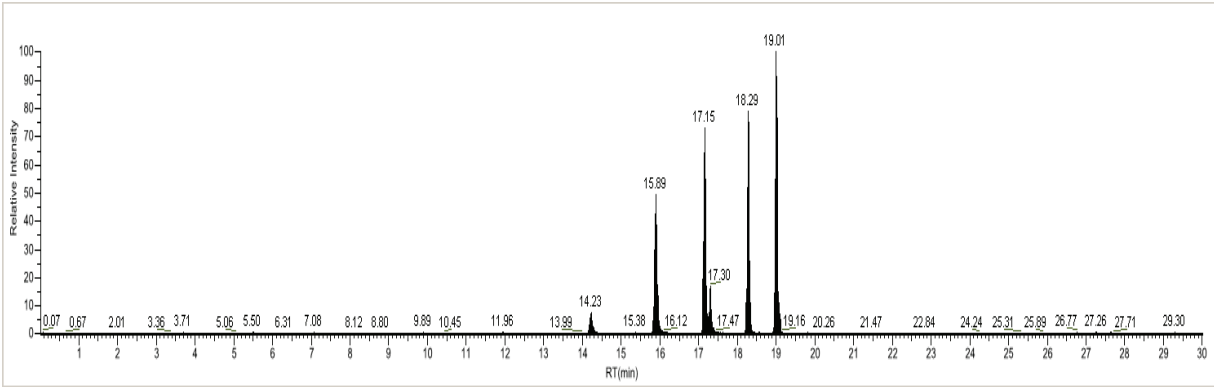
Manually integrated [ ] *** = Fail;Curve Type: A=Average RF; L=Linear; Q=Quadratic;R=Recovery limits exceeded**

Chromatogram Report

Chromatogram Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:8	SampleID008	500ppt-001	QC	D008	6/26/2007 9:16:35 PM	New Dilutions 6/26/2007 Hyp

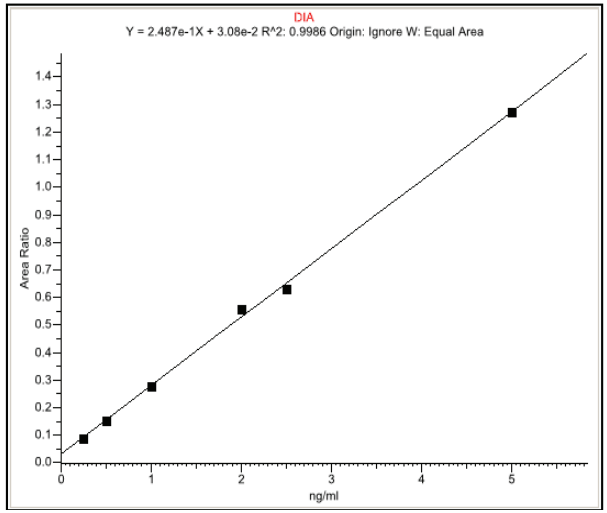


Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Compound Name: DIA



Linear
Pass

Level	Std Amount	Std Area	IS Amount	IS Area	Response ratio	Calc amt	Units	%CV	% RSD
c1	0.250	28757	1.000	318793	0.090	0.239	ng/ml	N/A	N/A
c2	0.500	50228	1.000	331167	0.152	0.486	ng/ml	N/A	N/A
c3	1.000	80437	1.000	290167	0.277	0.991	ng/ml	N/A	N/A
c4	2.000	158556	1.000	284217	0.558	2.119	ng/ml	N/A	N/A
c5	2.500	182117	1.000	287980	0.632	2.419	ng/ml	N/A	N/A
c6	5.000	371202	1.000	291439	1.274	4.997	ng/ml	N/A	N/A

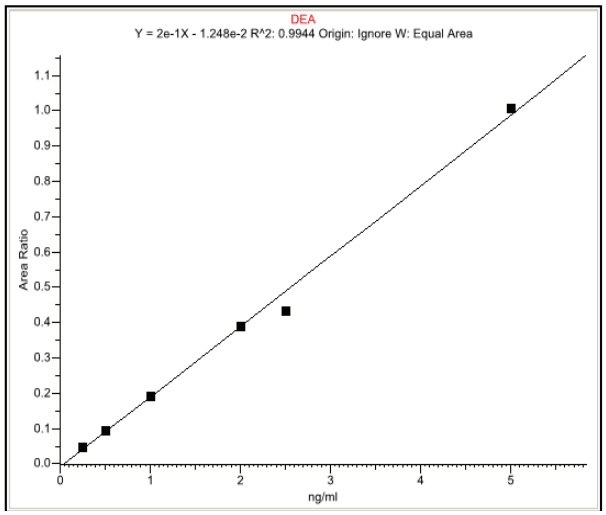
Manually Integrated: ☐ **Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount**

Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Compound Name: DEA



Linear
Fail A

Level	Std Amount	Std Area	IS Amount	IS Area	Response ratio	Calc amt	Units	%CV	% RSD
c1	0.250	92276	1.000	1835531	0.050	0.314	ng/ml	N/A	N/A A
c2	0.500	176402	1.000	1814511	0.097	0.549	ng/ml	N/A	N/A
c3	1.000	311422	1.000	1625976	0.192	1.020	ng/ml	N/A	N/A
c4	2.000	642652	1.000	1645818	0.390	2.015	ng/ml	N/A	N/A
c5	2.500	732057	1.000	1679937	0.436	2.241	ng/ml	N/A	N/A
c6	5.000	1583854	1.000	1568595	1.010	5.111	ng/ml	N/A	N/A

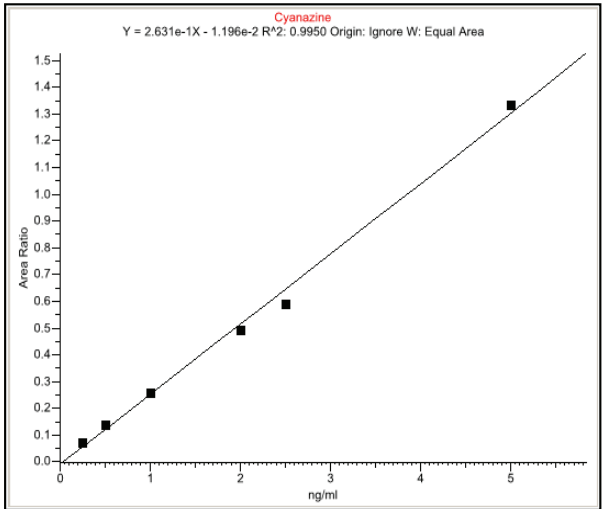
Manually Integrated: ☐ **Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount**

Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Compound Name: Cyanazine



Linear
Fail A

Level	Std Amount	Std Area	IS Amount	IS Area	Response ratio	Calc amt	Units	%CV	% RSD
c1	0.250	172415	1.000	2315307	0.074	0.329	ng/ml	N/A	N/A A
c2	0.500	336993	1.000	2452747	0.137	0.568	ng/ml	N/A	N/A
c3	1.000	568897	1.000	2208963	0.258	1.024	ng/ml	N/A	N/A
c4	2.000	1080890	1.000	2194598	0.493	1.918	ng/ml	N/A	N/A
c5	2.500	1331175	1.000	2255487	0.590	2.289	ng/ml	N/A	N/A
c6	5.000	2779559	1.000	2080823	1.336	5.123	ng/ml	N/A	N/A

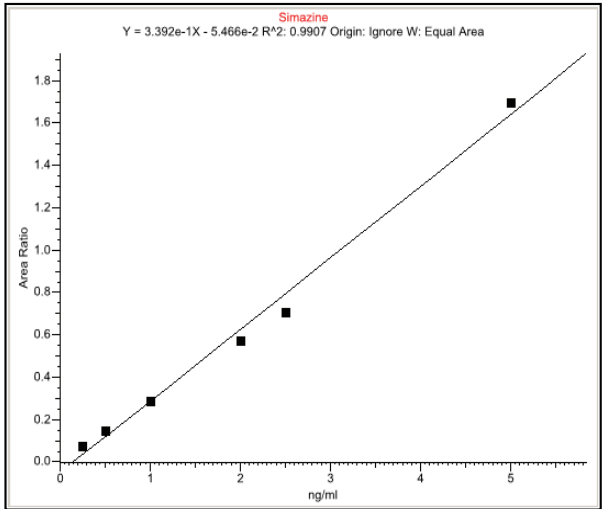
Manually Integrated: ☐ **Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount**

Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Compound Name: Simazine



Linear
Fail A

Level	Std Amount	Std Area	IS Amount	IS Area	Response ratio	Calc amt	Units	%CV	% RSD
c1	0.250	41086	1.000	564878	0.073	0.376	ng/ml	N/A	N/A A
c2	0.500	80784	1.000	545558	0.148	0.598	ng/ml	N/A	N/A
c3	1.000	142154	1.000	489931	0.290	1.016	ng/ml	N/A	N/A
c4	2.000	291272	1.000	508415	0.573	1.850	ng/ml	N/A	N/A
c5	2.500	352249	1.000	499551	0.705	2.240	ng/ml	N/A	N/A
c6	5.000	754439	1.000	443913	1.700	5.171	ng/ml	N/A	N/A

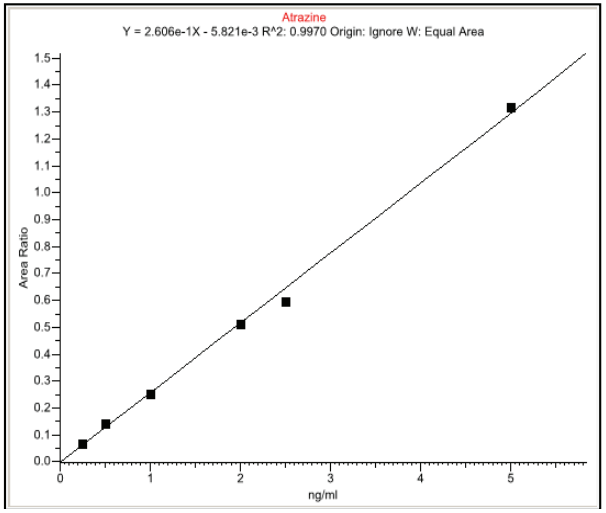
Manually Integrated: ☐ **Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount**

Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Compound Name: Atrazine



Linear
Pass

Level	Std Amount	Std Area	IS Amount	IS Area	Response ratio	Calc amt	Units	%CV	% RSD
c1	0.250	167583	1.000	2430347	0.069	0.287	ng/ml	N/A	N/A
c2	0.500	346827	1.000	2429903	0.143	0.570	ng/ml	N/A	N/A
c3	1.000	601232	1.000	2377500	0.253	0.993	ng/ml	N/A	N/A
c4	2.000	1173813	1.000	2279499	0.515	1.999	ng/ml	N/A	N/A
c5	2.500	1415179	1.000	2367556	0.598	2.316	ng/ml	N/A	N/A
c6	5.000	2942852	1.000	2231004	1.319	5.085	ng/ml	N/A	N/A

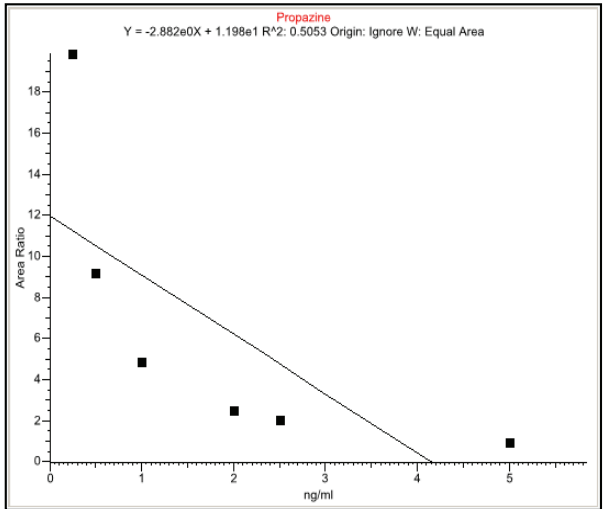
Manually Integrated: ☐ **Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount**

Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Compound Name: Propazine



Linear
Fail RA

Level	Std Amount	Std Area	IS Amount	IS Area	Response ratio	Calc amt	Units	%CV	% RSD
c1	0.250	2810520	1.000	141663	19.840	-2.728	ng/ml	N/A	N/A A
c2	0.500	2818642	1.000	306171	9.206	0.961	ng/ml	N/A	N/A A
c3	1.000	2674553	1.000	550388	4.859	2.469	ng/ml	N/A	N/A A
c4	2.000	2695746	1.000	1072853	2.513	3.283	ng/ml	N/A	N/A A
c5	2.500	2707903	1.000	1313475	2.062	3.439	ng/ml	N/A	N/A A
c6	5.000	2624723	1.000	2772239	0.947	3.826	ng/ml	N/A	N/A A

Manually Integrated: ☐ **Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount**

Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:2	SampleID-13	Cal001	c1	D-13	6/26/2007 5:38:40 PM	New Dilutions 6/26/2007 Hypersil Gold 100x2.
Tray1:3	SampleID002	Cal002	c2	D002	6/26/2007 6:09:47 PM	New Dilutions 6/26/2007 Hypersil Gold 100x2.
Tray1:4	SampleID003	Cal003	c3	D003	6/26/2007 6:40:58 PM	New Dilutions 6/26/2007 Hypersil Gold 100x2.
Tray1:5	SampleID004	Cal004	c4	D004	6/26/2007 7:12:06 PM	New Dilutions 6/26/2007 Hypersil Gold 100x2.
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hypersil Gold 100x2.
Tray1:7	SampleID006	Cal006	c6	D006	6/26/2007 8:14:20 PM	New Dilutions 6/26/2007 Hypersil Gold 100x2.

Manually Integrated:

Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount

Confirmation Report

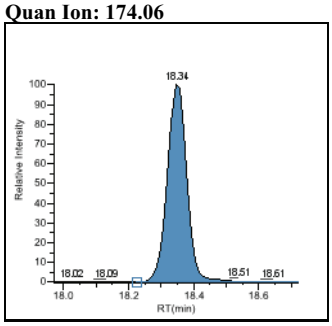
Confirmation Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali file: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:18	SampleID004	5ppb-004	N/A	D004	6/27/2007 2:28:00 AM	New Dilutions 6/26/2007

Atrazine

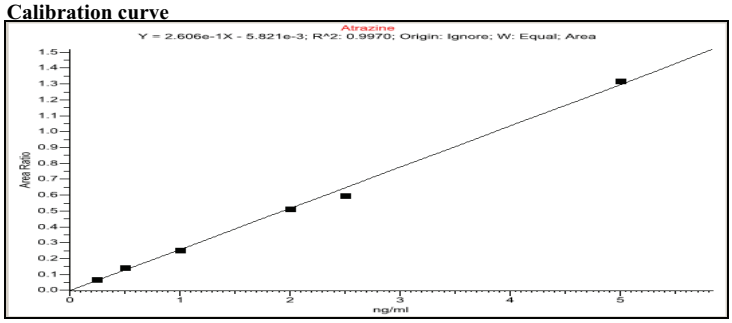
Quan Ion: 174.06



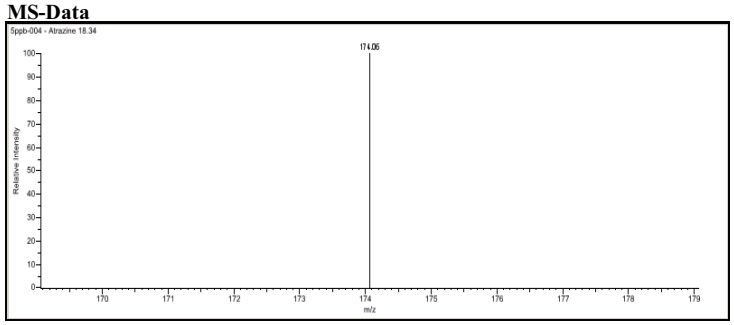
	Injected	Sample
Conc:	5.249 ng/ml	5.249 ng/ml

Retention time:	18.34
Area:	2905258
Height:	716288

Calibration curve



MS-Data



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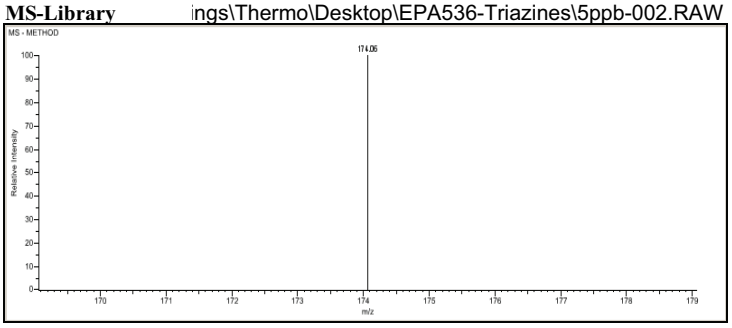


Confirmation Report 2

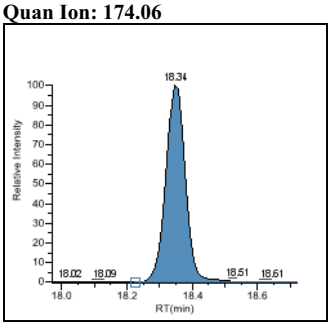
Confirmation Report 2

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali file: Preview2.calx

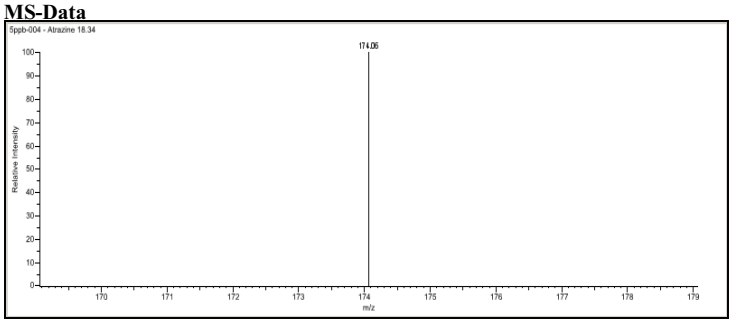
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:18	SampleID004	5ppb-004	N/A	D004	6/27/2007 2:28:00 AM	New Dilutions 6/26/2007

Compound Name: **Atrazine**
Injected Conc: 5.249 ng/ml
Sample Conc: 5.249 ng/ml
Retention time: 18.34
Area (Quan): 2905258
Height (Quan): 716288
Qual ratio 1: Pass
Qual ratio 2: Pass

Quan Ion: 174.06



MS-Data



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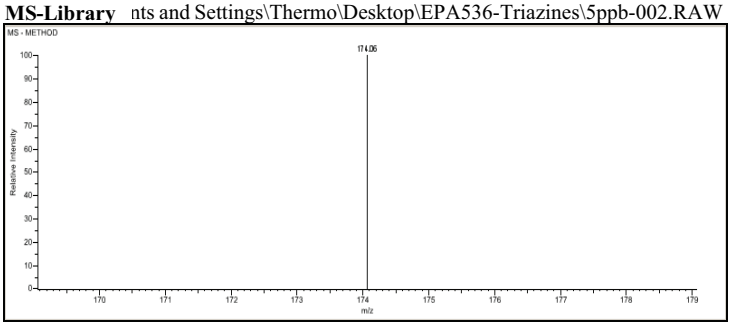


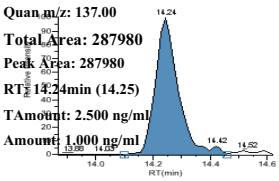
High Density Sample Report 1

High Density Sample Report 1

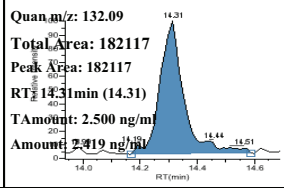
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hyp

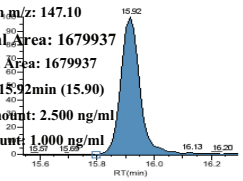
DIA D-5
Quan m/z: 137.00
Total Area: 287980
Peak Area: 287980
RT: 14.24min (14.25)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



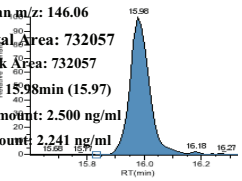
DIA
Quan m/z: 132.09
Total Area: 182117
Peak Area: 182117
RT: 14.31min (14.31)
TAmount: 2.500 ng/ml
Amount: 2.419 ng/ml



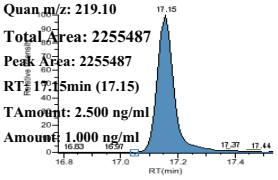
DEA D-7
Quan m/z: 147.10
Total Area: 1679937
Peak Area: 1679937
RT: 15.92min (15.90)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



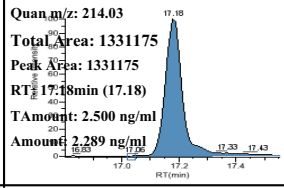
DEA
Quan m/z: 146.06
Total Area: 732057
Peak Area: 732057
RT: 15.98min (15.97)
TAmount: 2.500 ng/ml
Amount: 2.241 ng/ml



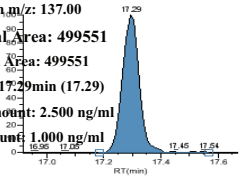
Cyanazine D-5
Quan m/z: 219.10
Total Area: 2255487
Peak Area: 2255487
RT: 17.15min (17.15)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



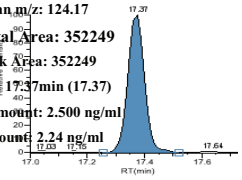
Cyanazine
Quan m/z: 214.03
Total Area: 1331175
Peak Area: 1331175
RT: 17.18min (17.18)
TAmount: 2.500 ng/ml
Amount: 2.289 ng/ml



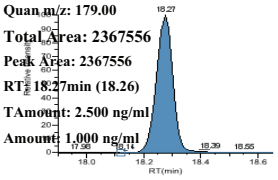
Simazine D-10
Quan m/z: 137.00
Total Area: 499551
Peak Area: 499551
RT: 17.29min (17.29)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



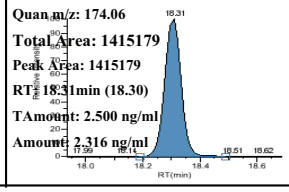
Simazine
Quan m/z: 124.17
Total Area: 352249
Peak Area: 352249
RT: 17.37min (17.37)
TAmount: 2.500 ng/ml
Amount: 2.24 ng/ml



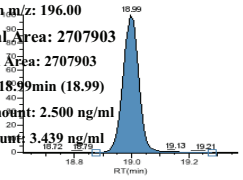
Atrazine D-5
Quan m/z: 179.00
Total Area: 2367556
Peak Area: 2367556
RT: 18.27min (18.26)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



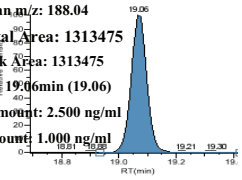
Atrazine
Quan m/z: 174.06
Total Area: 1415179
Peak Area: 1415179
RT: 18.31min (18.30)
TAmount: 2.500 ng/ml
Amount: 2.316 ng/ml



Propazine
Quan m/z: 196.00
Total Area: 2707903
Peak Area: 2707903
RT: 18.99min (18.99)
TAmount: 2.500 ng/ml
Amount: 3.439 ng/ml



Propazine D-14
Quan m/z: 188.04
Total Area: 1313475
Peak Area: 1313475
RT: 19.06min (19.06)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml

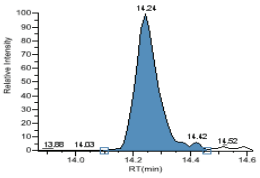


High Density Sample Report 1 Long

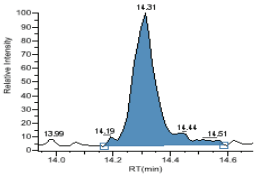
High Density Sample Report 1 Long

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

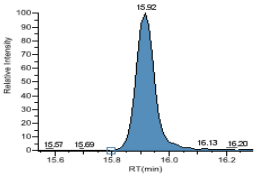
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy



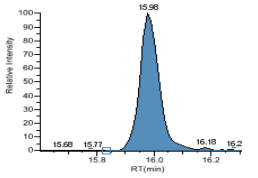
DIA D-5
Quan m/z: 137.00
Total Area: 287980
Peak Area: 287980
RT: 14.24min (14.25)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



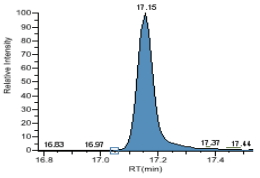
DIA
Quan m/z: 132.09
Total Area: 182117
Peak Area: 182117
RT: 14.31min (14.31)
TAmount: 2.500 ng/ml
Amount: 2.419 ng/ml



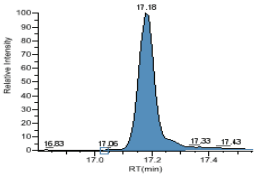
DEA D-7
Quan m/z: 147.10
Total Area: 1679937
Peak Area: 1679937
RT: 15.92min (15.90)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



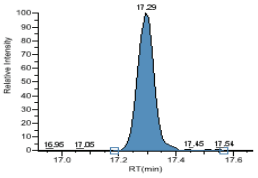
DEA
Quan m/z: 146.06
Total Area: 732057
Peak Area: 732057
RT: 15.98min (15.97)
TAmount: 2.500 ng/ml
Amount: 2.241 ng/ml



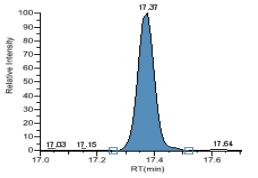
Cyanazine D-5
Quan m/z: 219.10
Total Area: 2255487
Peak Area: 2255487
RT: 17.15min (17.15)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



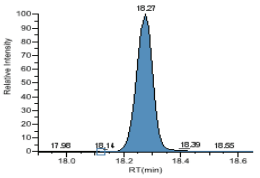
Cyanazine
Quan m/z: 214.03
Total Area: 1331175
Peak Area: 1331175
RT: 17.18min (17.18)
TAmount: 2.500 ng/ml
Amount: 2.289 ng/ml



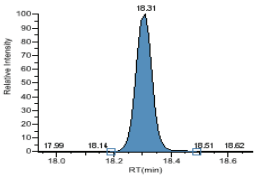
Simazine D-10
Quan m/z: 137.00
Total Area: 499551
Peak Area: 499551
RT: 17.29min (17.29)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



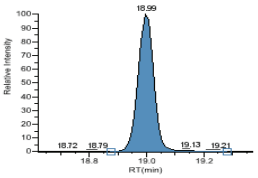
Simazine
Quan m/z: 124.17
Total Area: 352249
Peak Area: 352249
RT: 17.37min (17.37)
TAmount: 2.500 ng/ml
Amount: 2.24 ng/ml



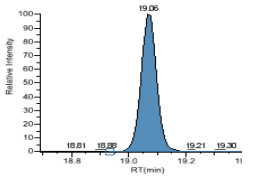
Atrazine D-5
Quan m/z: 179.00
Total Area: 2367556
Peak Area: 2367556
RT: 18.27min (18.26)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml



Atrazine
Quan m/z: 174.06
Total Area: 1415179
Peak Area: 1415179
RT: 18.31min (18.30)
TAmount: 2.500 ng/ml
Amount: 2.316 ng/ml



Propazine
Quan m/z: 196.00
Total Area: 2707903
Peak Area: 2707903
RT: 18.99min (18.99)
TAmount: 2.500 ng/ml
Amount: 3.439 ng/ml



Propazine D-14
Quan m/z: 188.04
Total Area: 1313475
Peak Area: 1313475
RT: 19.06min (19.06)
TAmount: 2.500 ng/ml
Amount: 1.000 ng/ml

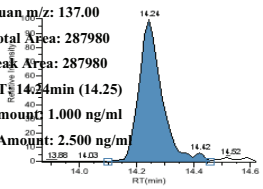
High Density Sample Report 2

High Density Sample Report 2

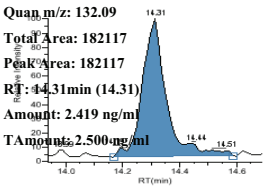
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hypersil Gold

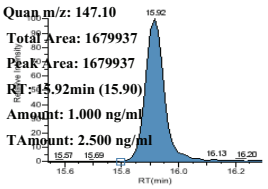
DIA D-5
Quan m/z: 137.00
Total Area: 287980
Peak Area: 287980
RT: 14.24min (14.25)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



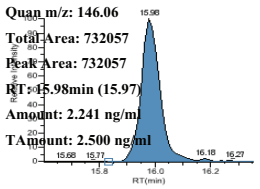
DIA
Quan m/z: 132.09
Total Area: 182117
Peak Area: 182117
RT: 14.31min (14.31)
Amount: 2.419 ng/ml
TAmount: 2.500 ng/ml



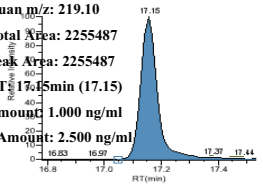
DEA D-7
Quan m/z: 147.10
Total Area: 1679937
Peak Area: 1679937
RT: 15.92min (15.90)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



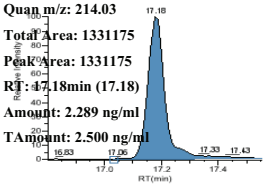
DEA
Quan m/z: 146.06
Total Area: 732057
Peak Area: 732057
RT: 15.98min (15.97)
Amount: 2.241 ng/ml
TAmount: 2.500 ng/ml



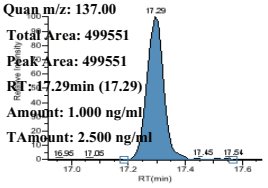
Cyanazine D-5
Quan m/z: 219.10
Total Area: 2255487
Peak Area: 2255487
RT: 17.15min (17.15)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



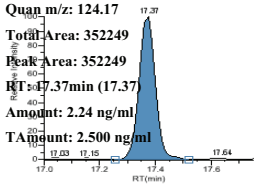
Cyanazine
Quan m/z: 214.03
Total Area: 1331175
Peak Area: 1331175
RT: 17.18min (17.18)
Amount: 2.289 ng/ml
TAmount: 2.500 ng/ml



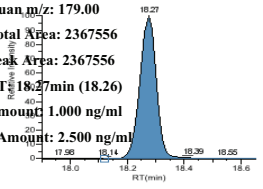
Simazine D-10
Quan m/z: 137.00
Total Area: 499551
Peak Area: 499551
RT: 17.29min (17.29)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



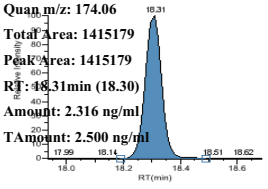
Simazine
Quan m/z: 124.17
Total Area: 352249
Peak Area: 352249
RT: 17.37min (17.37)
Amount: 2.24 ng/ml
TAmount: 2.500 ng/ml



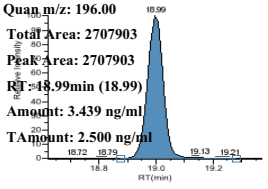
Atrazine D-5
Quan m/z: 179.00
Total Area: 2367556
Peak Area: 2367556
RT: 18.27min (18.26)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



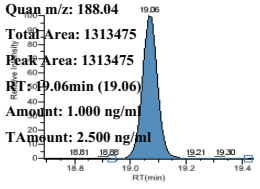
Atrazine
Quan m/z: 174.06
Total Area: 1415179
Peak Area: 1415179
RT: 18.31min (18.30)
Amount: 2.316 ng/ml
TAmount: 2.500 ng/ml



Propazine
Quan m/z: 196.00
Total Area: 2707903
Peak Area: 2707903
RT: 18.99min (18.99)
Amount: 3.439 ng/ml
TAmount: 2.500 ng/ml



Propazine D-14
Quan m/z: 188.04
Total Area: 1313475
Peak Area: 1313475
RT: 19.06min (19.06)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

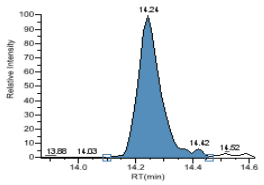


High Density Sample Report 2 Long

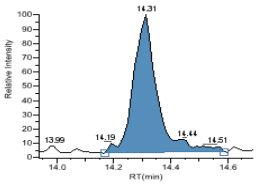
High Density Sample Report 2 Long

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

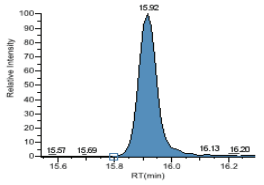
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy



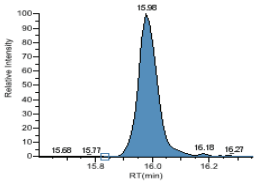
DIA D-5
Quan m/z: 137.00
Total Area: 287980
Peak Area: 287980
RT: 14.24min (14.25)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



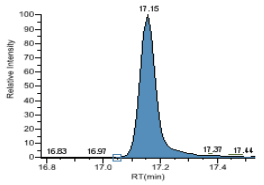
DIA
Quan m/z: 132.09
Total Area: 182117
Peak Area: 182117
RT: 14.31min (14.31)
Amount: 2.419 ng/ml
TAmount: 2.500 ng/ml



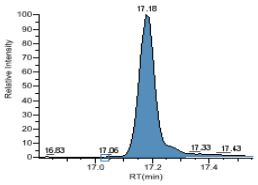
DEA D-7
Quan m/z: 147.10
Total Area: 1679937
Peak Area: 1679937
RT: 15.92min (15.90)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



DEA
Quan m/z: 146.06
Total Area: 732057
Peak Area: 732057
RT: 15.98min (15.97)
Amount: 2.241 ng/ml
TAmount: 2.500 ng/ml



Cyanazine D-5
Quan m/z: 219.10
Total Area: 2255487
Peak Area: 2255487
RT: 17.15min (17.15)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

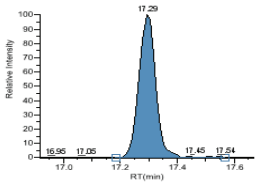


Cyanazine
Quan m/z: 214.03
Total Area: 1331175
Peak Area: 1331175
RT: 17.18min (17.18)
Amount: 2.289 ng/ml
TAmount: 2.500 ng/ml

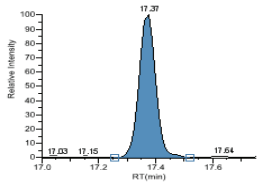
High Density Sample Report 2 Long

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

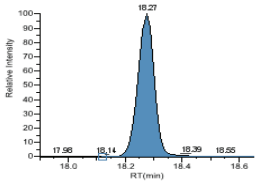
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy



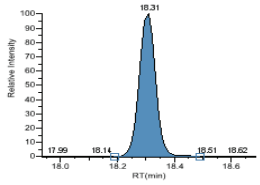
Simazine D-10
Quan m/z: 137.00
Total Area: 499551
Peak Area: 499551
RT: 17.29min (17.29)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



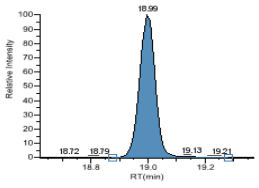
Simazine
Quan m/z: 124.17
Total Area: 352249
Peak Area: 352249
RT: 17.37min (17.37)
Amount: 2.24 ng/ml
TAmount: 2.500 ng/ml



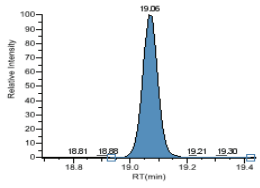
Atrazine D-5
Quan m/z: 179.00
Total Area: 2367556
Peak Area: 2367556
RT: 18.27min (18.26)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



Atrazine
Quan m/z: 174.06
Total Area: 1415179
Peak Area: 1415179
RT: 18.31min (18.30)
Amount: 2.316 ng/ml
TAmount: 2.500 ng/ml



Propazine
Quan m/z: 196.00
Total Area: 2707903
Peak Area: 2707903
RT: 18.99min (18.99)
Amount: 3.439 ng/ml
TAmount: 2.500 ng/ml



Propazine D-14
Quan m/z: 188.04
Total Area: 1313475
Peak Area: 1313475
RT: 19.06min (19.06)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

High Density Sample Report 3

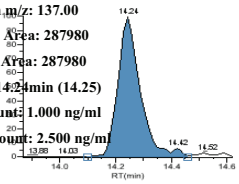
High Density Sample Report 3

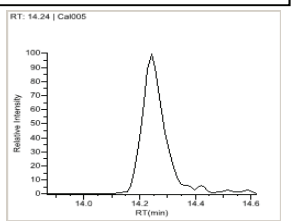
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy

DIA D-5

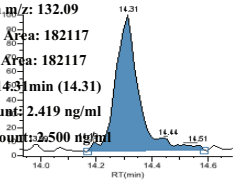
Quan m/z: 137.00
Total Area: 287980
Peak Area: 287980
RT: 14.24min (14.25)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

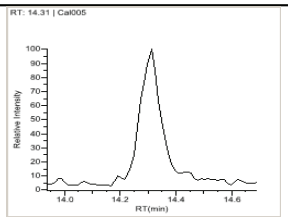




DIA

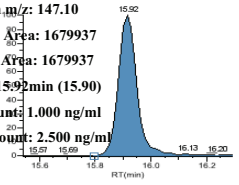
Quan m/z: 132.09
Total Area: 182117
Peak Area: 182117
RT: 14.31min (14.31)
Amount: 2.419 ng/ml
TAmount: 2.500 ng/ml

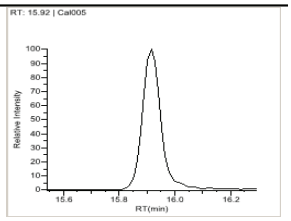




DEA D-7

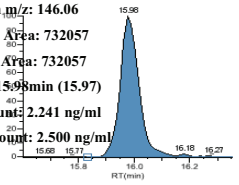
Quan m/z: 147.10
Total Area: 1679937
Peak Area: 1679937
RT: 15.92min (15.90)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

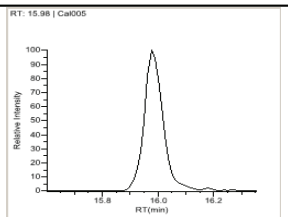




DEA

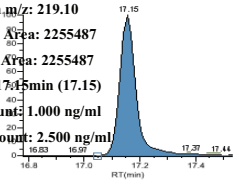
Quan m/z: 146.06
Total Area: 732057
Peak Area: 732057
RT: 15.98min (15.97)
Amount: 2.241 ng/ml
TAmount: 2.500 ng/ml

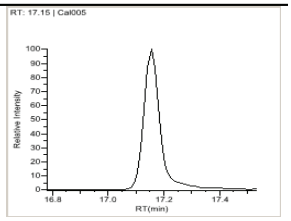




Cyanazine D-5

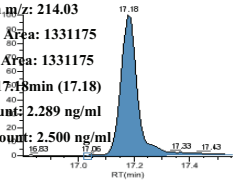
Quan m/z: 219.10
Total Area: 2255487
Peak Area: 2255487
RT: 17.15min (17.15)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

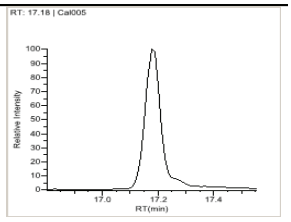




Cyanazine

Quan m/z: 214.03
Total Area: 1331175
Peak Area: 1331175
RT: 17.18min (17.18)
Amount: 2.289 ng/ml
TAmount: 2.500 ng/ml



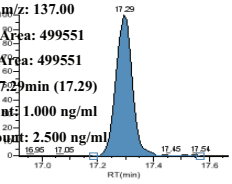


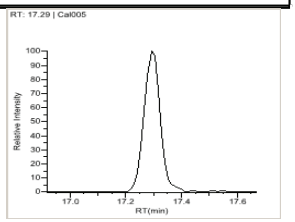
High Density Sample Report 3

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

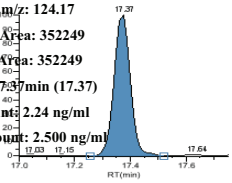
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hyp

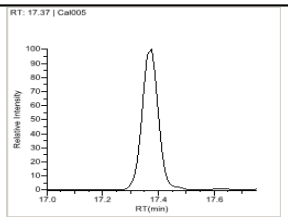
Simazine D-10
Quan m/z: 137.00
Total Area: 499551
Peak Area: 499551
RT: 17.29min (17.29)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



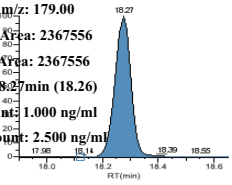


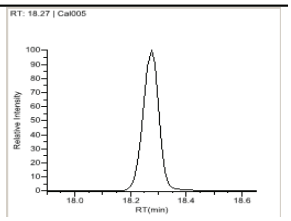
Simazine
Quan m/z: 124.17
Total Area: 352249
Peak Area: 352249
RT: 17.37min (17.37)
Amount: 2.24 ng/ml
TAmount: 2.500 ng/ml



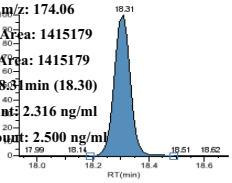


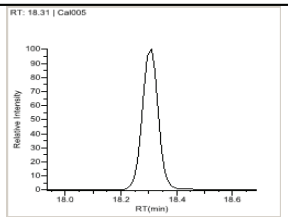
Atrazine D-5
Quan m/z: 179.00
Total Area: 2367556
Peak Area: 2367556
RT: 18.27min (18.26)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



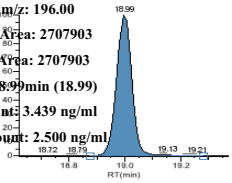


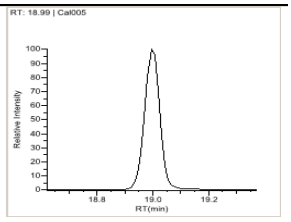
Atrazine
Quan m/z: 174.06
Total Area: 1415179
Peak Area: 1415179
RT: 18.31min (18.30)
Amount: 2.316 ng/ml
TAmount: 2.500 ng/ml



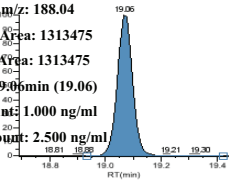


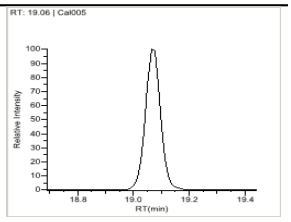
Propazine
Quan m/z: 196.00
Total Area: 2707903
Peak Area: 2707903
RT: 18.99min (18.99)
Amount: 3.439 ng/ml
TAmount: 2.500 ng/ml





Propazine D-14
Quan m/z: 188.04
Total Area: 1313475
Peak Area: 1313475
RT: 19.06min (19.06)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



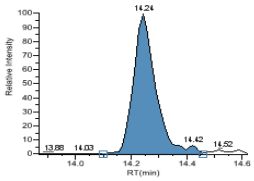


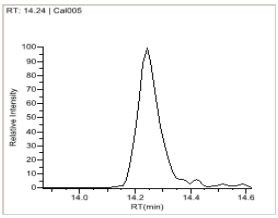
High Density Sample Report 3 Long

High Density Sample Report 3 Long

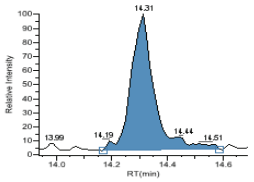
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

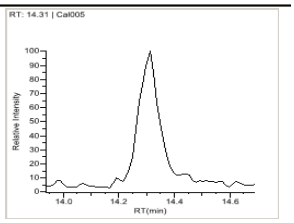
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy



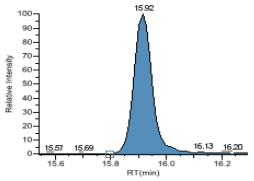


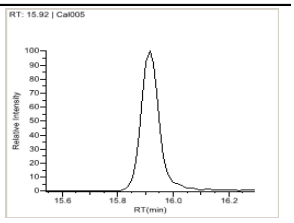
DIA D-5
Quan m/z: 137.00
Total Area: 287980
Peak Area: 287980
RT: 14.24min (14.25)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml





DIA
Quan m/z: 132.09
Total Area: 182117
Peak Area: 182117
RT: 14.31min (14.31)
Amount: 2.419 ng/ml
TAmount: 2.500 ng/ml



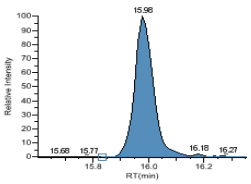


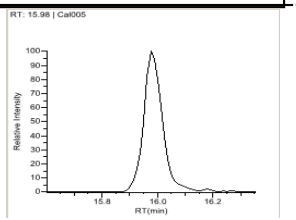
DEA D-7
Quan m/z: 147.10
Total Area: 1679937
Peak Area: 1679937
RT: 15.92min (15.90)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

High Density Sample Report 3 Long

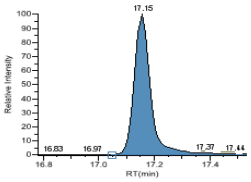
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

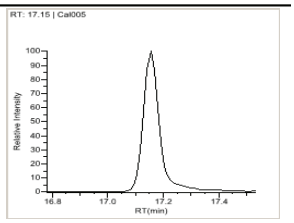
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy



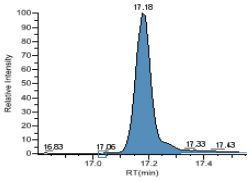


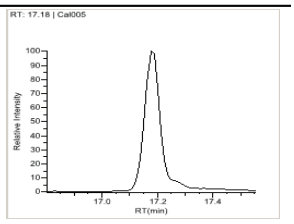
DEA
Quan m/z: 146.06
Total Area: 732057
Peak Area: 732057
RT: 15.98min (15.97)
Amount: 2.241 ng/ml
TAmount: 2.500 ng/ml





Cyanazine D-5
Quan m/z: 219.10
Total Area: 2255487
Peak Area: 2255487
RT: 17.15min (17.15)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml



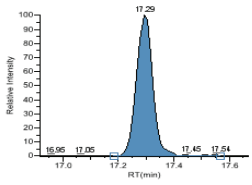


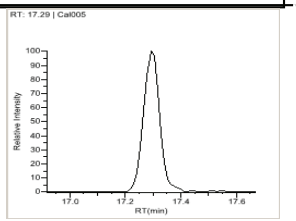
Cyanazine
Quan m/z: 214.03
Total Area: 1331175
Peak Area: 1331175
RT: 17.18min (17.18)
Amount: 2.289 ng/ml
TAmount: 2.500 ng/ml

High Density Sample Report 3 Long

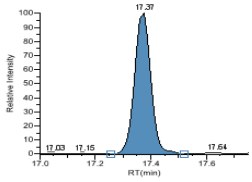
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

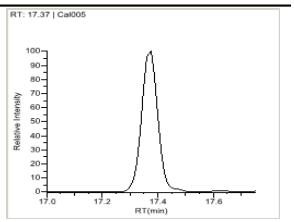
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy



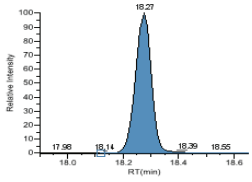


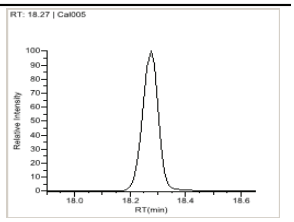
Simazine D-10
Quan m/z: 137.00
Total Area: 499551
Peak Area: 499551
RT: 17.29min (17.29)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml





Simazine
Quan m/z: 124.17
Total Area: 352249
Peak Area: 352249
RT: 17.37min (17.37)
Amount: 2.24 ng/ml
TAmount: 2.500 ng/ml



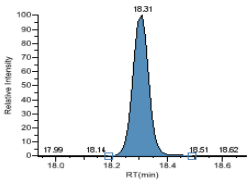


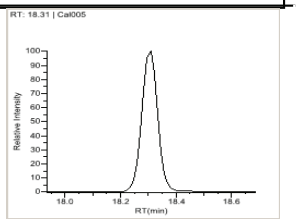
Atrazine D-5
Quan m/z: 179.00
Total Area: 2367556
Peak Area: 2367556
RT: 18.27min (18.26)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

High Density Sample Report 3 Long

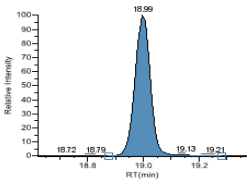
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

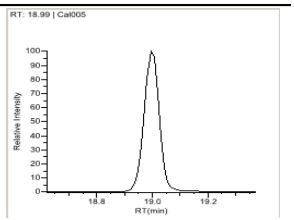
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy



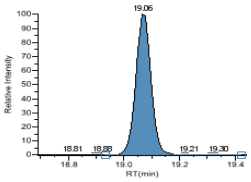


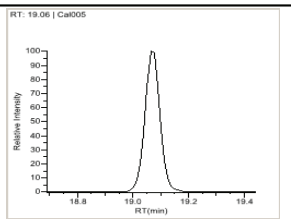
Atrazine
Quan m/z: 174.06
Total Area: 1415179
Peak Area: 1415179
RT: 18.31min (18.30)
Amount: 2.316 ng/ml
TAmount: 2.500 ng/ml





Propazine
Quan m/z: 196.00
Total Area: 2707903
Peak Area: 2707903
RT: 18.99min (18.99)
Amount: 3.439 ng/ml
TAmount: 2.500 ng/ml





Propazine D-14
Quan m/z: 188.04
Total Area: 1313475
Peak Area: 1313475
RT: 19.06min (19.06)
Amount: 1.000 ng/ml
TAmount: 2.500 ng/ml

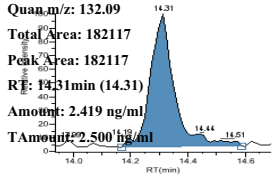
High Density Internal Standard Report

High Density Internal Standard Report

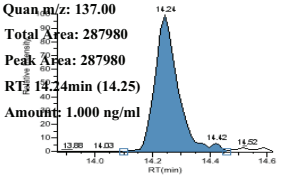
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hy

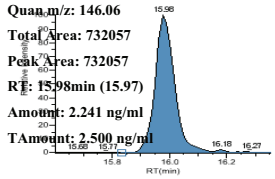
DIA
Quan m/z: 132.09
Total Area: 182117
Peak Area: 182117
RT: 14.31min (14.31)
Amount: 2.419 ng/ml
TAmount: 2.500 ng/ml



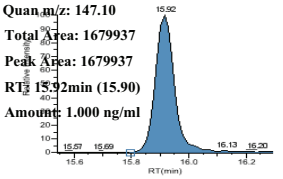
DIA D-5
Quan m/z: 137.00
Total Area: 287980
Peak Area: 287980
RT: 14.24min (14.25)
Amount: 1.000 ng/ml



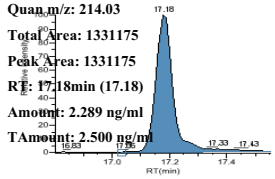
DEA
Quan m/z: 146.06
Total Area: 732057
Peak Area: 732057
RT: 15.98min (15.97)
Amount: 2.241 ng/ml
TAmount: 2.500 ng/ml



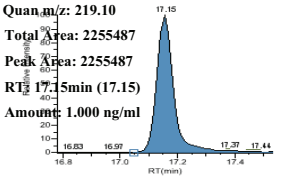
DEA D-7
Quan m/z: 147.10
Total Area: 1679937
Peak Area: 1679937
RT: 15.92min (15.90)
Amount: 1.000 ng/ml



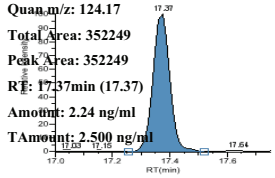
Cyanazine
Quan m/z: 214.03
Total Area: 1331175
Peak Area: 1331175
RT: 17.18min (17.18)
Amount: 2.289 ng/ml
TAmount: 2.500 ng/ml



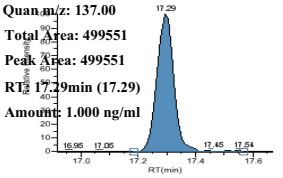
Cyanazine D-5
Quan m/z: 219.10
Total Area: 2255487
Peak Area: 2255487
RT: 17.15min (17.15)
Amount: 1.000 ng/ml



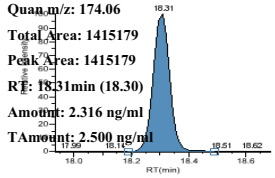
Simazine
Quan m/z: 124.17
Total Area: 352249
Peak Area: 352249
RT: 17.37min (17.37)
Amount: 2.24 ng/ml
TAmount: 2.500 ng/ml



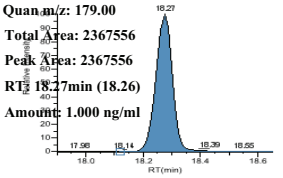
Simazine D-10
Quan m/z: 137.00
Total Area: 499551
Peak Area: 499551
RT: 17.29min (17.29)
Amount: 1.000 ng/ml



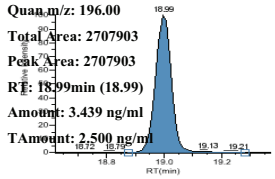
Atrazine
Quan m/z: 174.06
Total Area: 1415179
Peak Area: 1415179
RT: 18.31min (18.30)
Amount: 2.316 ng/ml
TAmount: 2.500 ng/ml



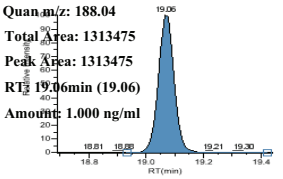
Atrazine D-5
Quan m/z: 179.00
Total Area: 2367556
Peak Area: 2367556
RT: 18.27min (18.26)
Amount: 1.000 ng/ml



Propazine
Quan m/z: 196.00
Total Area: 2707903
Peak Area: 2707903
RT: 18.99min (18.99)
Amount: 3.439 ng/ml
TAmount: 2.500 ng/ml



Propazine D-14
Quan m/z: 188.04
Total Area: 1313475
Peak Area: 1313475
RT: 19.06min (19.06)
Amount: 1.000 ng/ml



Internal Standard Summary Report

Internal Standard Summary Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hyp

Compound	Std Response	Min	Max	Sample Response
DIA D-5	300627	150314(50.00%)	450941(150.00%)	287980
DEA D-7	1695061	847531(50.00%)	2542592(150.00%)	1679937
Cyanazine D-5	2251321	1125660(50.00%)	3376981(150.00%)	2255487
Simazine D-10	508708	254354(50.00%)	763062(150.00%)	499551
Atrazine D-5	2352635	1176317(50.00%)	3528952(150.00%)	2367556
Propazine D-14	1026131	513066(50.00%)	1539197(150.00%)	1313475
	Std RT	**Min**	**Max**	**Sample RT**
DIA D-5	14.22	13.97(-0.25)	14.47(+0.25)	14.24
DEA D-7	15.90	15.65(-0.25)	16.15(+0.25)	15.92
Cyanazine D-5	17.15	16.90(-0.25)	17.40(+0.25)	17.15
Simazine D-10	17.29	17.04(-0.25)	17.54(+0.25)	17.29
Atrazine D-5	18.27	18.02(-0.25)	18.52(+0.25)	18.27
Propazine D-14	19.07	18.82(-0.25)	19.32(+0.25)	19.06

Ion Ratio Failure Report

Lab name: Example
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: test

Method: test
Cali File: test.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
12	16	09_0913	N/A	09_0913	6/17/2009 9:31:23 PM	

Compound	Response	Quan Ion	Quan Response	Qual Ion	Qual Response	Ratio	Range
Clothianidin	Area	169.10	15555	132.10	0	4.90	18.30-58.30
Acetamiprid	Area	126.10	812	99.00	0	83.40	23.64-63.64
Aldicarb	Area	116.05	1269	89.00	0	1169.97	27.25-67.25
Benoxacor	Area	149.10	1228	134.10	0	1.99	44.86-84.86
Chlorpyrifos_OA	Area	278.00	8491	197.90	4760	56.06	66.13-106.13

LCSLCSD Report

IMPORTANT When the Sample ID is the same for an unknown sample and an LCS or LCSD sample, the unknown sample is included in the LCSLCSD report. The report information for the unknown sample displays as zeros.

LCSLCSD Report Page 1 of 1

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:16	SampleID002	5ppb-002	N/A	D008	6/27/2007 1:25:44 AM	New Dilutions 6/26/2007 1
Tray1:9	SampleID002	500ppt-002	QC	D002	6/26/2007 9:47:43 PM	New Dilutions 6/26/2007 1
Tray1:3	SampleID002	Cal002	c2	D002	6/26/2007 6:09:47 PM	New Dilutions 6/26/2007 1
Tray1:15	SampleID008	5ppb-001	N/A	D008	6/27/2007 12:54:35 AM	New Dilutions 6/26/2007 1
Tray1:8	SampleID008	500ppt-001	QC	D008	6/26/2007 9:16:35 PM	New Dilutions 6/26/2007 1

SampleID002

Compound	Spike Amt	Lower Limit %	Upper Limit %	LCSD Conc	% Rec	RPD	Max RPD	Rec Fails	RPD Fails
DIA	0.500	50.00	150.00	**4.712**	**0.00**	**50.00**	**50.00**	0	**0**
DEA	0.500	50.00	150.00	**5.065**	**0.00**	**50.00**	**50.00**	0	**0**
Cyanazine	0.500	50.00	150.00	**5.127**	**0.00**	**50.00**	**50.00**	0	**0**
Simazine	0.500	50.00	150.00	**4.862**	**0.00**	**50.00**	**50.00**	0	**0**
Atrazine	0.500	50.00	150.00	**5.184**	**0.00**	**50.00**	**50.00**	0	**0**
Propazine	0.500	50.00	150.00	**3.829**	**0.00**	**50.00**	**50.00**	0	**0**

SampleID008

Compound	Spike Amt	LCS Conc	% Rec	Lower Limit %	Upper Limit %	LCSD Conc	% Rec	RPD	Max RPD	Rec Fails	RPD Fails
DIA	0.500	**4.754**	**0.00**	50.00	150.00	**4.712**	**0.00**	**0.00**	**50.00**	0	**0**
DEA	0.500	**4.960**	**0.00**	50.00	150.00	**5.065**	**0.00**	**0.00**	**50.00**	0	**0**
Cyanazine	0.500	**5.218**	**0.00**	50.00	150.00	**5.127**	**0.00**	**0.00**	**50.00**	0	**0**
Simazine	0.500	**4.839**	**0.00**	50.00	150.00	**4.862**	**0.00**	**0.00**	**50.00**	0	**0**
Atrazine	0.500	**5.178**	**0.00**	50.00	150.00	**5.184**	**0.00**	**0.00**	**50.00**	0	**0**
Propazine	0.500	**3.829**	**0.00**	50.00	150.00	**3.829**	**0.00**	**0.00**	**50.00**	0	**0**

Manual Integration Report

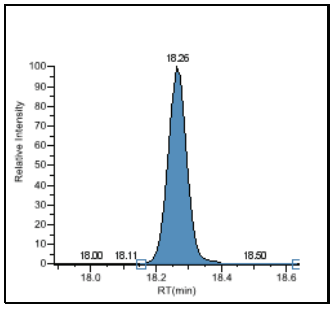
Manual Integration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

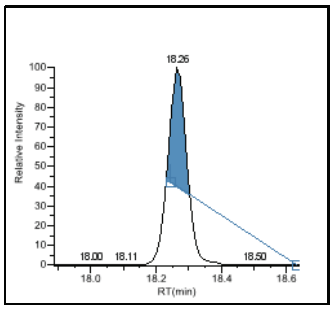
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:4	SampleID003	Cal003	c3	D003	6/26/2007 6:40:58 PM	New Dilutions 6/26/2007 I

Atrazine D-5
m/z: 179.00



Method integration

Apex RT:	18.26
Height:	608261
Area:	2377500



Manual integration

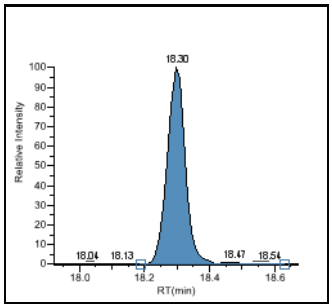
Apex RT:	18.26
Height:	361974
Area:	860754

Manual Integration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

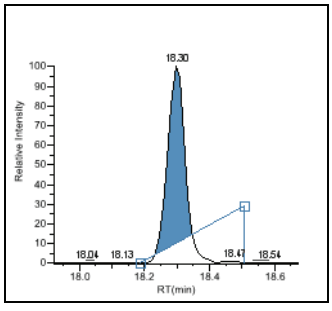
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Atrazine
m/z: 174.06



Method integration

Apex RT:	18.30
Height:	160397
Area:	601232



Manual integration

Apex RT:	18.30
Height:	144422
Area:	457354

Method Detection Limit Report

Method Detection Limit Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Method Detection Limit Summary

Compound	Avg Conc	Std Dev	t-stat	% RSD	MDL	
DIA D-5	290218	0		0.00		IS
DIA	0.095	0.000	0.000	0.00	0.000	<<<
DEA D-7	1704578	0		0.00		IS
DEA	0.065	0.000	0.000	0.00	0.000	<<<
Cyanazine D-5	2204710	0		0.00		IS
Cyanazine	0.062	0.000	0.000	0.00	0.000	<<<
Simazine D-10	513521	0		0.00		IS
Simazine	0.168	0.000	0.000	0.00	0.000	<<<
Atrazine D-5	2292164	0		0.00		IS
Atrazine	0.023	0.000	0.000	0.00	0.000	<<<
Propazine	-1069.216	0.000	0.000	0.00	0.000	<<<
Propazine D-14	826	0		0.00		IS

Manually integrated

Method Detection Limit Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Method Validation Report Data

Compound	1
DIA D-5	290218
DIA	0.095
DEA D-7	1704578
DEA	0.065
Cyanazine D-5	2204710
Cyanazine	0.062
Simazine D-10	513521
Simazine	0.168
Atrazine D-5	2292164
Atrazine	0.023
Propazine	-1069.216
Propazine D-14	826

Manually integrated ☐

Method Detection Limit Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:1	SampleID007	Cal007	N/A	D007	6/26/2007 8:45:28 PM	New Dilutions 6/26/2007 I

Manually integrated

Method Report

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 1 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Compound identification:

Compound	Quan mass	RT	Window	View Width	Use as reference	Reference compound
DIA D-5	137.00	14.25	30.00	0.75	No	
DIA	132.09	14.31	30.00	0.75	No	
DEA D-7	147.10	15.90	30.00	0.75	No	
DEA	146.06	15.97	30.00	0.75	No	
Cyanazine D-5	219.10	17.15	30.00	0.75	No	
Cyanazine	214.03	17.18	30.00	0.75	No	
Simazine D-10	137.00	17.29	30.00	0.75	No	
Simazine	124.17	17.37	30.00	0.75	No	
Atrazine D-5	179.00	18.26	30.00	0.75	No	
Atrazine	174.06	18.30	30.00	0.75	No	
Propazine	196.00	18.99	30.00	0.75	No	
Propazine D-14	188.04	19.06	30.00	0.75	No	

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 2 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Compound calibration:

Compound	Response	Calibration	Curve type	Weighting	Origin	Units	ISTD Name	ISTD Units
DIA	Area	Internal	Linear	Equal	Ignore	ng/ml	DIA D-5	ng/ml
DEA	Area	Internal	Linear	Equal	Ignore	ng/ml	DEA D-7	ng/ml
Cyanazine	Area	Internal	Linear	Equal	Ignore	ng/ml	Cyanazine D-5	ng/ml
Simazine	Area	Internal	Linear	Equal	Ignore	ng/ml	Simazine D-10	ng/ml
Atrazine	Area	Internal	Linear	Equal	Ignore	ng/ml	Atrazine D-5	ng/ml
Propazine	Area	Internal	Linear	Equal	Ignore	ng/ml	Propazine D-14	ng/ml

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 3 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Flags Quan:

Compound	LOD	LOQ	LOR	ULOL	Carryover
DIA	5.000	10.000	20.000	1000000.000	2000.000
DEA	5.000	10.000	20.000	1000000.000	2000.000
Cyanazine	5.000	10.000	20.000	1000000.000	2000.000
Simazine	5.000	10.000	20.000	1000000.000	2000.000
Atrazine	5.000	10.000	20.000	1000000.000	2000.000
Propazine	5.000	10.000	20.000	1000000.000	2000.000

Method Report

Method name:	Preview2_EPA536-Triazines			**Page number:**	Page 4 of 15
Master method name:	EPA536-Triazines				
Current calibration file:	Preview2.calx				
Assay type:	Assay name	**Ion range calc method:**	Manual		
Inj vol:	100.000				
Instrument method:	EPA536Triazines				
Tune/Breakdown method	EPA536Triazines				

Groups:

Method Report

Method name:	Preview2_EPA536-Triazines			**Page number:**	Page 5 of 15
Master method name:	EPA536-Triazines				
Current calibration file:	Preview2.calx				
Assay type:	Assay name	**Ion range calc method:**	Manual		
Inj vol:	100.000				
Instrument method:	EPA536Triazines				
Tune/Breakdown method	EPA536Triazines				

Report options:

Quan report options

Report concentration:	Always
Decimal places to be reported:	3
Show chromatogram on Quantitation report:	True
Display valid compound only:	False

Qual options

Sort Qual results by:	Reverse Search Index
Enable limiting peaks:	True
Limit Peaks to :	Top 1 by Height

User interface options

Shade row when sample is outside of evaluation criteria:	False
Separate ion overlay display :	True
Use alternative calibration report format:	False
Show quan flags and legend:	False

Trace Finder settings

Quan flags

Flag values below LOD:	True
Flag values below LOQ:	True
Flag values above LOR:	True
Flag values above ULOL:	True
Flag values above Carryover:	True
Flag values between LOD and LOQ:	True

Correct for surrogates option

Correct for surrogates:	False

Tune time tracking options

Enable tune time tracking:	True
Tune file lifetime (hrs):	12

Method Report

Method name:	Preview2_EPA536-Triazines			**Page number:**	Page 6 of 15
Master method name:	EPA536-Triazines				
Current calibration file:	Preview2.calx				
Assay type:	Assay name	**Ion range calc method:**	Manual		
Inj vol:	100.000				
Instrument method:	EPA536Triazines				
Tune/Breakdown method	EPA536Triazines				

Flags calibration:

Compound	Max RSD (%)	Min RF	R^2 threshold	Max amt diff (%)
DIA	20.00	0.00	0.990	20.000
DEA	20.00	0.00	0.990	20.000
Cyanazine	20.00	0.00	0.990	20.000
Simazine	20.00	0.00	0.990	20.000
Atrazine	20.00	0.00	0.990	20.000
Propazine	20.00	0.00	0.990	20.000

Method Report

Method name:	Preview2_EPA536-Triazines			**Page number:**	Page 7 of 15
Master method name:	EPA536-Triazines				
Current calibration file:	Preview2.calx				
Assay type:	Assay name	**Ion range calc method:**	Manual		
Inj vol:	100.000				
Instrument method:	EPA536Triazines				
Tune/Breakdown method	EPA536Triazines				

Flags check standard:

Compound	Max RF diff (%)	Min RF	Max amt diff (%)
DIA	20.00	10.000	20.000
DEA	20.00	10.000	20.000
Cyanazine	20.00	10.000	20.000
Simazine	20.00	10.000	20.000
Atrazine	20.00	10.000	20.000
Propazine	20.00	10.000	20.000

Method Report

Method name:	Preview2_EPA536-Triazines			**Page number:**	Page 8 of 15
Master method name:	EPA536-Triazines				
Current calibration file:	Preview2.calx				
Assay type:	Assay name	**Ion range calc method:**	Manual		
Inj vol:	100.000				
Instrument method:	EPA536Triazines				
Tune/Breakdown method	EPA536Triazines				

Flags Blank (for GC):

Compound	Criterion	Max value
DIA	% of LOQ	0.200
DEA	% of LOQ	0.200
Cyanazine	% of LOQ	0.200
Simazine	% of LOQ	0.200
Atrazine	% of LOQ	0.200
Propazine	% of LOQ	0.200

Method Report

Method name:	Preview2_EPA536-Triazines			**Page number:**	Page 9 of 15
Master method name:	EPA536-Triazines				
Current calibration file:	Preview2.calx				
Assay type:	Assay name	**Ion range calc method:**	Manual		
Inj vol:	100.000				
Instrument method:	EPA536Triazines				
Tune/Breakdown method	EPA536Triazines				

Flags ISTD:

Compound	Min recovery (%)	Max recovery (%)	Min RT (-min)	Max RT (+min)
DIA D-5	50.00	150.00	0.25	0.25
DEA D-7	50.00	150.00	0.25	0.25
Cyanazine D-5	50.00	150.00	0.25	0.25
Simazine D-10	50.00	150.00	0.25	0.25
Atrazine D-5	50.00	150.00	0.25	0.25
Propazine D-14	50.00	150.00	0.25	0.25

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 10 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Flags solvent blank:

Compound	Method	Upper Limit %
DIA D-5	Quan Ion RT	2
DIA	Quan Ion RT	2
DEA D-7	Quan Ion RT	2
DEA	Quan Ion RT	2
Cyanazine D-5	Quan Ion RT	2
Cyanazine	Quan Ion RT	2
Simazine D-10	Quan Ion RT	2
Simazine	Quan Ion RT	2
Atrazine D-5	Quan Ion RT	2
Atrazine	Quan Ion RT	2
Propazine	Quan Ion RT	2
Propazine D-14	Quan Ion RT	2

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 11 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Flags surrogates:

Compound	Theo Conc	Min Recovery (%)	Max Recovery (%)

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 12 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Flags matrix spike:

Compound	Theo Conc	Min Recovery (%)	Max Recovery (%)	Max RPD
DIA	0.500	50.00	150.00	50.00
DEA	0.500	50.00	150.00	50.00
Cyanazine	0.500	50.00	150.00	50.00
Simazine	0.500	50.00	150.00	50.00
Atrazine	0.500	50.00	150.00	50.00
Propazine	0.500	50.00	150.00	50.00

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 13 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Flags lab control:

Compound	Theo Conc	Min Recovery (%)	Max Recovery (%)	Max RPD
DIA	0.500	50.00	150.00	50.00
DEA	0.500	50.00	150.00	50.00
Cyanazine	0.500	50.00	150.00	50.00
Simazine	0.500	50.00	150.00	50.00
Atrazine	0.500	50.00	150.00	50.00
Propazine	0.500	50.00	150.00	50.00

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 14 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Flags method validation:

Compound	Theo Conc	Min Recovery (%)	Max Recovery (%)	Max RSD
DIA	0.500	50.00	150.00	20.00
DEA	0.500	50.00	150.00	20.00
Cyanazine	0.500	50.00	150.00	20.00
Simazine	0.500	50.00	150.00	20.00
Atrazine	0.500	50.00	150.00	20.00
Propazine	0.500	50.00	150.00	20.00

Method Report

Method name: Preview2_EPA536-Triazines **Page number:** Page 15 of 15
Master method name: EPA536-Triazines
Current calibration file: Preview2.calx
Assay type: Assay name **Ion range calc method:** Manual
Inj vol: 100.000
Instrument method: EPA536Triazines
Tune/Breakdown method EPA536Triazines

Breakdown Groups

GroupName	Max % breakdown

Members

Method Validation Report

Method Validation Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines EPA536-Triazines
Cali File: Preview2.calx

Method Validation Summary

Compound	Avg Conc	Theo Conc	% Diff	Min Conc	Max Conc	% RSD	Max % RSD	
DIA D-5	295652					0.00		IS
DIA	0.358	0.500	-28.34	0.250	0.750	0.00	20.00	
DEA D-7	1778658					0.00		IS
DEA	0.602	0.500	20.45	0.250	0.750	0.00	20.00	
Cyanazine D-5	2224244					0.00		IS
Cyanazine	0.565	0.500	12.90	0.250	0.750	0.00	20.00	
Simazine D-10	505462					0.00		IS
Simazine	0.607	0.500	21.49	0.250	0.750	0.00	20.00	
Atrazine D-5	2334865					0.00		IS
Atrazine	0.512	0.500	2.46	0.250	0.750	0.00	20.00	
Propazine	0.757	0.500	51.41	0.250	0.750	0.00	20.00	<<<
Propazine D-14	272050					0.00		IS

Manually integrated ☐

<<< = Failure

Method Validation Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Method Validation Report Data

Compound	1
DIA D-5	295652
DIA	0.358
DEA D-7	1778658
DEA	0.602
Cyanazine D-5	2224244
Cyanazine	0.565
Simazine D-10	505462
Simazine	0.607
Atrazine D-5	2334865
Atrazine	0.512
Propazine	0.757
Propazine D-14	272050

Manually integrated ☐

<<< = Failure

Method Validation Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:10	SampleID003	500ppt-003	N/A	D003	6/26/2007 10:18:49 PM	New Dilutions 6/26/2007 F

Manually integrated ☐ **<<< = Failure**

MSMSD Report

MSMSD Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:1	SampleID021	DACTTest001	N/A	D021	6/27/2007 11:42:07 AM	New dilution of DACT

SampleID021

Compound	Unknown Conc	Spike Amt	MS Conc	% Rec	Lower Limit %	Upper Limit %	Rec Fails
DIA	0.000	0.500	0.000	0.00	50.00	150.00	0
DEA	0.000	0.500	0.000	0.00	50.00	150.00	0
Cyanazine	0.000	0.500	0.000	0.00	50.00	150.00	0
Simazine	0.000	0.500	0.000	0.00	50.00	150.00	0
Atrazine	0.000	0.500	0.000	0.00	50.00	150.00	0
Propazine	0.000	0.500	0.000	0.00	50.00	150.00	0

QC Standard Report

QC Standard Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jim.edwards
Batch: fs_int_5212008_a
Methods: fs_int_5212008_a_fs_int
fs_int
Cali File: fs_int_5212008_a.calx

Row	Sample ID	Filename	Sample Name	File Date	Comment
6	qc std = 50 ng/uL	qc_std_50		5/21/2008 8:47:04 PM	

Compound	Type	Daily RF	Mean RF	Min RF	RF %D	Max RF % D	Inj amt	Calc amt	Amt %D	Max Amt %D	Flag
Pentachloroethane	L	0.508		0.000			50.000	47.006	-5.99	15.00	Pass
1,3-Dichlorobenzene	L	1.604		0.000			50.000	47.186	-5.63	15.00	Pass
1,4-Dichlorobenzene	L	1.639		0.000			50.000	47.755	-4.49	15.00	Pass
1,2-Dichlorobenzene	L	1.529		0.000			50.000	46.925	-6.15	15.00	Pass
Hexachloroethane	L	0.520		0.000			50.000	47.320	-5.36	15.00	Pass
Nitrobenzene-d5	L	0.263		0.000			50.000	48.636	-2.73	15.00	Pass
1,2,4-Trichlorobenzene	L	0.336		0.000			50.000	47.525	-4.95	15.00	Pass
Hexachloropropene	L	0.192		0.000			50.000	46.293	-7.41	15.00	Pass
Hexachlorobutadiene	L	0.152		0.000			50.000	48.356	-3.29	15.00	Pass
1,2,4,5-Tetrachlorobenzene	L	0.579		0.000			50.000	47.572	-4.86	15.00	Pass
Hexachlorocyclopentadiene	L	0.292		0.000			50.000	44.738	-10.52	15.00	Pass
2-Fluorobiphenyl	L	1.367		0.000			50.000	50.479	0.96	15.00	Pass
2-Chloronaphthalene	L	1.739		0.000			50.000	46.413	-7.17	15.00	Pass
Pentachlorobenzene	L	0.428		0.000			50.000	47.702	-4.60	15.00	Pass
Hexachlorobenzene	L	0.198		0.000			50.000	50.951	1.90	15.00	Pass
p-Terphenyl-d14	L	0.968		0.000			50.000	48.576	-2.85	15.00	Pass

Internal standard summary:

Compound	Std Response	Min	Max	Sample Response
1,4-Dichlorobenzene-d4	14404699	7202349(50.00%)	21607048(150.00%)	16845174
Naphthalene-d8	54661104	27330552(50.00%)	81991657(150.00%)	65021230
Acenaphthene-d10	29970209	14985104(50.00%)	44955313(150.00%)	36089270
Phenanthrene-d10	56249845	28124923(50.00%)	84374768(150.00%)	64155577
Chrysene-d12	31711250	15855625(50.00%)	47566875(150.00%)	35263190
Perylene-d12	27504889	13752444(50.00%)	41257333(150.00%)	29857492
	Std RT	**Min**	**Max**	**Sample RT**
1,4-Dichlorobenzene-d4	4.45	4.20(-0.25)	4.70(+0.25)	4.45
Naphthalene-d8	5.96	5.71(-0.25)	6.21(+0.25)	5.96
Acenaphthene-d10	7.96	7.71(-0.25)	8.21(+0.25)	7.95
Phenanthrene-d10	9.60	9.35(-0.25)	9.85(+0.25)	9.60
Chrysene-d12	12.53	12.28(-0.25)	12.78(+0.25)	12.53
Perylene-d12	13.99	13.74(-0.25)	14.24(+0.25)	13.99

Surrogate recovery:

Compound	Conc added	Conc recovered	% Recovered	Limits

Manually integrated [ ] *** = Fail;R=Recovery limits exceeded;Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard**

QC Standard Report

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	**Methods:**	fs_int_5212008_a_fs_int
User:	AMER\jim.edwards		fs_int
Batch:	fs_int_5212008_a	**Cali File:**	fs_int_5212008_a.calx

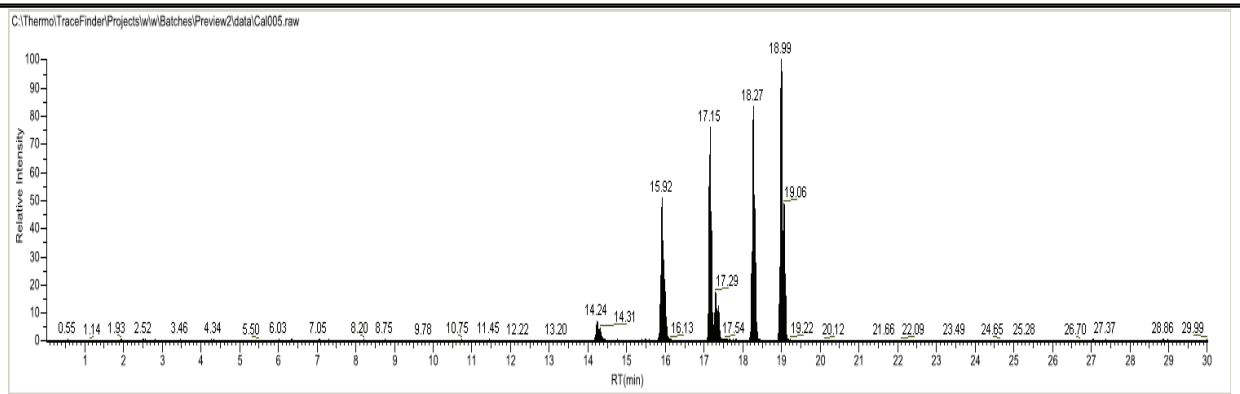
Quantitation Report

Quantitation Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:6	SampleID005	Cal005	c5	D005	6/26/2007 7:43:12 PM	New Dilutions 6/26/2007 Hypersil Gold 100x2



Internal Standards	RT	QIon	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
DIA D-5	14.24	137.00	287980	Linear	0.000	1.000	ng/ml	1.000	ng/ml
DEA D-7	15.92	147.10	1679937	Linear	0.000	1.000	ng/ml	1.000	ng/ml
Cyanazine D-5	17.15	219.10	2255487	Linear	0.000	1.000	ng/ml	1.000	ng/ml
Simazine D-10	17.29	137.00	499551	Linear	0.000	1.000	ng/ml	1.000	ng/ml
Atrazine D-5	18.27	179.00	2367556	Linear	0.000	1.000	ng/ml	1.000	ng/ml
Propazine D-14	19.06	188.04	1313475	Linear	0.000	1.000	ng/ml	1.000	ng/ml

Target Compounds	RT	QIon	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
DIA	14.31	132.09	182117	Linear	0.632	2.419	ng/ml	2.419	ng/ml
DEA	15.98	146.06	732057	Linear	0.436	2.241	ng/ml	2.241	ng/ml
Cyanazine	17.18	214.03	1331175	Linear	0.590	2.289	ng/ml	2.289	ng/ml
Simazine	17.37	124.17	352249	Linear	0.705	2.24	ng/ml	2.24	ng/ml

Manually integrated ☐

Quantitation Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Target Compounds	RT	QIon	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
Atrazine	18.31	174.06	1415179	Linear	0.598	2.316	ng/ml	2.316	ng/ml
Propazine	18.99	196.00	2707903	Linear	2.062	3.439	ng/ml	3.439	ng/ml

Manually integrated ☐

Solvent Blank Report

Solvent Blank Report

Page 1 of 1

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:1	SampleID-14	FreshBlankWednesday	N/A	D-14	6/27/2007 4:38:40 PM	New Dilutions 6/26/2007 Hyp

Internal Standards	RT	QIon	Response	Method	Upper Limit	
DIA D-5	14.18	137.00	14705	Quan Ion RT	2	**Fail**
DEA D-7	15.83	147.10	234369	Quan Ion RT	2	**Fail**
Cyanazine D-5	17.07	219.10	1007120	Quan Ion RT	2	**Fail**
Simazine D-10	17.29	137.00	65	Quan Ion RT	2	**Fail**
Atrazine D-5	18.20	179.00	422464	Quan Ion RT	2	**Fail**
Propazine D-14	19.11	188.04	386	Quan Ion RT	2	**Fail**

Target Compounds	RT	QIon	Response	Method	Upper Limit	
DIA	14.38	132.09	773	Quan Ion RT	2	**Fail**
DEA	N/F	146.06	N/F	Quan Ion RT	2	**Pass**
Cyanazine	17.19	214.03	1956	Quan Ion RT	2	**Fail**
Simazine	N/F	124.17	N/F	Quan Ion RT	2	**Pass**
Atrazine	N/F	174.06	N/F	Quan Ion RT	2	**Pass**
Propazine	18.93	196.00	230619	Quan Ion RT	2	**Fail**

Manually integrated

Surrogate Recovery Report

Surrogate Recovery Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:7	SampleID006	Cal006	c6	D006	6/26/2007 8:14:20 PM	New Dilutions 6/26/2007

Compound	Conc added	Conc recovered	% Recovered	Limits	
DIA D-5	0.500	0.000	0.00	50.00 - 150.00	
DIA	0.500	0.000	100.00	50.00 - 150.00	
DEA	0.500	5.111	100.00	50.00 - 150.00	R
Cyanazine	0.500	5.123	100.00	50.00 - 150.00	R

Manually integrated ☐ **R=Recovery limits exceeded**

Using Copy Down and Fill Down

This appendix describes the Copy down and Fill down commands that you can use to make entering column values easier.

You can use the Fill down command for the Sample name, Sample ID, Vial position, and Sample level columns.

You can use the Copy down command for the Sample type, Vial position, Injection volume, Conv factor, and Sample level columns.

Use the following procedures

- To automatically enter sequential column values
- To automatically copy column values
- To use Copy down or Fill down for a range of samples

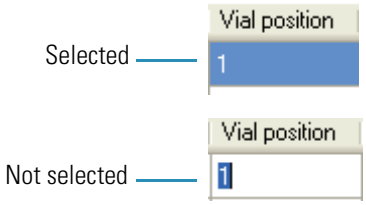
❖ To automatically enter sequential column values

1. Enter a value for the first row of the fill down sequence.

   This does not have to be the first sample row. You can begin the fill down procedure from any row in the sequence.

2. Select the cell whose value is the first in the fill down sequence.

   Observe that this cell is selected.



   You can repeatedly use the **Fill down** command to create multiple sequences. See "Example 1" on page 277.

3. Right-click and choose **Fill down** from the shortcut menu.

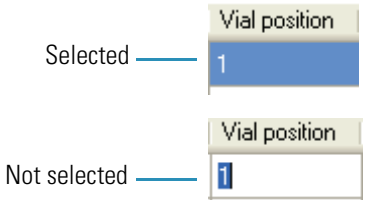
   The application enters sequential column values starting with the value in the selected row and ending with the last row in the column.

Note If you use the Fill down command for the Vial position column and you have an autosampler configured, the TraceFinder application knows the number of vial positions configured in your autosampler and numbers the positions accordingly. See "Example 2" on page 277.

❖ To automatically copy column values

1. Select the cell whose value you want to copy to all cells below it.

   Observe that this cell is selected.



2. Right-click and choose **Copy down** from the shortcut menu.

   The value is copied to all rows below the selected row.

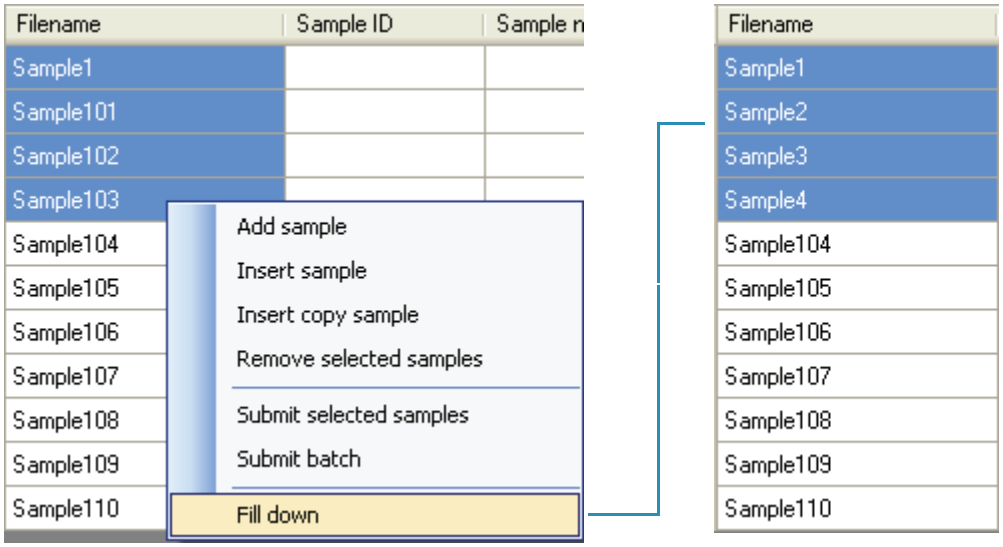
❖ To use Copy down or Fill down for a range of samples

1. To select a range of sample values, do one of the following:
   - Drag your cursor to select a contiguous group of sample values.

     –Or–

   - Hold down the SHIFT key to select a contiguous group of sample values.
2. Right-click and choose the appropriate command from the shortcut menu.

   The column values are copied or entered sequentially starting with the value in the first selected row and ending with the last selected row.



Example 1

You can repeatedly use the Fill down command to create multiple sequences.

Vial position
A:A1
A:A2
A:A1
A:A2
A:A1
A:A2
A:A3
A:A4

Example 2

The TraceFinder application knows the number of vial positions configured in your autosampler and numbers the positions accordingly.

Vial position
A:A1
A:A2
A:A3
A:A4
A:A5
A:A6
A:A7
A:A8
A:A9
A:A10
A:A11
A:A12
A:B1
A:B2
A:B3
A:B4
A:B5
A:B6

Using Filter Criteria

The filter criteria tool is available from the compound datastore in the Configuration mode and the acquisition list in the Method Development mode.

❖ To filter the compound list

1. To display only a filtered list of compounds, click the funnel icon,  , in the column header.

   For each column, a list of filterable criteria is displayed. On all columns, your filter choice are All, Blanks, and NonBlanks. Other filter criteria is specific to the individual columns.

2. To create a custom filter based on compound values in a specific column, choose **Custom** from the column list box.

   The Enter filter criteria dialog box opens. See "Enter Filter Criteria" on page 280.

3. From the Operator list box, select an operator.

4. From the Operand list box, select an operand.

5. When all conditions are defined, click **OK**.

   The complete filter string is displayed at the bottom of the dialog box. For example:

   ```
   chemical formula = Blanks
   ```

Enter Filter Criteria

The Enter filter criteria dialog box is specifically named for the column on which you are filtering. In this example, the selected column is the Compound Name column.

Figure 9. Enter filter criteria dialog box

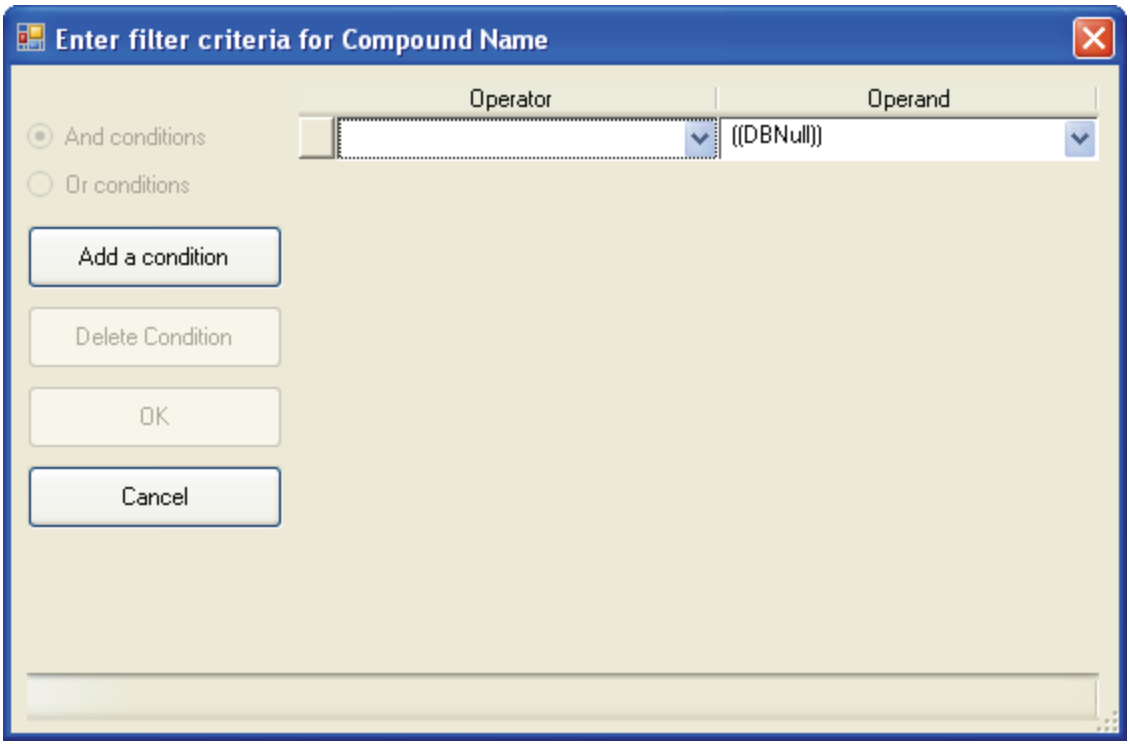


Table 43. Filter criteria parameters

Parameter	Description
And conditions	Requires that all filter criteria must be met.
Or conditions	Requires that any of the specified filter criteria be met.
Add a condition	Adds a new, empty condition to the filter criteria.
Delete condition	Deletes the selected condition. Click the box at the left of the row to select the condition.
Operator	The mathematical function applied to the operand.
Operand	The arguments to which the operator is applied.

Index

Symbols

A

B

C

D

E

F

G

H

I

L

M

N

O

P

Q

R

S

T

U

V

W