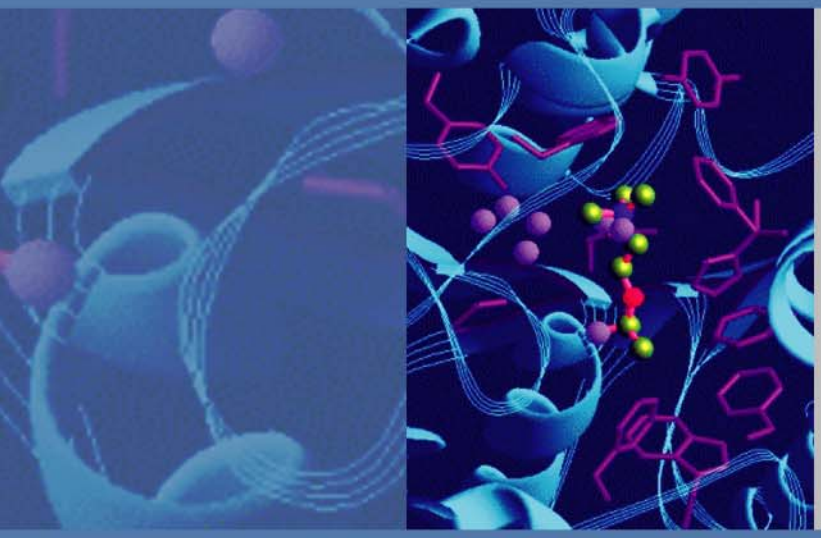

Thermo

TraceFinder

Version 1.1

User Guide

XCALI-97357 Revision A June 2011

DOCUMENTATION SURVEY

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Thermo SCIENTIFIC

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Release history: Revision A

Minimum software requirements: Xcalibur 2.1.0 SP1; Microsoft Windows XP Professional SP 3; (optional) LC Devices 2.5

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

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Preface

The TraceFinder application is the newest application in the series of Thermo Scientific LC/MS analytical software.

Contents

- Related Documentation
- Special Notices
- System Requirements
- System Activation
- Contacting Us

❖ **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

The TraceFinder documentation includes Help that you can access from the application and also includes the *TraceFinder User Guide* and four quick reference guides as PDF files that you can access from the TraceFinder Help menu and the Windows Start menu.

❖ **To view the TraceFinder user guide or quick reference guides**

Go to **Start > All Programs > Thermo TraceFinder > Manuals** and choose one of the following documents:

- *TraceFinder User Guide*
- *TraceFinder Administrator Quick Reference Guide*
- *TraceFinder Acquisition Quick Reference Guide*
- *TraceFinder Data Review Quick Reference Guide*
- *TraceFinder Shortcut Menus Quick Reference Guide*
- *TraceFinder Custom Reports Tutorial*

❖ **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, visit www.thermo.com. You can find application notes at www.thermo.com/appnotes.

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.

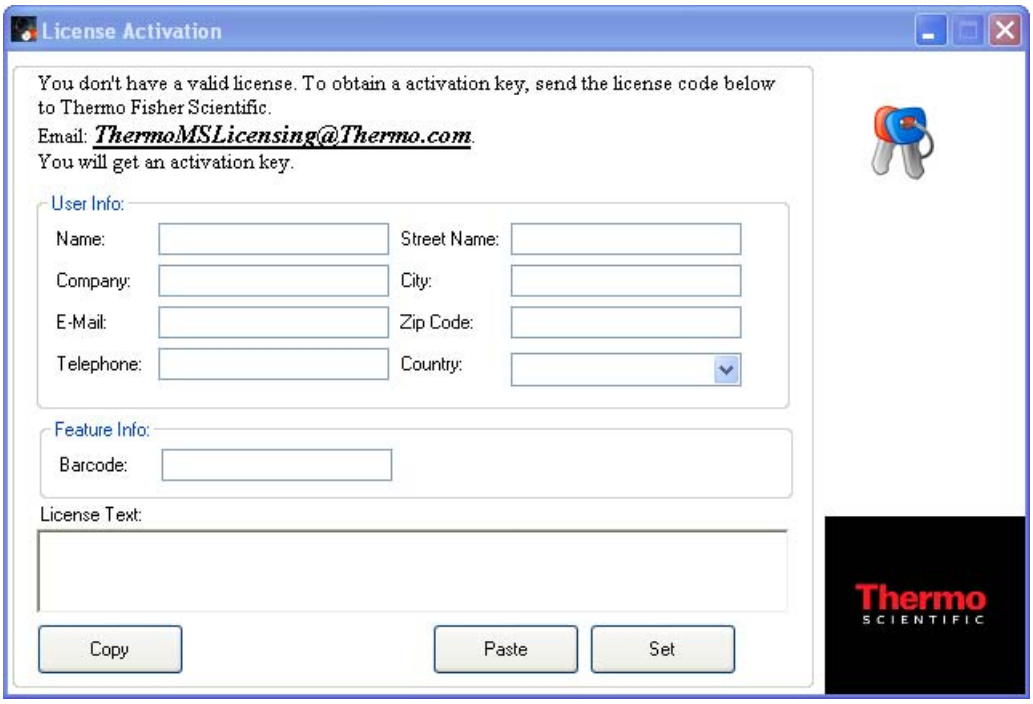
System Requirements

Your system must meet these minimum requirements.

System	Requirements
Computer	• 2.33 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)	• AS3000 autosampler
Software	• Microsoft™ Windows™ XP Professional SP3 • Microsoft Office 2007 SP2 or Excel™ 2007 SP2 • Microsoft .NET Framework 3.5 SP 1 • Thermo Foundation™ 1.1 (available on the Xcalibur 2.1.0 CD) • Thermo Xcalibur™ 2.1 and Xcalibur 2.1.QF • Adobe Reader 9.0 • NIST 2008

System Activation

When you first start the TraceFinder application, a dialog box displays the number of days remaining on your 30-day free trial. If your free trial has expired, the License Activation window opens.



Note You can open the License Activation window at any time during your trial period by choosing **Help > License Activation** from the TraceFinder menu. If you already have a permanent license, a message tells you that your product is fully licensed.

Two types of licenses are available:

- 30-Day Evaluation Version (free of charge)
- Full Version Single License

The evaluation version is full-featured and automatically expires 30 days after activation. Any attempt to set back the system date automatically terminates this version. You can purchase and then activate the full version of the TraceFinder application at any time, during or after the free evaluation, without reinstalling the software.

Each activation key is valid only for a single license. Any additional installation generates a different license and requires a different activation key.

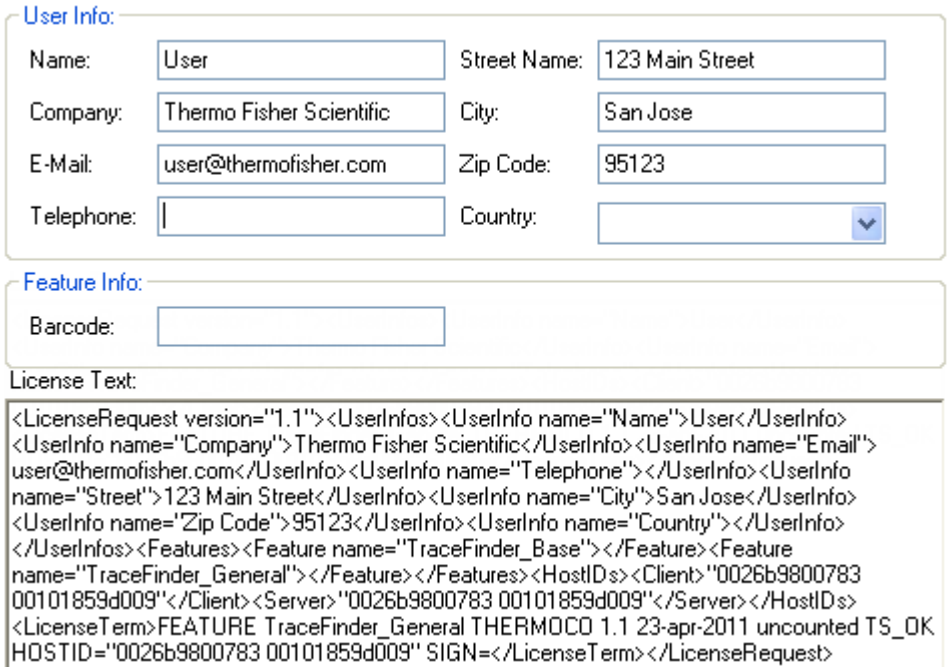
For questions regarding activation, contact Thermo Fisher Scientific Technical Support in San Jose, CA:

- E-mail: ThermoMSLicensing@thermofisher.com
- Fax: 408-965-6120

❖ To request an activation key

1. In the License Activation window, enter your information in the User Info area.

   As you type, the License Text box creates an XML text string with your information.



2. In the barcode box, type the barcode printed on the TraceFinder CD.

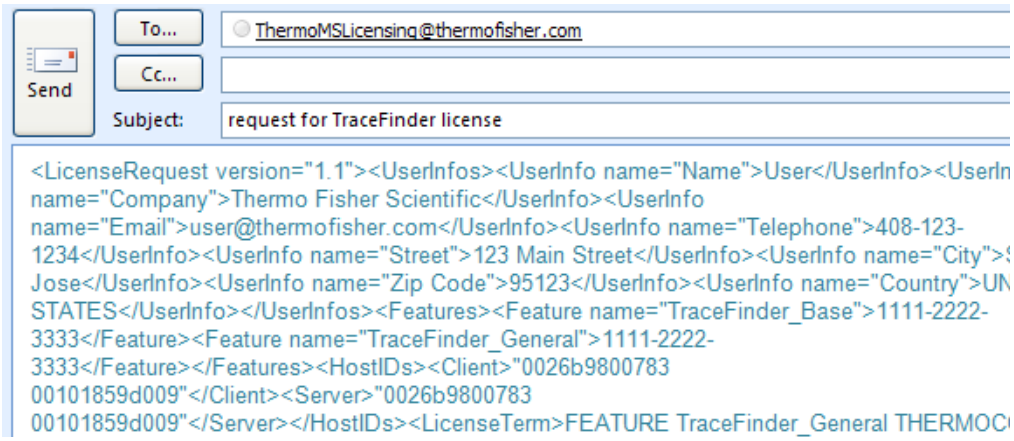
   The form of the barcode number is either *xxxx-xxxx-xxxx* or *xxxx-xxxx-xxxx-xxxx*.

3. When you finish entering all your information, click **Copy**.

   The application copies this XML text to the Clipboard.

   If you have not completed all the information, a pop-up box opens, identifying the missing information.

4. Paste this XML text in the body of an e-mail and send the e-mail to ThermoMSLicensing@thermofisher.com.



❖ To use your activation key

Note You must run the TraceFinder application with ITAdmin or LabDirector rights when entering the activation key.

1. When you receive your activation key, copy it from the e-mail.
2. Choose **Help > License Activation** from the TraceFinder menu.

   The License Activation window opens.
3. Click **Paste**.

   The application pastes the contents of the Clipboard to the License Text box.
4. Click **Set.**

   The application is activated according to the type of authorization your license gives you.

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 get local contact information for sales or service

Go to www.thermoscientific.com/wps/portal/ts/contactus.

❖ To copy manuals from the Internet

Go to mssupport.thermo.com, agree to the Terms and Conditions, and then 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 www.surveymonkey.com/s/PQM6P62.
- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

Introduction

This chapter describes the general features of TraceFinder software.

Contents

- About the TraceFinder Application
- TraceFinder Feature Summary
- TraceFinder Workflow
- Reporting Features

About the TraceFinder Application

The TraceFinder application targets general quantitation and environmental markets, creating the workflows that laboratories use. It supports a focused workflow for specific non-bioanalytical laboratory use, instrument control, and method development functionality in a single software package. The TraceFinder application is the primary application for the TSQ Quantum™ XLS triple quadrupole mass spectrometers.

The TraceFinder application can export SRM data in .xml format so that other applications 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 the Xcalibur data system
- Compounds from files that use the datastore (.xml) format
- Batches or methods from the TraceFinder 1.0.1 application

The TraceFinder application checks the 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

The TraceFinder application supports the following file types:

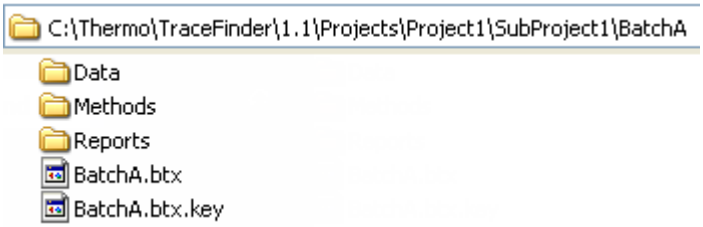
- Comma-separated values (.csv): A set of file formats used to store tabular data in which numbers and text are stored in plain textual form that can be read in a text editor. Lines in the text file represent rows of a table, and commas in a line separate fields in the tables row.
- Extensible Markup 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.
- Instrument method (.meth): A proprietary file format for the Xcalibur software suite with specific instructions that enable scientific instruments to perform data acquisition.
- Processing method (.pmd): A proprietary file format for the Xcalibur software suite with specific instructions on processing data that was acquired through the instruments attached to the system.
- Raw data (.raw): The file type for acquired samples on the system.

TraceFinder Directory Structure

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

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

Figure 1. Example batch directory structure



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 both the general quantitation and the environmental and food safety applications. The application has a fully automated acquisition mode and a manual data 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, reviewing, and reporting. In addition, it can compare the mass spectral and integrate the processes of data review and reporting.

Key features include the following:

- Role-based authorization for LabDirector, ITAdmin, Supervisor, Technician, and QAQC (quality assurance) roles
- Configuration mode for user administration, project administration, datastore administration, and application administration
- Method Development mode for editing instrument methods, setting processing and error flag parameters, and setting report options
- Acquisition mode that acts as a wizard to guide you in creating batches and running samples
- Data Review mode with batch views, data review, local method views, and report views
- Database-capable method development
- Quantification workflows, supporting capabilities present in the LCquan and LabForms applications
- Standard and customized report formats

Features of the common workflow core include the following:

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

TraceFinder Workflow

The TraceFinder application 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 that you expect to run in your lab. When you are ready to run a particular type of sample, select the appropriate method and begin.

When using the TraceFinder application, follow these basic steps:

1. Create and save a master method in the Method Development mode.

   A master method combines the instrument method and processing method that define how the raw data is acquired and processed, how the error checking information evaluates the results, and how the results appear in reports.

2. Create and submit a batch in the Acquisition mode.

   A batch lists 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.

   Note At any time, you can quickly view the system status by looking in the lower right corner of the TraceFinder window. This area displays a green, yellow, or red LED and a description of the number of samples in the queue (if any).

4. Evaluate the data in the Acquisition mode.

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

5. View and print reports in the Report View of the Acquisition mode.

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

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, helping to track the performance of LC systems and methods. The reports divide into three groups: Standard, Custom, and Target Screening.

For additional information about standard, custom, and target screening reports and a sample of each standard report type, see "Reports" on page 353. Examples of standard reports (as PDFs) are also located in the C:\Thermo\TraceFinder\1.1\ExampleReports folder.

Standard Report Types

- Batch Report
- Batch Report Rev 1
- Blank Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- Confirmation Report 2
- High Density Calibration Report
- 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 (Environmental and Food Safety only)
- Manual Integration Report
- Method Detection Limit Report (Environmental and Food Safety only)
- Method Report
- Method Validation Report (Environmental and Food Safety only)
- MSMSD Report (Environmental and Food Safety only)
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary Report

Custom Report Types

- AltCalibrationReport
- Alternate BatchReport
- Alternate CalibrationReport
- Alternate ConfirmationReport
- Alternate MatrixSpikeReport
- Alternate SampleReport
- Alternate SummaryReport
- BatchReport
- BlankReport
- CalibrationDensityReport
- CalibrationReport
- CheckStandardReport
- CompoundCalibrationReport
- ConfirmationReport
- ConfirmationReport2
- HighDensitySampleReport1Long
- HighDensitySampleReport2Long
- HighDensitySampleReport3Long
- HighDensitySampleReport4
- HighDensitySampleReport5
- QuantitationReport
- SteroidAnalysisReport

Target Screening Report Types

Target Screening reports are available only when you enable the Target Screening features. See "Enabling Target Screening" on page 83.

- Target Screening Long Report
- Target Screening Summary Report

Getting Started

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

Contents

- Installing the TraceFinder Application
- Installing the QED and NIST Libraries
- Launching the NIST Library Browser
- Launching the Qual Browser
- Converting Legacy Data
- Choosing a Mode

Installing the TraceFinder Application

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

❖ To install the TraceFinder application

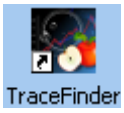
1. Follow the instructions on the included CDs to install the Xcalibur 2.1 data system and your instrument drivers.
2. Install the driver for your LC device and autosampler.
3. Insert the TraceFinder CD in the drive, and follow the on-screen instructions.

   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 > TraceFinder** or **TraceFinder EFS**.

   By default, user security is not enabled and the application does not require a password. To enable user security, see "Specifying User Security" on page 66.

❖ To log on to the TraceFinder application (when user security is enabled)

1. Enter your assigned user name.

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

   IMPORTANT If you are the administrator logging on for the first time with user security enabled, use **Administrator/Password** as the *username/password*.

2. Enter your password.

   If your user name or 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 25.

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

Figure 2. TraceFinder logon screen

Table 1. Logon screen parameters

Parameter	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	Closes the TraceFinder application without logging on.

Installing the QED and NIST Libraries

When you are using triple quad instruments, follow these instructions to install the NIST and QED libraries.

❖ To install the NIST library

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

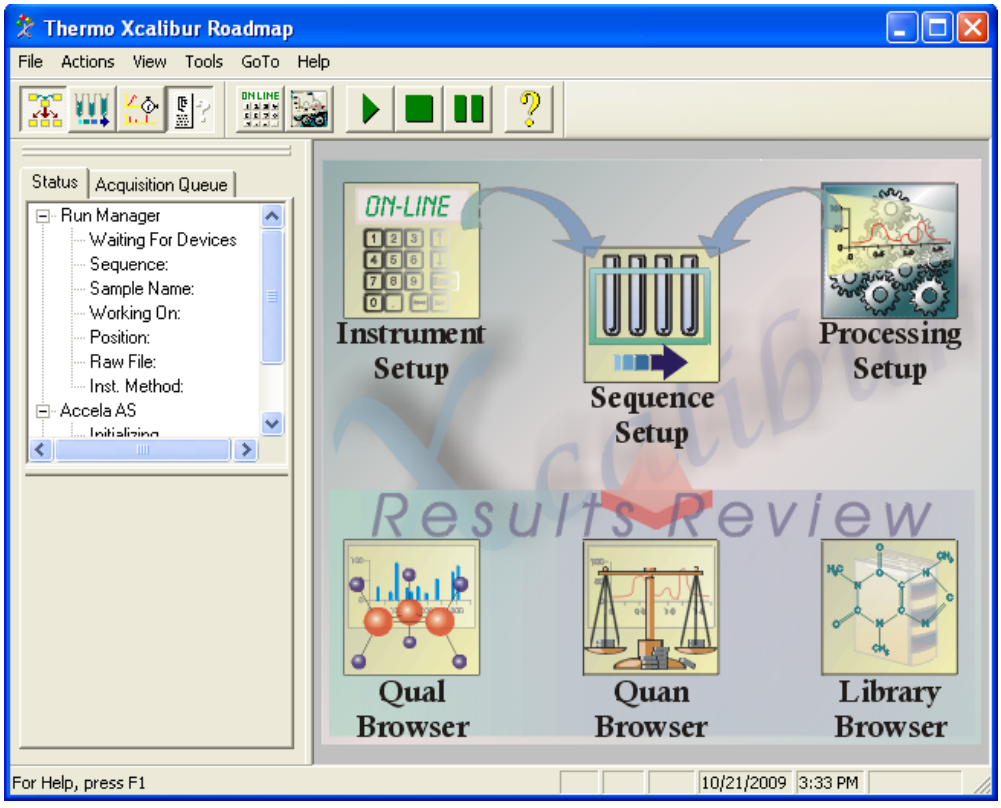
   The NIST 08 MS Search and AMDIS Setup wizard opens.
3. Follow the instructions in the setup wizard.
4. When the wizard prompts you to select a program folder, select **C:\Thermo**.

❖ To install the QED library

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

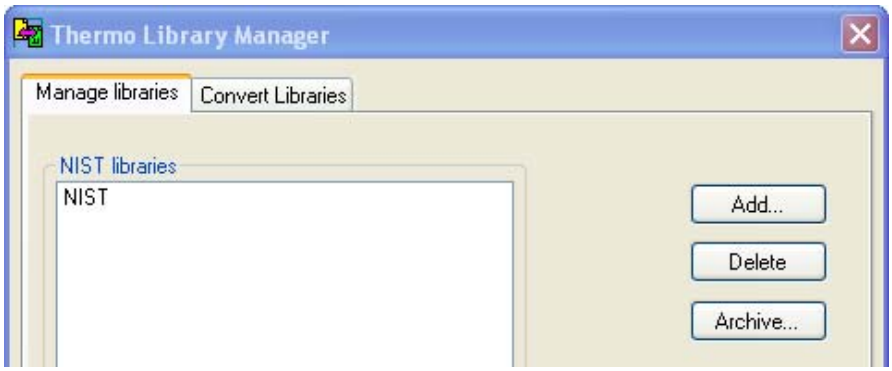
.

   The Thermo Xcalibur Roadmap opens.



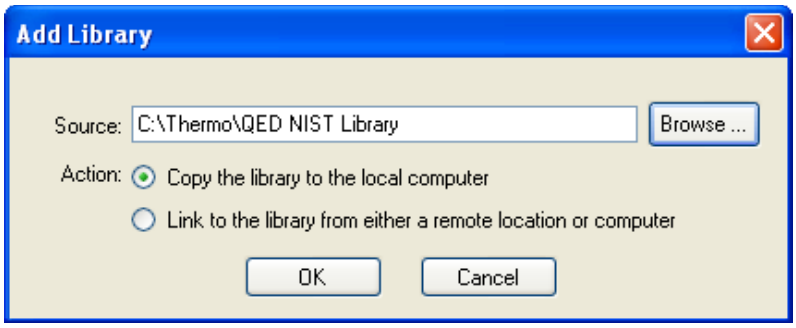
2. Select **Tools > Library Manager**.

   The Thermo Library Manager dialog box opens. The NIST library is displayed in the NIST Libraries list.



3. Click **Add**.

   The Add Library dialog box opens.



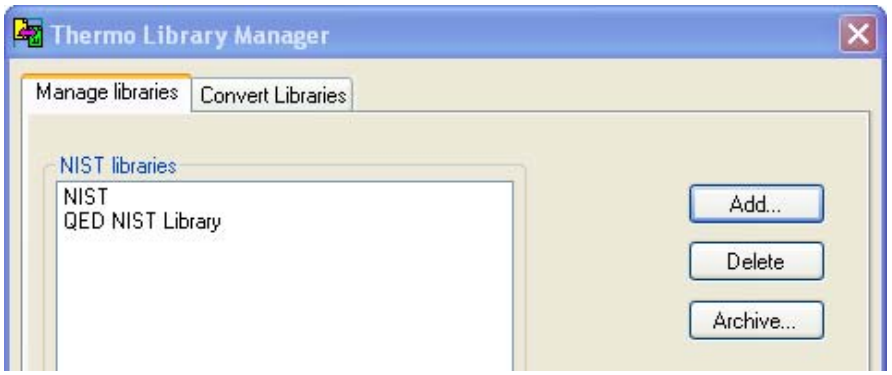
4. Click **Browse**, and locate your QED library in the C:\Thermo folder.

5. Click **OK**.

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

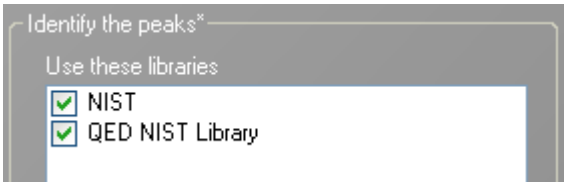
6. Click **Dismiss** to close the message box.

   The application adds the QED library to the NIST Libraries list in the Library Manager dialog box.



7. Click **Exit** in the Thermo Library Manager dialog box.
8. Start the TraceFinder application.
9. Go to the Method Development mode.
10. Click **Method View** in the navigation pane.
11. Choose **File > New > Method Template** from the main menu.

    The QED NIST Library is listed in the Use These Libraries list in the Method Template Editor.



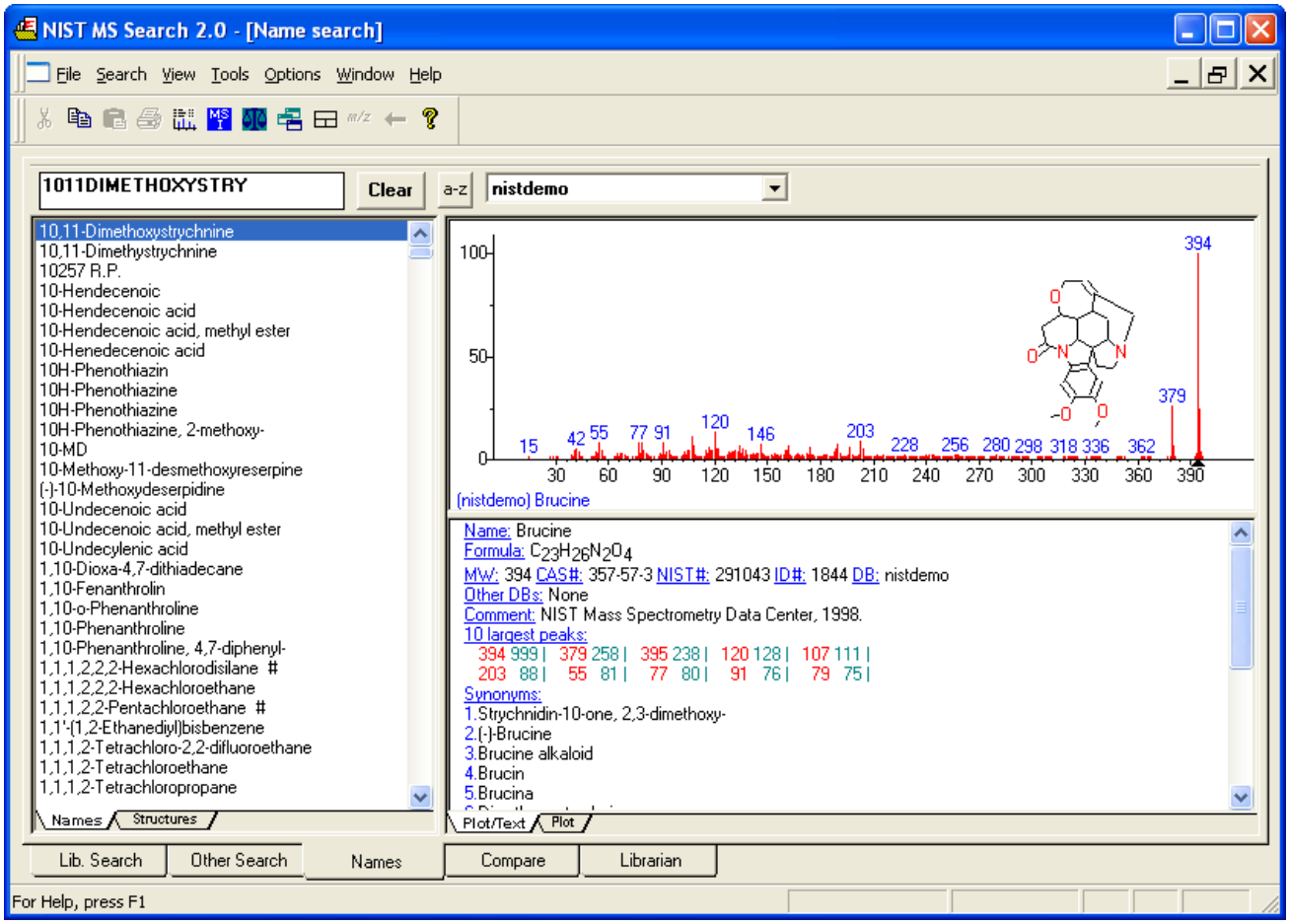
Launching the NIST Library Browser

Use the NIST MS Search tool to search the NIST library.

❖ To open the NIST library browser

1. Choose **Go > Launch Library Browser** from the main menu.

   The NIST MS Search window opens.



For detailed instructions about using the library browser, refer to the NIST MS Search window Help.

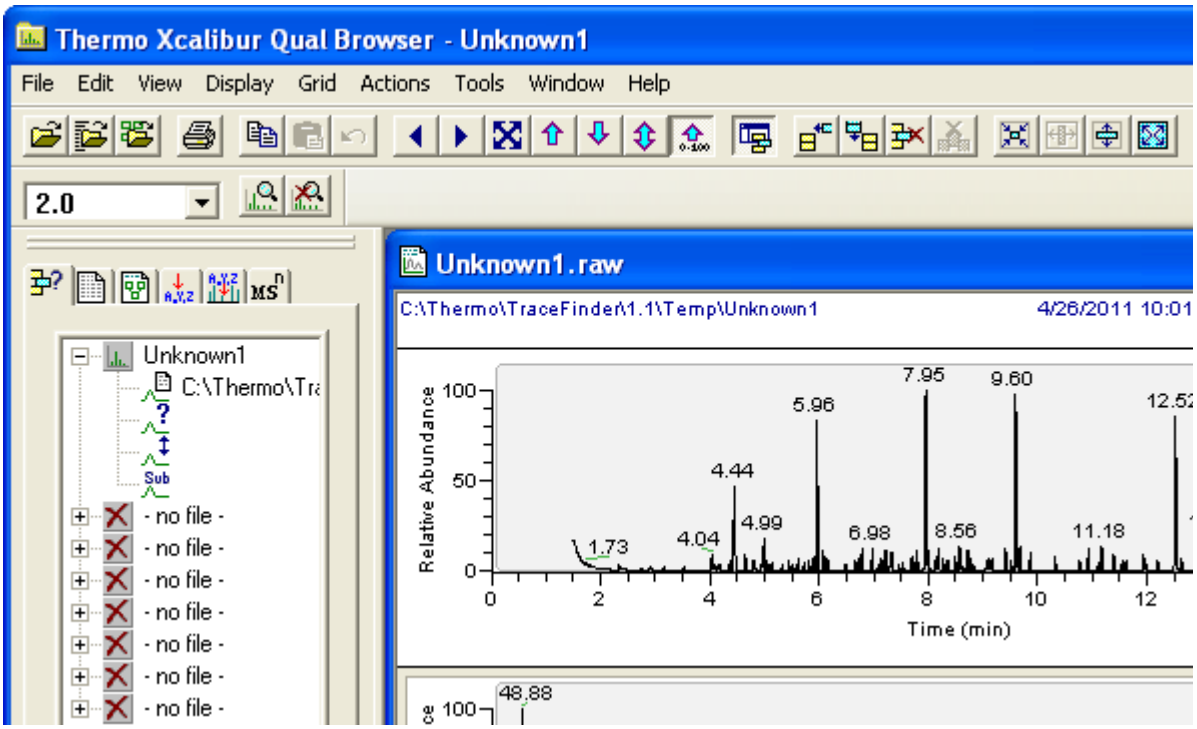
Launching the Qual Browser

Use the Qual Browser to view chromatograms and spectra from raw data files or qualitative processing results.

❖ To open the Qual Browser

1. Choose **Go > Launch Qual Browser** from the main menu.

   The Thermo Xcalibur Qual Browser opens.



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

Converting Legacy Data

Use the TraceFinder Legacy Data Converter to convert methods, batches, method templates, or batch templates from a previous version of TraceFinder to the current version.

To open the TraceFinder Legacy Data Converter, choose **Go > Launch Legacy Data Converter** from the main menu.

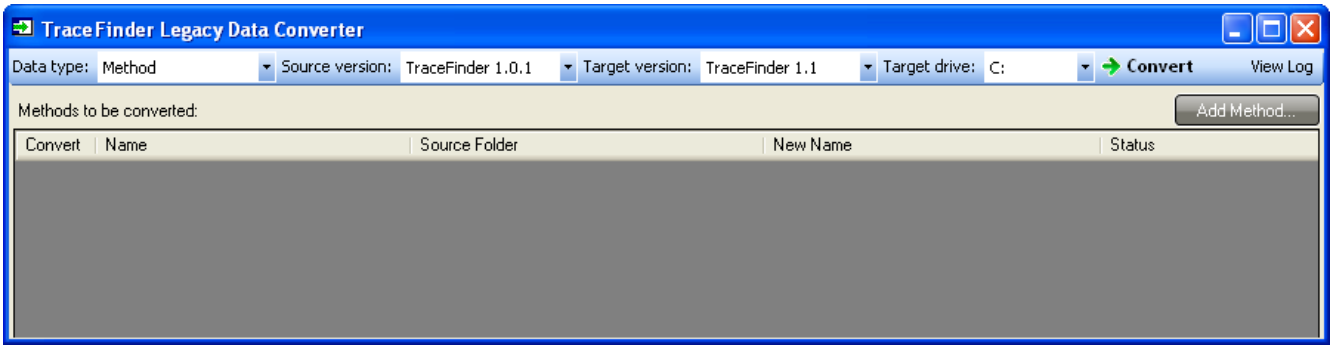
Use the following procedures:

- To convert a method
- To convert a batch
- To convert a method template
- To convert a batch template

❖ To convert a method

1. In the Data Type list, select **Method**.

   The TraceFinder Legacy Data Converter displays the interface for converting methods.



2. In the Source Version list, select a legacy version.

   The legacy version defaults to TraceFinder 1.0.1.

3. In the Target Version list, select **TraceFinder 1.1**.

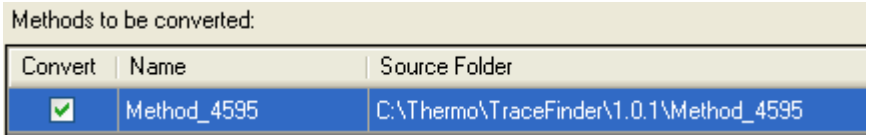
4. In the Target Drive list, select a fixed drive.

   You cannot write the converted files to a mapped drive.

5. Click **Add Method** and browse to a method folder.

6. Select the method folder and click **OK**.

   The application adds the method to the Methods to be Converted list:



7. Repeat step 6 for each method you want to convert.
8. (Optional) In the New Name column, type a new name for each method that you want converted.

   If you leave this column blank, the converted method keeps the old name.
9. Select the check box for each method you will convert, and click Convert.

   When the conversion process begins, the application displays a status bar and a Cancel button. You can cancel pending conversions, but not the method that is currently converting.

   When the Status column reports that the method is successfully converted, the application writes the converted file to the C:\Thermo\TraceFinder\1.1\Methods folder.
10. To view a log of the conversion, click **View Log**.

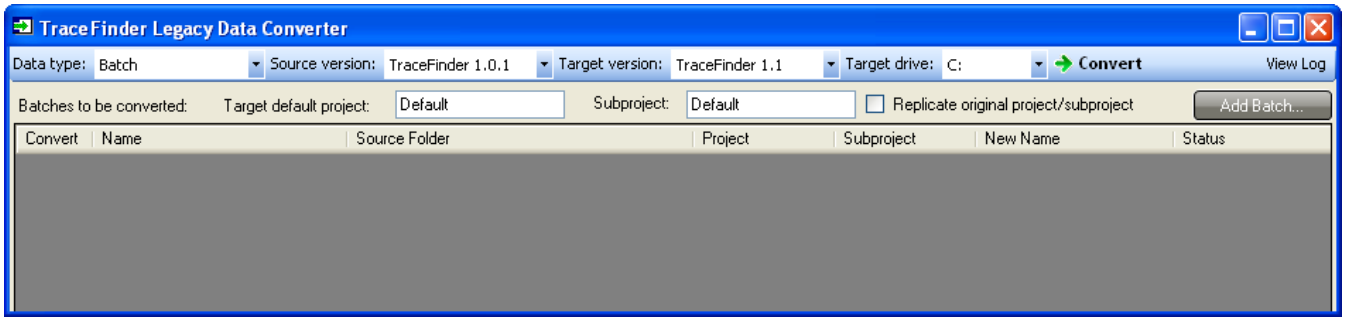
    The application opens a log file for the session in a Notepad text editor window:

```
====== Start Converting Method from TraceFinder 1.0.1 to TraceFinder 1.1 ==========
Converting master method from 'C:\Thermo\TraceFinder\1.0.1\Method_4595\Method_4595.mmx'
Creating master method
Importing properties of object 'MethodData' from XML file 'C:\Thermo\TraceFinder\1.0.1\Method_4595\Meth
Saving master method
Copying instrument method
Successfully converted master method from 'C:\Thermo\TraceFinder\1.0.1\Method_4595\Method_4595.mmx'
'C:\Thermo\TraceFinder\1.1\Methods\Method_4595_new\Method_4595_new.mmx'
```

❖ To convert a batch

1. In the Data Type list, select **Batch**.

   The TraceFinder Legacy Data Converter displays the interface for converting batches.



2. In the Source Version list, select a legacy version.

   The legacy version defaults to TraceFinder 1.0.1.
3. In the Target Version list, select **TraceFinder 1.1**.

4. In the Target Drive list, select a fixed drive.

   You cannot write the converted files to a mapped drive.

5. Do one of the following to create a project and subproject for the converted batch:

   In the Target Default Project and Subproject boxes, type the name of a project and subproject.

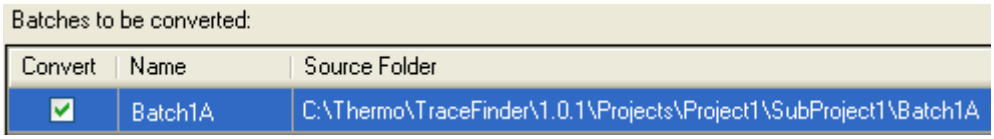
   –Or–

   Select the Replicate Original Project/Subproject check box.

6. Click **Add Batch** and browse to a batch folder.

7. Select the batch folder and click **OK**.

   The application adds the batch to the Batches to be Converted list:



8. Repeat step 7 for each batch you want to convert.

9. (Optional) In the New Name column, type a new name for each batch that you want converted.

   If you leave this column blank, the converted batch keeps the old name with "_1" appended.

10. Select the check box for each batch you will convert, and click

.

    When the conversion process begins, the application displays a status bar and a Cancel button. You can cancel pending conversions, but not the batch that is currently converting.

    When the Status column reports that the batch is successfully converted, the application writes the converted batch to the C:\Thermo\TraceFinder\1.1\Projects folder using either the original project and subproject names or the new names you entered.

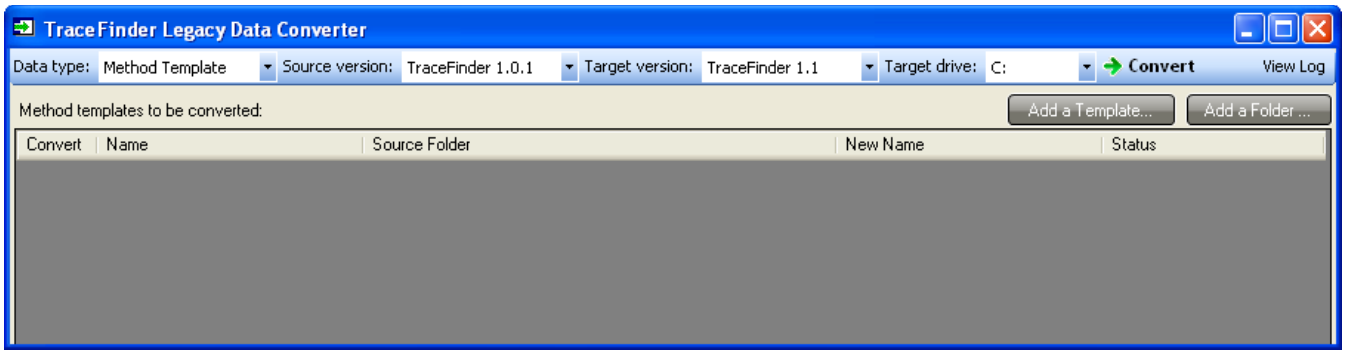
11. To view a log of the conversion, click **View Log**.

    The application opens a log file for the session in a Notepad text editor window.

❖ To convert a method template

1. In the Data Type list, select **Method Template**.

   The TraceFinder Legacy Data Converter displays the interface for converting method templates.



2. In the Source Version list, select a legacy version.

   The legacy version defaults to TraceFinder 1.0.1.

3. In the Target Version list, select **TraceFinder 1.1**.

4. In the Target Drive list, select a fixed drive.

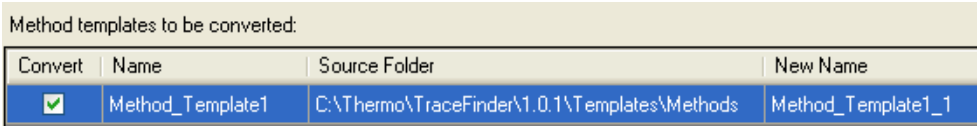
   You cannot write the converted files to a mapped drive.

5. To add a single method template, do the following:

   a. Click **Add a Template** and browse to the C:\Thermo\TraceFinder\1.0.1\Templates\Methods folder.

   b. Select the method template (.pmtx) file and click **Open**.

   The application adds the method template to the Method Templates to be Converted list:



6. To add all the method templates in the Methods folder, do the following:

   a. Click **Add a Folder** and browse to the C:\Thermo\TraceFinder\1.0.1\Templates folder.

   b. Select the **Methods** folder and click **OK**.

Note The default folder for saved method templates is Templates\Methods. If you have templates in other folders, you can navigate to your folder.

The application adds all the method templates in the folder to the Method Templates to be Converted list:

Method templates to be converted:

Convert	Name	Source Folder	New Name
☑	Method_Template1	C:\Thermo\TraceFinder\1.0.1\Templates\Methods	Method_Template1_1
☑	Method_Template2	C:\Thermo\TraceFinder\1.0.1\Templates\Methods	Method_Template2_1
☑	Method_Template3	C:\Thermo\TraceFinder\1.0.1\Templates\Methods	Method_Template3_1
☑	Method_Template_DDS	C:\Thermo\TraceFinder\1.0.1\Templates\Methods	Method_Template_DDS_1
☑	Method_Template_DDS_off	C:\Thermo\TraceFinder\1.0.1\Templates\Methods	Method_Template_DDS_off_1
☑	Method_Template_DDS_on	C:\Thermo\TraceFinder\1.0.1\Templates\Methods	Method_Template_DDS_on_1

7. Repeat step 6 for each method template you want to convert.
8. (Optional) In the New Name column, type a new name for each method template that you want converted.

   If you leave this column blank, the converted template keeps the old name with "_1" appended.
9. Select the check box for each method template you will convert, and click **Convert**.

   When the conversion process begins, the application displays a status bar and a Cancel button. You can cancel pending conversions, but not the template that is currently converting.

   When the Status column reports that the template is successfully converted, the application writes the converted template to the C:\Thermo\TraceFinder\1.1\Templates\Methods folder.
10. To view a log of the conversion, click **View Log**.

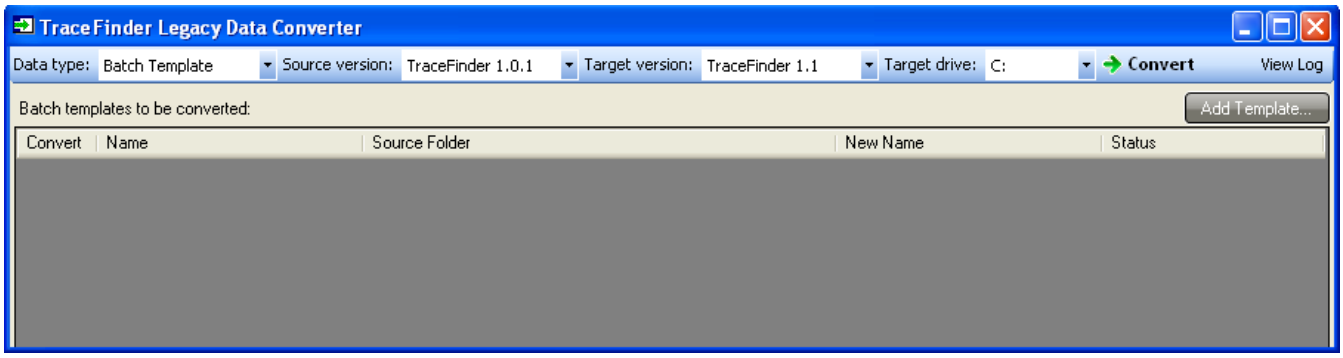
    The application opens a log file for the session in a Notepad window:

```
====== Start Converting Method Template from TraceFinder 1.0.1 to TraceFinder 1.1 ==========
Converting method template from 'C:\Thermo\TraceFinder\1.0.1\Templates\Methods\Method_Template1.pmtx'
Importing properties of object 'ProcMethodTemplateData' from XML file 'C:\Thermo\TraceFinder\1.0.1\Temp
Saving the method template
Successfully converted method template from 'C:\Thermo\TraceFinder\1.0.1\Templates\Methods\Method_Tem
to 'C:\Thermo\TraceFinder\1.1\Templates\Methods\Method_Template1_1.pmtx'
```

❖ To convert a batch template

1. In the Data Type list, select **Batch Template**.

   The TraceFinder Legacy Data Converter displays the interface for converting batch templates.



2. In the Source Version list, select a legacy version.

   The legacy version defaults to TraceFinder 1.0.1.

3. In the Target Version list, select **TraceFinder 1.1**.

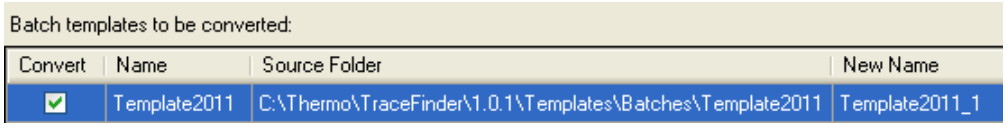
4. In the Target Drive list, select a fixed drive.

   You cannot write the converted files to a mapped drive.

5. Click **Add Template** and browse to the C:\Thermo\TraceFinder\1.0.1\Templates\Batches folder.

6. Select the batch template folder and click **OK**.

   The application adds the batch template to the Batch Templates to be Converted list:



7. Repeat step 6 for each batch template you want to convert.

8. (Optional) In the New Name column, type a new name for each batch template that you want converted.

   If you leave this column blank, the converted template keeps the old name with "_1" appended.

9. Select the check box for each batch template you will convert, and click

.

   When the conversion process begins, the application displays a status bar and a Cancel button. You can cancel pending conversions, but not the template that is currently converting.

When the Status column reports that the template is successfully converted, the application writes the converted template folder to the C:\Thermo\TraceFinder\1.1\Templates\Batches folder.

10. To view a log of the conversion, click **View Log**.

    The application opens a log file for the session in a Notepad text editor window:

```
====== Start Converting Batch Template from TraceFinder 1.0.1 to TraceFinder 1.1 ==========
Converting batch template from 'C:\Thermo\TraceFinder\1.0.1\Templates\Batches\Template_15\Template_15.
Importing properties of object 'BatchData' from XML file 'C:\Thermo\TraceFinder\1.0.1\Templates\Batches\
---------- Importing sample 'Unknown1' [1/1] ----------
Importing properties of object 'SampleData' from XML file 'C:\Thermo\TraceFinder\1.0.1\Templates\Batches
---------- Completed sample import ----------
Saving batch data for 'Template_15_1'
Importing local method for 'Template_15_1'
```

Choosing a Mode

When user security is enabled, the dashboard provides the current user with options applicable to the role assigned to 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
LabDirector	×	×	×	×
ITAdmin				×
Supervisor	×	×	×	
Technician		×	×	
QAQC			×	

Note When user security is not enabled, all modes are available to all users.

Use the following procedures:

- To choose a mode
- To display a log of instrument errors
- To monitor the instrument status
- To watch the real-time display from the dashboard

❖ To choose a mode

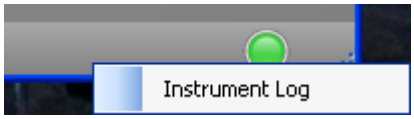
1. From the dashboard, click the mode in which you want to work.

   Your dashboard shows only the modes that you have permission to use. See "TraceFinder Dashboard" on page 25.

2. To change modes from within any of the TraceFinder application modes, click a mode button in the navigation pane.

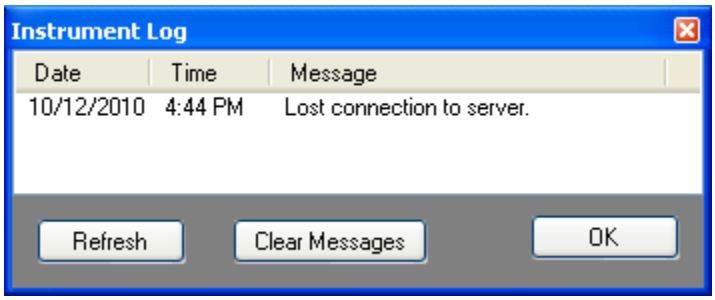
❖ To display a log of instrument errors

1. Right-click the status light in the lower right corner of any mode.



2. Select **Instrument Log**.

   The Instrument Log dialog box opens.



   The Instrument Log displays all instrument errors that have occurred since the TraceFinder application started or since the last time you cleared the message log.

3. Do any of the following:
   - Click **Refresh** to display errors that occur after you open the Instrument Log dialog box.
   - Click **Clear Messages** to remove messages from the Instrument Log display.

     The application clears messages only from the Instrument Log display. These messages remain in the following log file:

     C:\Thermo\TraceFinder\1.1\Logs\TraceFinder.log
   - Click **OK** to dismiss the Instrument Log dialog box.

❖ To monitor the instrument status

To get immediate information about the instrument status, look at the LED in the lower right corner of the TraceFinder window.

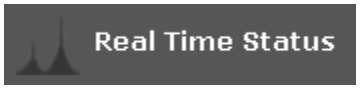
Green: Indicates that the instrument is ready.

Yellow: Indicates that the instrument is in standby mode.

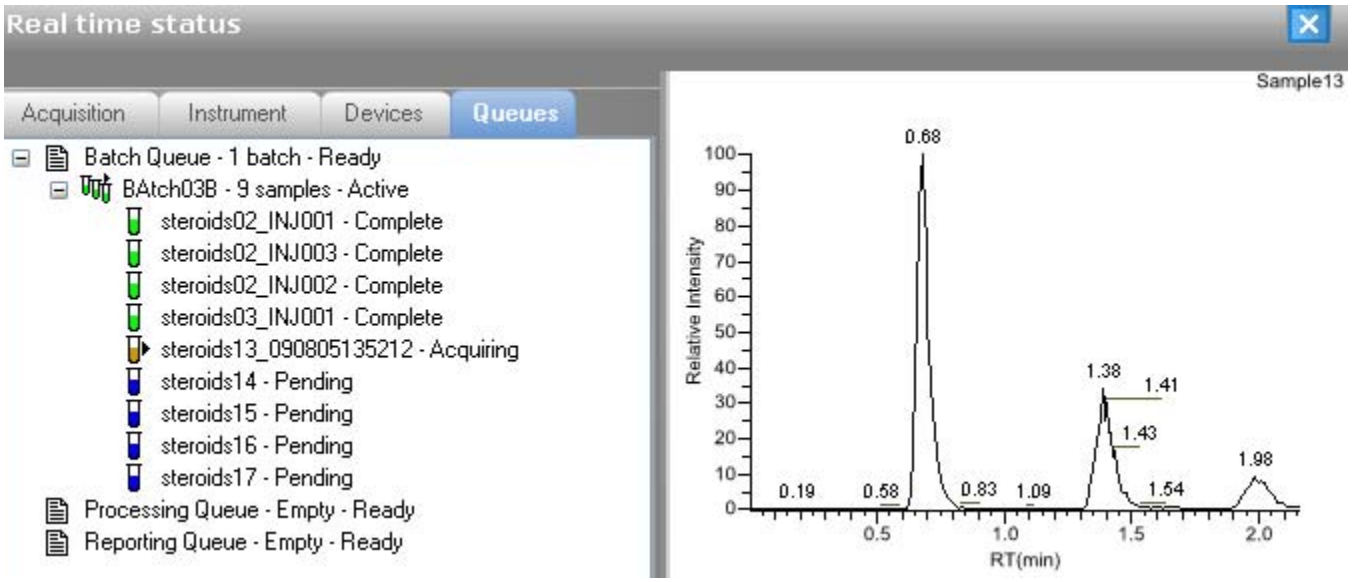
Red: Indicates that the instrument is turned off or no device is configured.

❖ 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 246.

TraceFinder Dashboard

A dashboard for a user in the LabDirector role looks like this:

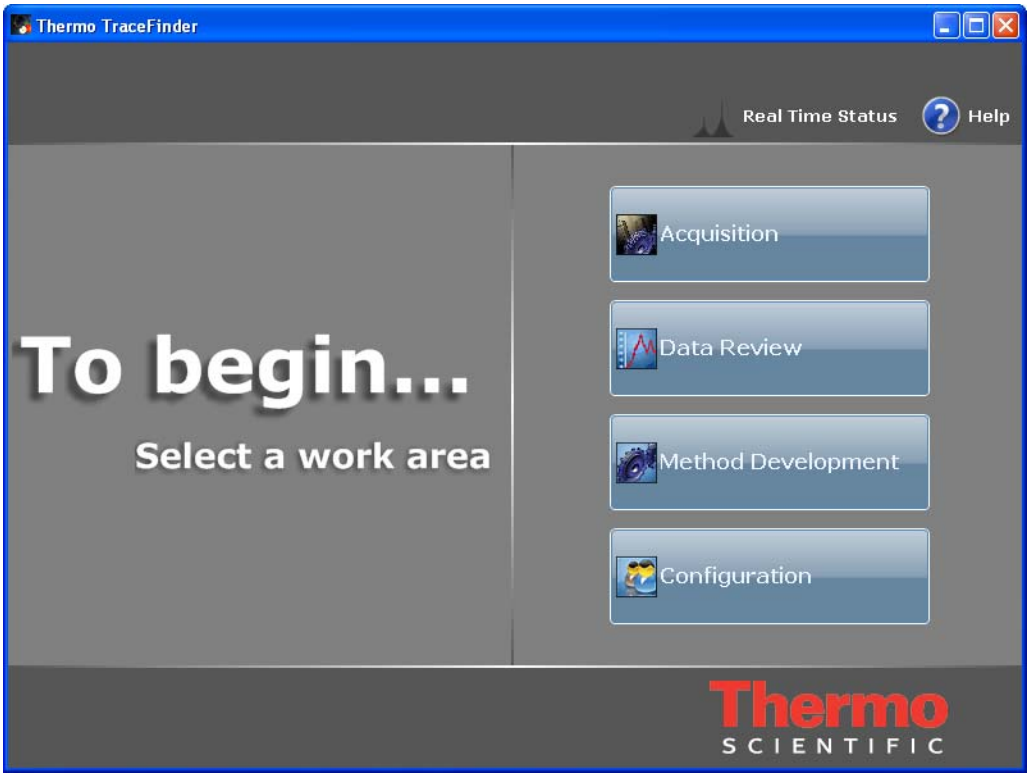


Table 3. TraceFinder dashboard screen parameters (Sheet 1 of 2)

Parameter	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 logon screen. This function is available only when user security is enabled. See "Specifying User Security" on page 66.
Acquisition	Opens the Acquisition mode where you can create and review batches, batch data, reports, and local methods. See Chapter 5, "Using the Acquisition Mode."
Data Review	Opens the Data Review mode where you can review batches, batch data, reports, and local methods. See Chapter 6, "Using the Data Review Mode."

Table 3. TraceFinder dashboard screen parameters (Sheet 2 of 2)

Parameter	Description
Method Development	Opens the Method Development mode where you can create a master method, an instrument method, or a development batch. See Chapter 4, "Using the Method Development Mode."
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. See Chapter 3, "Using the Configuration Mode."

Using the Configuration Mode

This chapter discusses the configuration tasks assigned to the ITAdmin and LabDirector roles.

Contents

- User Administration
- Project Administration
- Compound Datastore
- Application Configuration

Users in the role of ITAdmin or LabDirector 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 mode navigation pane opens.

Figure 3. Configuration mode navigation pane

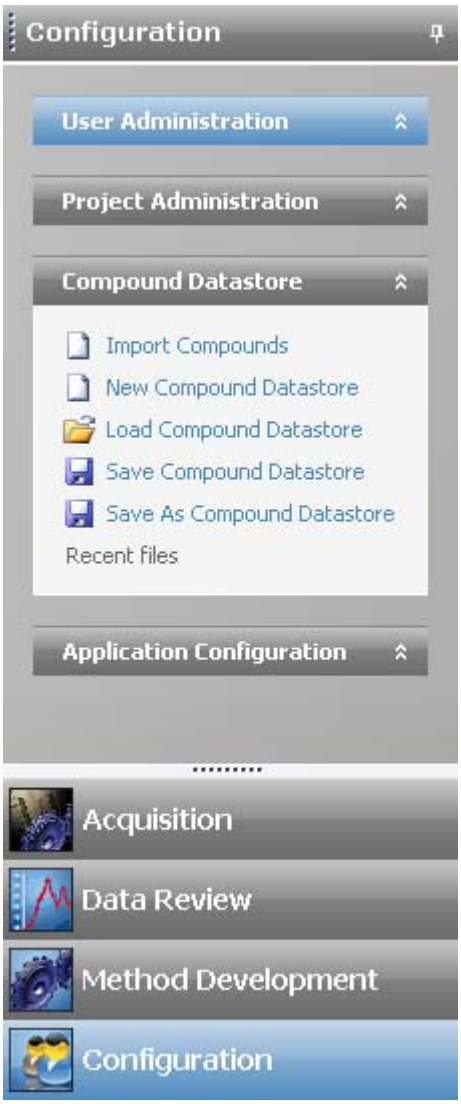


Table 4. Configuration mode navigation pane functions (Sheet 1 of 2)

Function	Description
User Administration	Opens the User Administration view where you can add, remove, or edit user accounts and permissions. See "User Administration" on page 30. This task pane is available only when you have selected Enable User Security on the General page of the Application Configuration view. See "Application Configuration" on page 56.
Project Administration	Opens the Project Administration view where you can create and manage projects and subprojects. See "Project Administration" on page 39.

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

Function	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 44. This task pane is available only when you have selected Enable Compound Datastore on the General page of the Application Configuration view. See "Application Configuration" on page 56.
Application Configuration	Opens the Application Configuration view where you can specify available reports, user security, compound datastore, reporting defaults, multiplexing, detection algorithms, and target screening. See "Application Configuration" on page 56.

User Administration

In the User Administration view of the Configuration mode, users in the role of LabDirector or ITAdmin 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 "Choosing User Roles" on page 36.

Use the following procedures:

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

❖ To open the User Administration view

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

The Configuration navigation pane opens.

> **Note** The User Administration view is available only when you enable user security. Follow the instructions "To enable user security" on page 66.

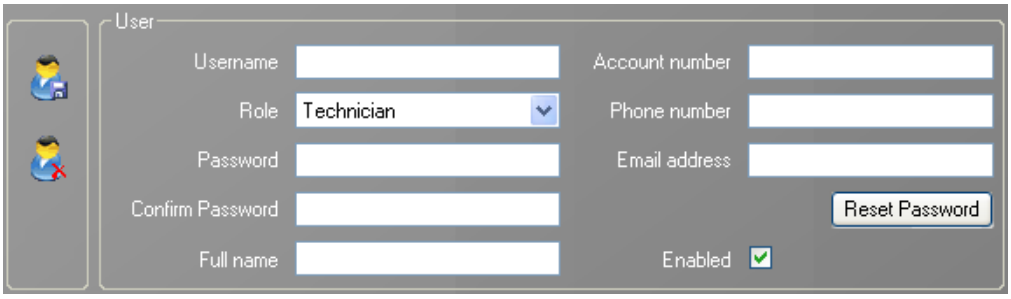
2. Click the **User Administration** task pane.

The User Administration view opens. See "User Administration view" on page 34.

❖ To add a user

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

The application enables the parameters in the User area at the bottom of the view.



2. Type 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 "Choosing User Roles" on page 36.

4. Type the user's password and type it again to the confirm it.

   Make sure to communicate the password to the user.

5. (Optional) Type the user's full name, account number, phone number, and e-mail address.

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

   You can disable a user logon without deleting the user's information. Follow the instructions "To edit user information" on page 31.

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.

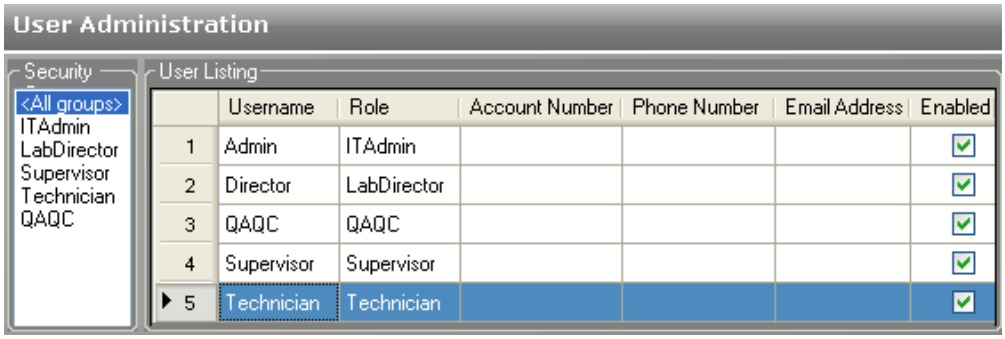
   –Or–

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

   The application discards all information and the parameters in the User area are unavailable.

❖ To edit user information

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

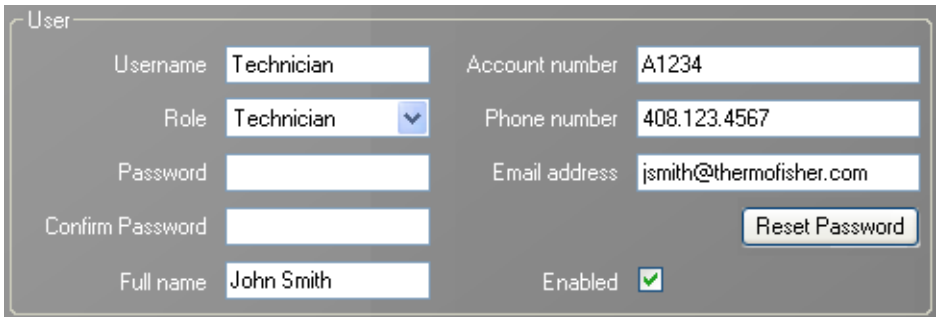


Note Clicking anywhere in the row selects the user.

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

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

   The application enables the parameters in the User area.



3. Edit any of the parameter values.

   If you are editing your own 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.

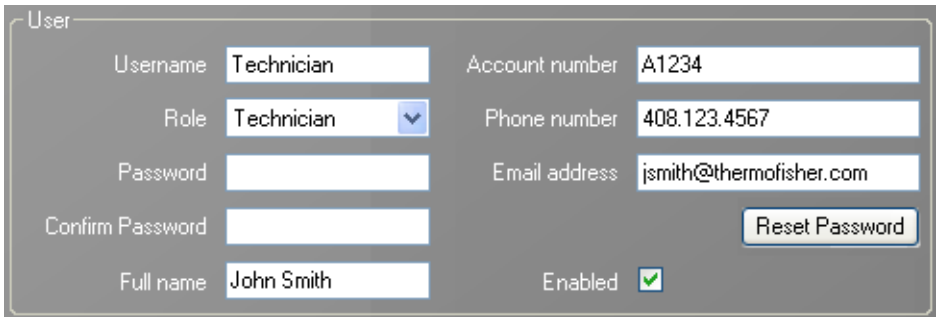
❖ To change a user password

1. In the User Listing table, select a 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. Click **Reset Password**.

   The application makes the password and confirming password visible as a string of asterisks ******.

4. In the Password box, select the ****** and type a new password.

5. In the Confirm Password box, select the ****** and retype the new password.

6. Click the **Save Changes** icon, .

   Make sure to communicate the new password to the user.

❖ 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 logon without removing all the user information from the system. Follow the instructions "To edit user information" on page 31.

Figure 4. User Administration view

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

Parameter	Description
Security Groups	All permission levels defined in the TraceFinder application. For detailed descriptions of user permissions, see "Choosing User Roles" on page 36.
User Listing	
Username	User logon 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	Logon name for the current user.
Role	Security group that defines the current user's permissions.
Password	Logon password for the current user.
Full name	The the current user's actual name.
Account number	Optional account number for the current user.
Phone number	Optional telephone number for the current user.

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

Parameter		Description
Email address		E-mail address for the current 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.
Reset Password		Makes the password visible as a string of asterisks so that you can select and change it.
Icon	**Function**	
	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 the 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.

Choosing User Roles

This section describes the responsibilities for five different user roles when user security is enabled: LabDirector, ITAdmin, Supervisor, Technician, and QAQC.

IMPORTANT User roles are in effect only when user security is enabled. When user security is not enabled, all users have access to all modes.

User Permissions

A laboratory 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
LabDirector	×	×	×	×
ITAdmin				×
Supervisor	×	×	×	
Technician		×	×	
QAQC			×	

LabDirector

In the LabDirector role, you review graphically applicable data and manipulate data, batches, methods, and instruments.

A laboratory 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

ITAdmin

In the ITAdmin role, you set security, manage users into roles, and manipulate the various databases. You are 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

In the Supervisor role, you are responsible for setting up the instrument samples 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 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 giving intermediate approval and sending the data to management
- Modifying new compounds or adjusting methods for specific result sets

Technician

In the Technician role, you are responsible for setting up the instrument samples and using previously built sequences and methods for processing and acquiring data. You also edit existing methods for processing and acquiring data, are responsible for reviewing collected data, and distinguishing between the need to rerun samples or pass reports up to the supervisor. On a daily basis, you are 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

In the QAQC role, you review graphically applicable data and interpret the data, but you do not manipulate the data.

A QAQC technician 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 to management
- Receiving instructions for new sets of samples for the TraceFinder application to analyze after finishing the current analysis

Note In the QAQC role, you cannot submit batches for acquisition from the Acquisition mode.

Project Administration

In the LabDirector or ITAdmin role, you can create and manage projects and subprojects on fixed or network drives in the Project Administration view of the Configuration mode.

This section includes the following topics:

- Working with Drives
- Working with Projects

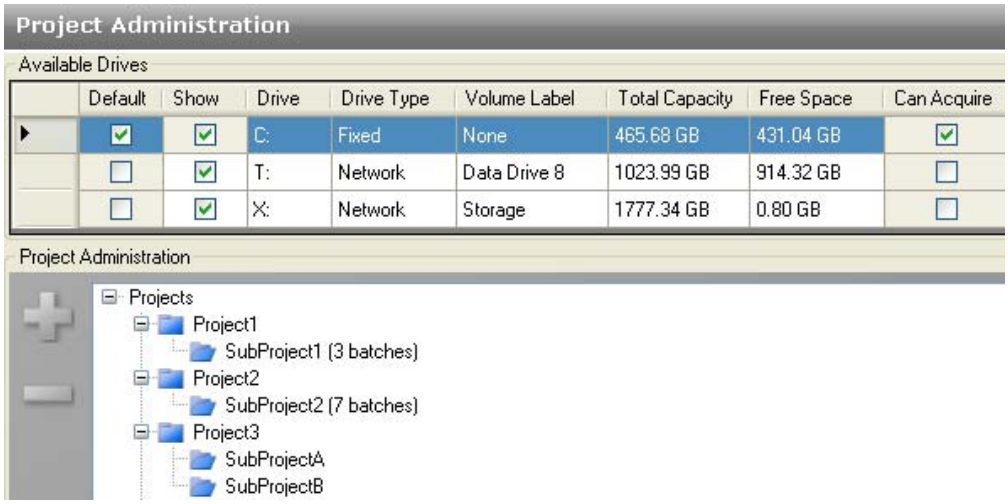
❖ To open the Project Administration view

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

   The Configuration navigation pane opens.

2. In the Configuration navigation pane, click **Project Administration**.

   The Project Administration view opens.

   By default, all projects are created under a main Projects folder on the C: drive:

   C:\Thermo\TraceFinder\1.1\Projects

Working with Drives

Drives can be any of the following:

- Fixed: Directly connected to your computer.
- Network: Either a remote box or a mapped drive. A shared folder that is mapped to a drive letter might physically exist on your computer, but because it is mapped, it is considered to be a Network drive.
- Removable: Temporary drives such as a 3.5-inch disk or USB drive.

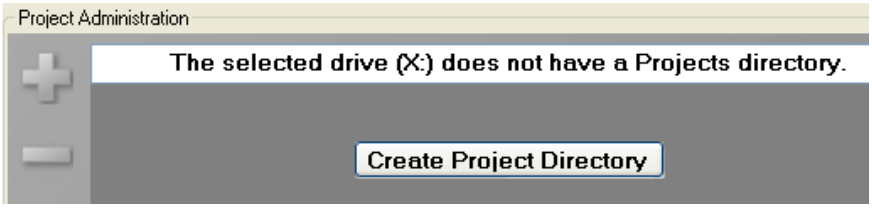
Use the following procedures:

- To choose a drive
- To change the default drive
- To hide a drive from display
- To refresh the drives display

❖ To choose a drive

1. In the Available Drives area, click any drive other than the default C: drive.

   If you have not created a Projects directory on this drive, you see this message:



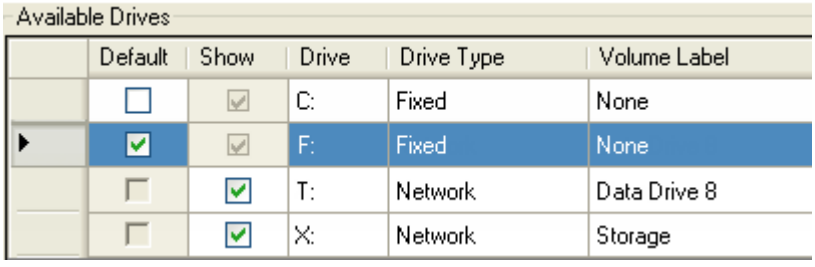
2. Click **Create Projects Directory**.

   The TraceFinder application adds a new Projects directory to the selected drive. To create projects and subprojects on this drive, see "To create projects or subprojects" on page 42.

❖ To change the default drive

Select the check box in the Default column.

Only fixed drives can be set as the default drive. The default drive is the first drive listed in all drive lists and is the only drive that you can use to acquire data.



❖ To hide a drive from display

Clear the check box in the Show column.

The application does not list the hidden drive in drive lists. You cannot hide the default drive.

❖ To refresh the drives display

Right-click and choose **Refresh** from the shortcut menu.

The Available Drives table refreshes to show any drives that have changed, for example, if you have inserted a USB drive. You can now configure any new drives.

Working with Projects

When you create a batch, the application stores the data files, local method, and reports in a project and subproject that you create in the C:\Thermo\TraceFinder\1.1\Projects folder.

Use the following procedures:

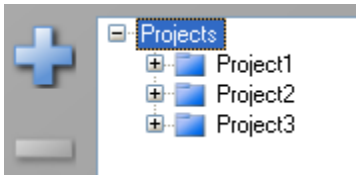
- To create projects or subprojects
- To delete projects or subprojects
- To remove all empty folders
- To copy the folder hierarchy from another drive

❖ 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 the existing projects and create a subproject under it.

   When you select a project folder, the application enables the plus sign icon, , indicating that you can create a folder within the selected folder.



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.

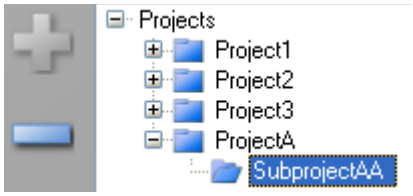
   Project names are limited to 30 characters and can contain spaces and special characters, except for the following special characters: \ / : * ? " < > |

   Note After you add a subproject to a project, you cannot rename the project.

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

❖ To delete projects or subprojects

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



You can delete projects that do not have subprojects. You can delete subprojects that do not have batches. When the selected project or subproject is available for deletion, the application enables the minus sign icon, .

2. Click the minus sign, or right-click and choose **Remove Project** from the shortcut menu.
3. At the prompt, click **Yes** to remove the selected project or subproject.

❖ To remove all empty folders

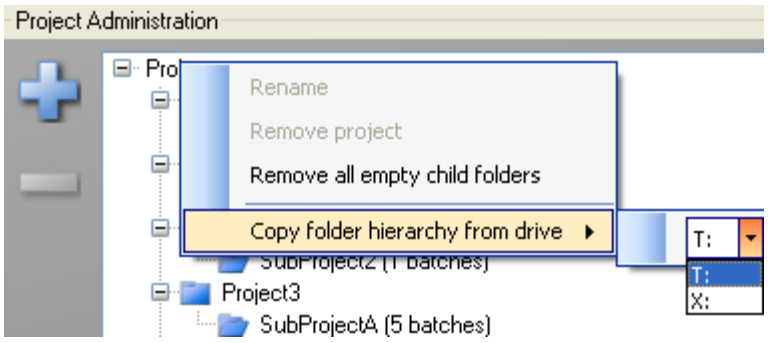
1. Select the project or subproject that contains empty folders.
2. Right-click and choose **Remove All Empty Child Folders** from the shortcut menu.

   A dialog box asks if you want to remove all empty folders.
3. Click **OK**.

   The application removes all folders that have no folders or files. There is no undo for this command.

❖ To copy the folder hierarchy from another drive

1. Select the top-level Projects directory in the Project Administration area.
2. Right-click and choose **Copy Folder Hierarchy from Drive** from the shortcut menu.
3. Choose a drive from the list of available drives.



At the prompt, you must confirm that you want to create a folder hierarchy that matches that of the specified drive.

4. Click **OK**.

   To replicate the hierarchy from the specified drive, the application will add new folders to the current hierarchy, but it will not remove folders.

IMPORTANT The **Copy Folder Hierarchy from Drive** command copies only the project and subproject folders; it does not copy batches within the folders.

Compound Datastore

In the LabDirector or ITAdmin role, you can manage compound definitions in the current datastore in the Compound Datastore view.

This section includes the following topics:

- Opening and Saving a Datastore
- Adding Compounds, Quan Peaks, and Confirming Ions to a Datastore
- Choosing Experiment Types

For a description of all the parameters in the Compound Datastore view, see "Compound Datastore View" on page 48.

Opening and Saving a Datastore

You can use the default datastore or you can create your own datastore.

Use the following procedures:

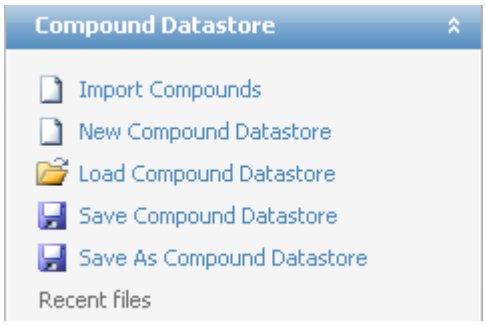
- To open the Compound Datastore editor
- To open a compound datastore
- To create a new compound datastore
- To save a datastore
- To save a datastore to a new name

❖ To open the Compound Datastore editor

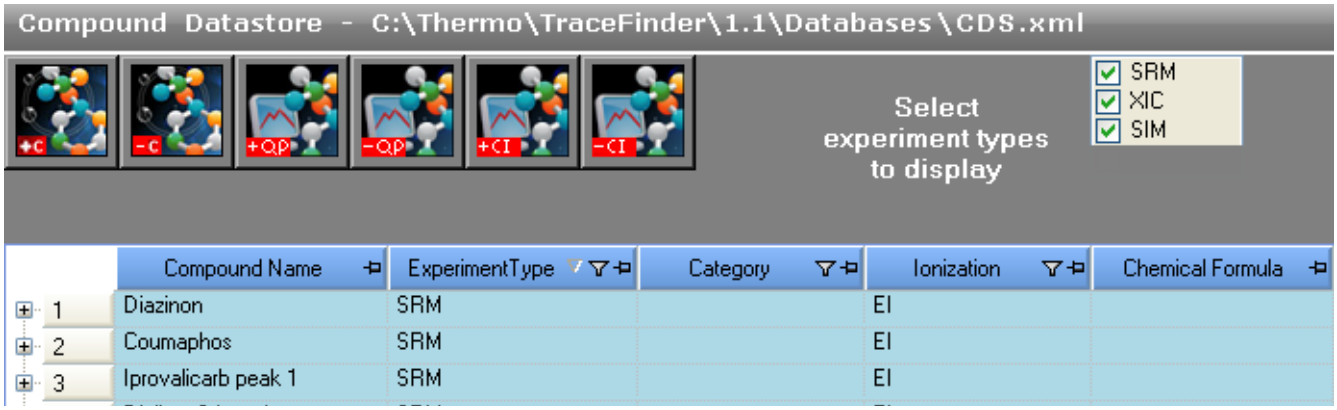
1. Click **Configuration** from the dashboard or the navigation pane.

The Configuration navigation pane opens.

2. Click the **Compound Datastore** task pane.



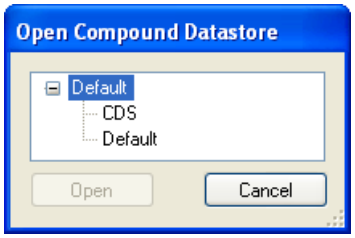
The current datastore opens in the Compound Datastore view. For a detailed list of all parameters and functions on the compound Datastore view, see "Compound Datastore View" on page 48.



❖ To open a compound datastore

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

   The Open Compound Datastore dialog box opens.



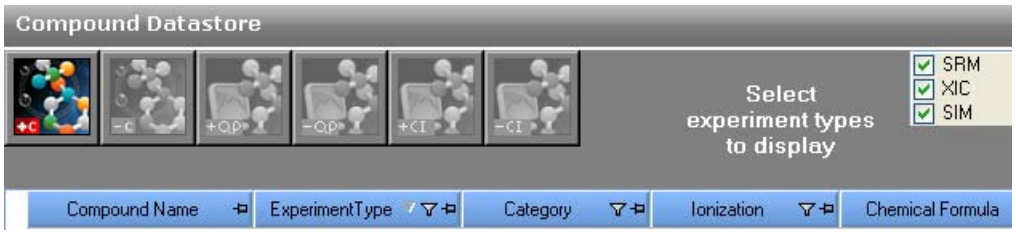
2. Double-click the name of the datastore you want to open.

   The selected datastore opens in the Compound Datastore view. See "Compound Datastore View" on page 48.

❖ 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 (following the instructions, To import compounds), or you can manually add compounds one at a time (following the instructions, To add a compound to the datastore).

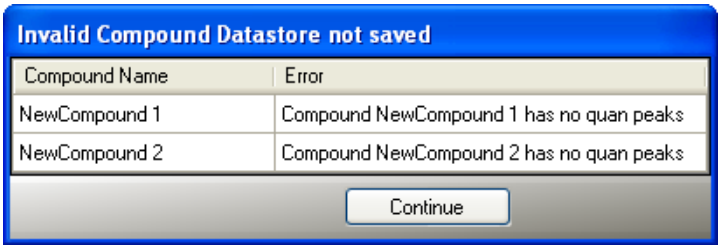
❖ To save a datastore

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

   The application stores the database as

   …\Thermo\TraceFinder\1.1\Databases*filename*.xml

   If the datastore contains any compounds that do not have associated quan peaks, the Invalid Compound Datastore Not Saved dialog box opens, listing the compounds.



2. To add a quan peak row to the listed compounds, click **Continue**.

   The application returns you to the Compound Datastore view.

3. Add quan peaks to the incomplete compounds before you save the datastore.

   See "To add a quan peak to a compound" on page 53.

❖ 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.

2. Type a file name for the new compound datastore.

3. Click **Save**.

   The application stores the database as

   …\Thermo\TraceFinder\1.1\Databases*filename*.xml

Figure 5. Save Compound Datastore dialog box

Table 7. Select Compound Datastore dialog box parameters

Parameter	Description
Compound Datastore name	Lists the file name for the new datastore.
Overwrite	Overwrites the selected datastore.
OK	Writes the new datastore to the Databases folder.
Cancel	Closes the dialog box and makes no changes to the datastore.

Figure 6. Compound Datastore View

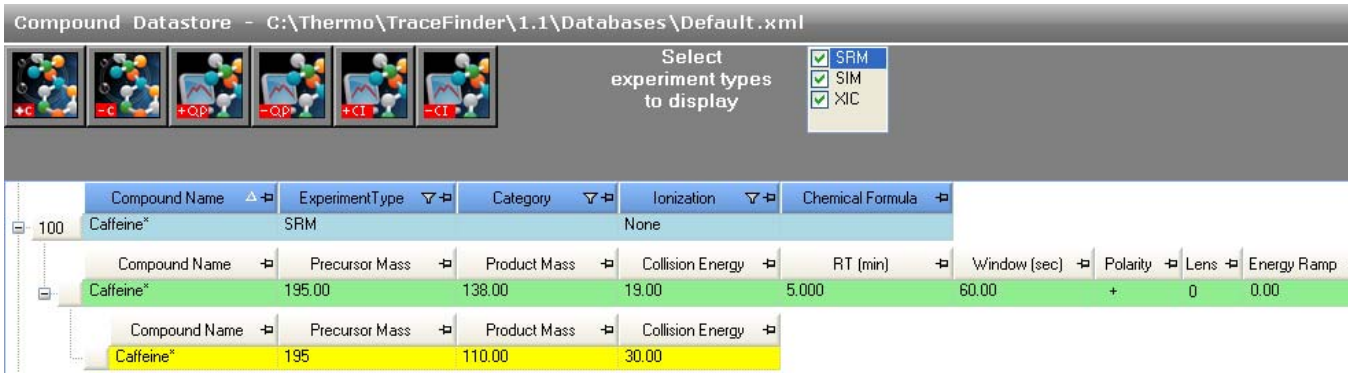


Table 8. Compound Datastore view parameters (Sheet 1 of 3)

Parameter	Description
Function icons	
	Adds a new compound row.
	Removes the selected row and all quan peak and confirming ion rows within it.
	Adds a new quan peak row to the compound. Each compound requires at least one quan peak.
	Removes the selected row and all confirming ion rows within it.
	Adds a new confirming ion row to the quan peak.
	Removes the selected confirming ion row.
Select experiment types to display	Specifies one of these experiment types that each use a different structure for the mass filter. See "Choosing Experiment Types" on page 55. • SRM: Selected Reaction Monitoring • XIC: Extracted Ion Chromatogram • SIM: Single Ion Monitoring
Compound parameters	
Compound Name	Alphanumeric name assigned to the compound.
Experiment Type	Experiment type: SRM, XIC, or SIM.
Category	(Optional) Alphanumeric identifier.
Ionization	(Optional) Alphanumeric identifier. Valid values: None, ESI, APCI, EI, CI, APPI Default: None
Chemical Formula	(Optional) Alphanumeric chemical identifier.

Table 8. Compound Datastore view parameters (Sheet 2 of 3)

Parameter	Description
Quan peak parameters	
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. In confirming ion rows, the precursor mass is a noneditable copy of the quan peak precursor mass. Available only for SRM experiments. 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. Available only for SRM experiments. Default: 0.0 Range: 10.000 to 2999.999
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. Available only for XIC and SIM experiments. Default: 0.0 Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00
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)	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
Polarity	+ (positive) or – (negative)
Lens	(Optional) Range: –400 to 400
Energy Ramp	(Optional) Available only for SRM experiments. Range: 0.00 to 200.00

Table 8. Compound Datastore view parameters (Sheet 3 of 3)

Parameter	Description
Confirming ion parameters	
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. Available as a noneditible field only for SRM experiments. 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. Available only for SRM experiments. Default: 0.0 Range: 10.000 to 2999.999
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. Available only for XIC and SIM experiments. Default: 0.0 Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00

Adding Compounds, Quan Peaks, and Confirming Ions to a Datastore

In the Compound Datastore view, you can import compounds into the datastore, add or remove compounds from the datastore, add quan peaks and confirming ions to a compound, or remove quan peaks or confirming ions from a compound.

Use the following procedures:

- To import compounds
- To add a compound to the datastore
- To remove a compound
- To add a quan peak to a compound
- To remove a quan peak
- To add a confirming ion to a quan peak
- To remove a confirming ion

❖ To import compounds

1. Click **Import Compounds** in the Compound Datastore task pane.
2. Browse to a .csv or .xml compounds file and click **Open**.

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

   When the application imports a compound that contains multiple quan peaks and confirming ions, it lists all the peaks under a single compound name, as in this example for Monuron:

	Compound Name	ExperimentType	Category	Ionization	Ch
3	Monuron	SRM	Class 1	ESI	

Compound Name	Precursor Mass	Product Mass	Collision Energy	
Monuron	199.09	46.182	16.00	6.00

Compound Name	Precursor Mass	Product Mass	Collision Energy
Monuron	199.09	72.105	16.00
Monuron	199.09	74.104	16.00

Compound Name	Precursor Mass	Product Mass	Collision Energy	
Monuron	200.09	46.182	16.00	6.00

Compound Name	Precursor Mass	Product Mass	Collision Energy
Monuron	200.09	72.105	16.00
Monuron	200.09	74.112	16.00

❖ To add a compound to the datastore

1. Click the **Add Compound** button, , or right-click the compounds list and choose **Add Compound** from the shortcut menu.

   The application adds a new, empty compound row to the compounds table.

2. Click the first table cell, and enter the required Compound Name parameter.
3. (Optional) Change the value for the Experiment Type.

   The default is SRM. For descriptions of available experiment types, see "Choosing Experiment Types" on page 55.

   After you add a quan peak to the compound, you cannot change the experiment type, even if you cancel the quan peak.
4. (Optional) Type a value or select a value from the Category list.

   You can use any alphanumeric string. After you type a new Category value, that value is available from the list.
5. (Optional) Change the values for Ionization.

   The default is None.
6. (Optional) Type a value for the Chemical Formula.

   You can use any alphanumeric string.

Each compound requires at least one quan peak.

❖ To remove a compound

1. Select the compound row you want to delete.
2. Click the **Remove Compound** button, , or right-click and choose **Remove Compound** from the shortcut menu.
3. If you are sure you want to delete the selected row, at the prompt, click **OK**.

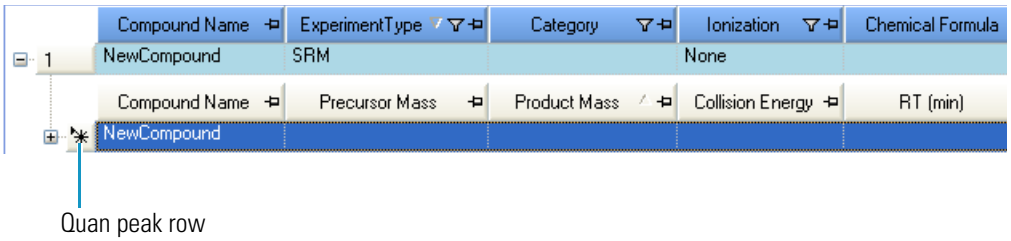
   The application removes the selected row and all quan peak and confirming ion rows within it.

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

❖ To add a quan peak to a compound

1. Select the compound.
2. Click the **Add Quan Peak** button, , or right-click and choose **Add Quan Peak** from the shortcut menu.

   The application adds a new quan peak row to the compound. A quan peak includes quantitative values for the compound. Each compound requires at least one quan peak.



3. Enter all required parameters.

   For a list of required and optional parameters, see the list of "Compound Datastore view parameters" on page 48.

   Tip You cannot add another new compound or save the compound datastore until you enter all required quan peak parameters or remove incomplete quan peaks from the compound.

4. Repeats steps 2 through 3 to add as many as six quan peaks to the compound.

❖ To remove a quan peak

1. Select the row of the quan peak you want to delete.
2. Click the **Remove Quan Peak** button, , or right-click and choose **Remove Quan Peak** from the shortcut menu.
3. If you are sure you want to delete the selected row, at the prompt, click **OK**.

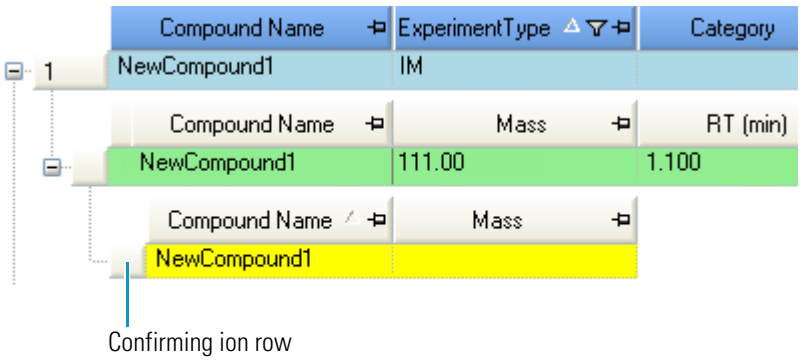
   The application removes the selected row and all confirming ion rows within it.

   Tip If you add a row of quan peak 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 quan peak rows.

❖ To add a confirming ion to a quan peak

1. Click the **Add Confirming Ion** icon, , or right-click the quan peak row and choose **Add Confirming Ion** from the shortcut menu.

   The application adds a new confirming ion row to the quan peak. A confirming ion includes a mass value.



2. Type the required column values for the confirming ion.

   The required confirming ion values differ for each experiment type. See "Choosing Experiment Types" on page 55.

3. Repeats steps 1 through 2 to add as many as 10 confirming ions to the quan peak.

❖ To remove a confirming ion

1. Select the confirming ion row you want to delete.
2. Click the **Remove Confirming Ion** icon, , or right-click and choose **Remove Confirming Ion** from the shortcut menu.
3. If you are sure you want to delete the selected row, at the prompt, click **OK**.

   The application removes the selected confirming ion row.

> **Tip** If you add a row of confirming ion 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 confirming ion rows.

❖ To filter a list

To display a filtered list of compound names, experiment types, categories, or ionization methods, click the funnel icon, , in the column header.

For each column, filterable criteria are displayed in a list. In all lists, you can choose to view all criteria or a specific type of criterion for that column.

Choosing Experiment Types

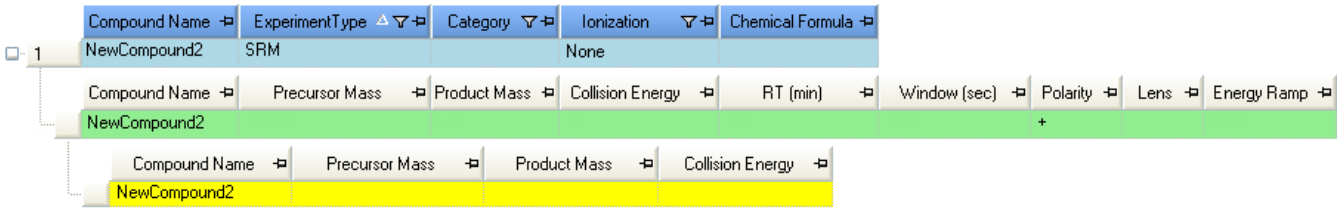
The TraceFinder application uses three experiment types: SRM, XIC, and SIM.

A compound datastore can include multiple experiment types for a single compound; however, each compound name and experiment type combination must be unique.

SRM – Selected Reaction Monitoring

The SRM experiment type supports triple quadrupole LC/MS. The mass filter includes precursor mass and narrow mass ranges to identify product masses. Imported compounds with no experiment type are treated as SRM data.

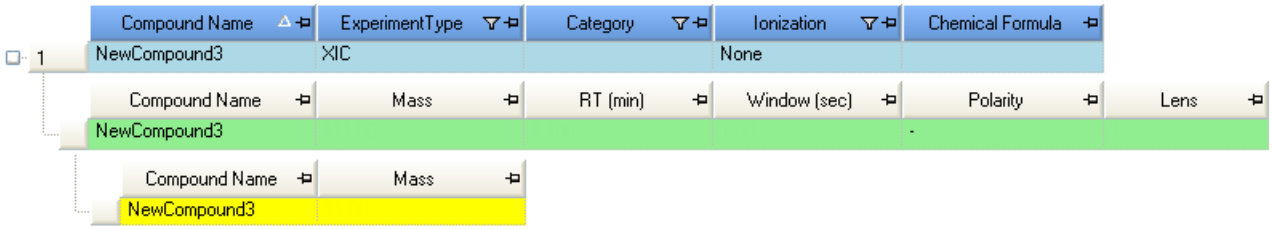
Confirming ions include values for product mass, collision energy, and a noneditable precursor mass.



XIC – Extracted Ion Chromatogram

The mass filter is a single, full scan which is post-processed to extract a peak for the ions of interest.

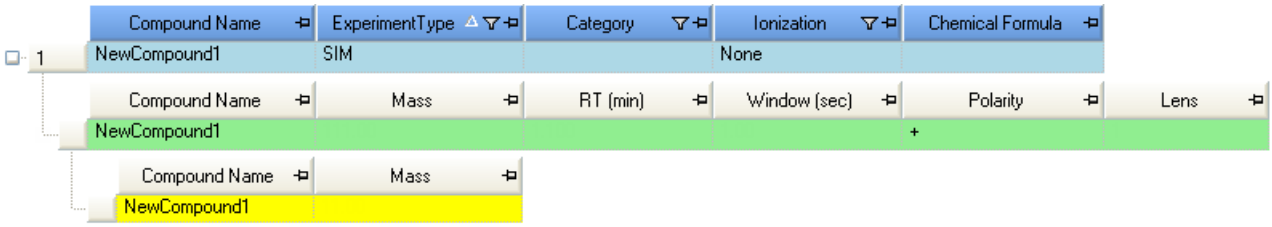
Confirming ions include a single mass value.



SIM – Single Ion Monitoring

The SIM experiment type supports single quadrupole LC/MS and Exactive™ systems. The mass filter includes narrow mass ranges to identify product masses.

Confirming ions include a single mass value.



Application Configuration

In the LabDirector or ITAdmin role, you can enable features such as available reports, user security, compound datastore, reporting defaults, multiplexing, detection algorithms, and target screening. You can also choose the reports that are available to users, the application defaults, and the defaults used for peak detection.

This section includes the following tasks:

- Specifying the Reports Configuration
- Specifying User Security
- Enabling a Compound Datastore
- Specifying Configuration Defaults
- Specifying Multiplexing Parameters
- Specifying Detection Parameters
- Enabling Target Screening

❖ To open the Application Configuration view

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

The Configuration navigation pane opens.

2. Click **Application Configuration**.

The Application Configuration view opens.

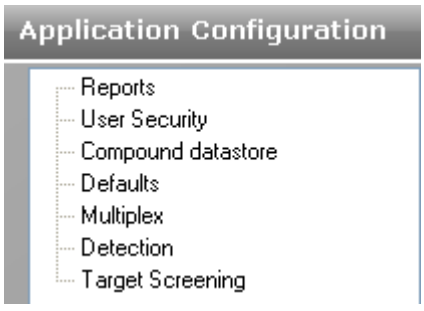


Table 9. Application Configuration pages (Sheet 1 of 2)

Page	
Reports	See "Specifying the Reports Configuration" on page 58.
User Security	See "Specifying User Security" on page 66.
Compound Datastore	See "Enabling a Compound Datastore" on page 67.

Table 9. Application Configuration pages (Sheet 2 of 2)

Page	
Defaults	See "Specifying Configuration Defaults" on page 68.
Multiplex	See "Specifying Multiplexing Parameters" on page 70.
Detection	See "Specifying Detection Parameters" on page 71.

3. In the Application Configuration list, click the type of information you want to configure.

Specifying the Reports Configuration

In the LabDirector or ITAdmin role, you can configure a list of reports that are available to users when they generate reports from the Method Development, Data Review, and Acquisition modes. From the Reports page, you can configure the standard, custom, or target screening reports.

Example PDFs of report formats are located in the following folder:

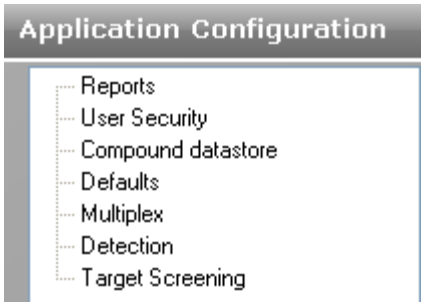
C:\Thermo\TraceFinder\1.1\ExampleReports

Use the following procedures:

- To open the Reports page
- To specify which reports are available
- To import new reports

❖ To open the Reports page

In the Application Configuration view, click **Reports**.



The Reports page of the Application Configuration view opens.

- For a list of General Quantitation reports, see "General Quantitation Reports" on page 60.
- For a list of Environmental and Food Safety reports, see "Environmental and Food Safety Reports" on page 63.

❖ To specify which reports are available

1. Use the directional arrows to move reports from the Installed Reports pane to the Displayed Reports pane.

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

   In the Method Development, Data Review, and Acquisition modes, users can access all reports in the Displayed Reports pane.

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

   Rather than creating separate reports for each sample, the application uses a composite of the data from all the samples to create a single report for the entire batch. Batch-level reports are prepended with a **B** to differentiate them.

   Note Only reports with the ability to aggregate data at the batch level have the **Batch Level** check box enabled.

3. Do one of the following:

   To apply the current selections, do the following:

   a. Click **Apply**.

      A message reminds you that you must restart the TraceFinder application before a user can access the reports you selected for the Method Development, Data Review, and Acquisition modes.

   b. To restart the TraceFinder application now, click **Yes,** or to remain on the Reports page, click **No**.

   –Or–

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

❖ To import new reports

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

   The application writes the imported report to the TraceFinder installation directory and displays the new report in the Installed Reports pane.

General Quantitation Reports

The General Quantitation configuration uses the following standard, custom, and target screening reports. For descriptions of the parameters on the Reports page, see "General Quantitation Reports page parameters" on page 62.

Figure 7. General Quantitation Reports page showing standard reports

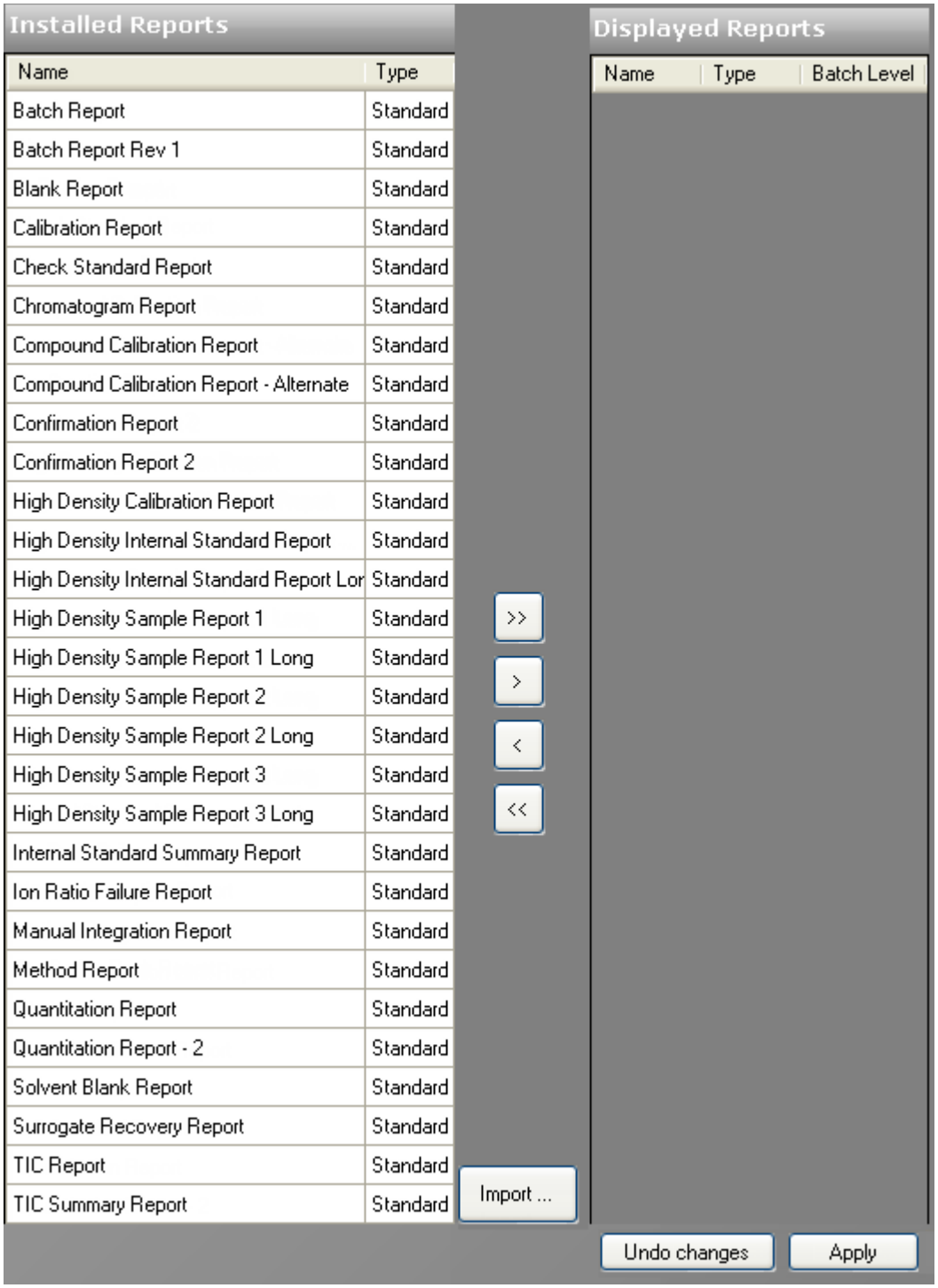


Figure 8. General Quantitation Reports page showing custom reports

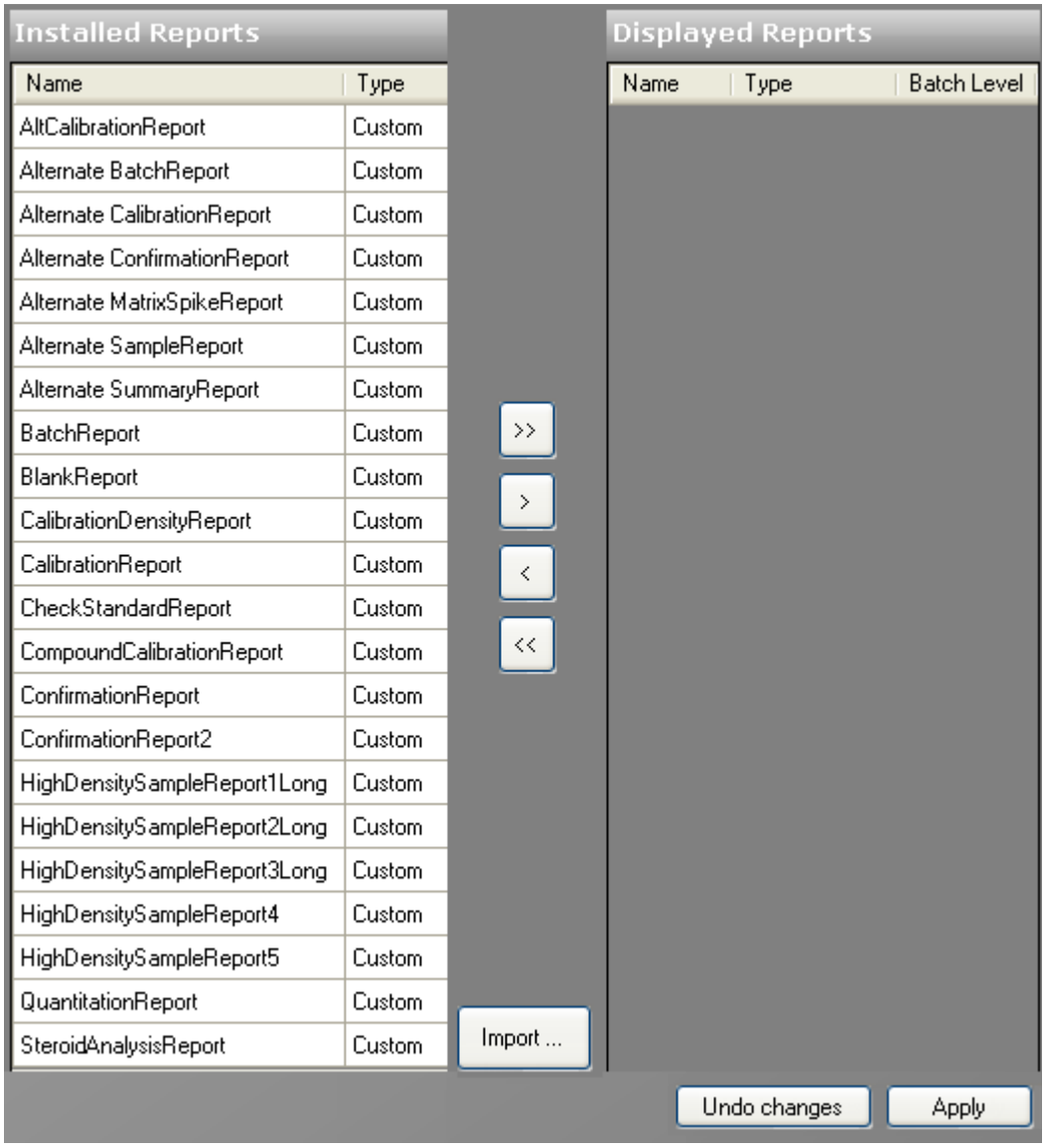
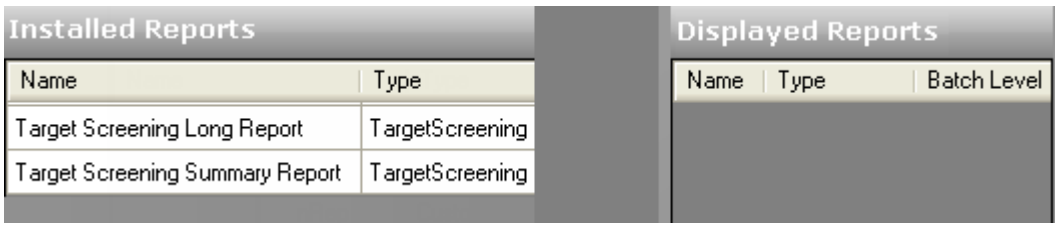


Figure 9. General Quantitation Reports page showing target screening reports



Note Target Screening reports are available only when you enable target screening. See "Enabling Target Screening" on page 83.

Table 10. General Quantitation Reports page parameters

Parameter	Description
Installed reports	All reports listed in the Installed Reports pane are potentially available but are not selected for use in the application.
Displayed reports	All reports listed in the Displayed Reports pane are selected for use in the application.
>>	Moves all reports from the Installed Reports list to the Displayed Reports list.
>	Moves the selected reports from the Installed Reports list to the Displayed Reports list.
<	Moves the selected reports from the Displayed Reports list to the Installed Reports list.
<<	Moves all reports from the Displayed Reports list to the Installed Reports list.
Import	Opens a browser where you can select a report file to add to the Installed 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 TraceFinder application before a user can access the reports you selected for the Method Development, Data Review, and Acquisition modes.

Environmental and Food Safety Reports

The Environmental and Food Safety configuration uses the following standard, custom, and target screening reports. For descriptions of the parameters on the Reports page, see "Environmental and Food Safety Reports page parameters" on page 65.

Figure 10. Environmental and Food Safety Reports page showing standard reports

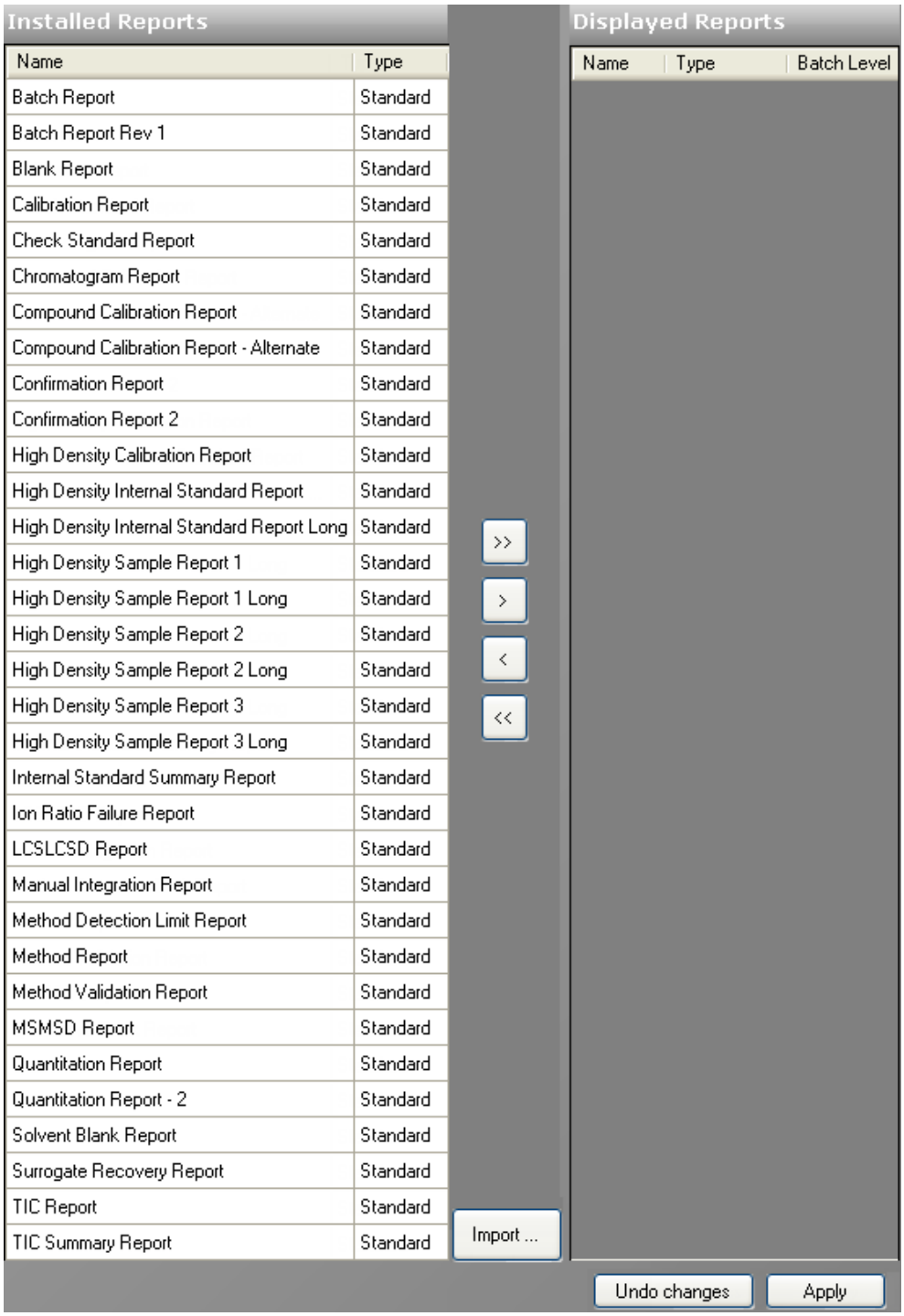


Figure 11. Environmental and Food Safety Reports page showing custom reports

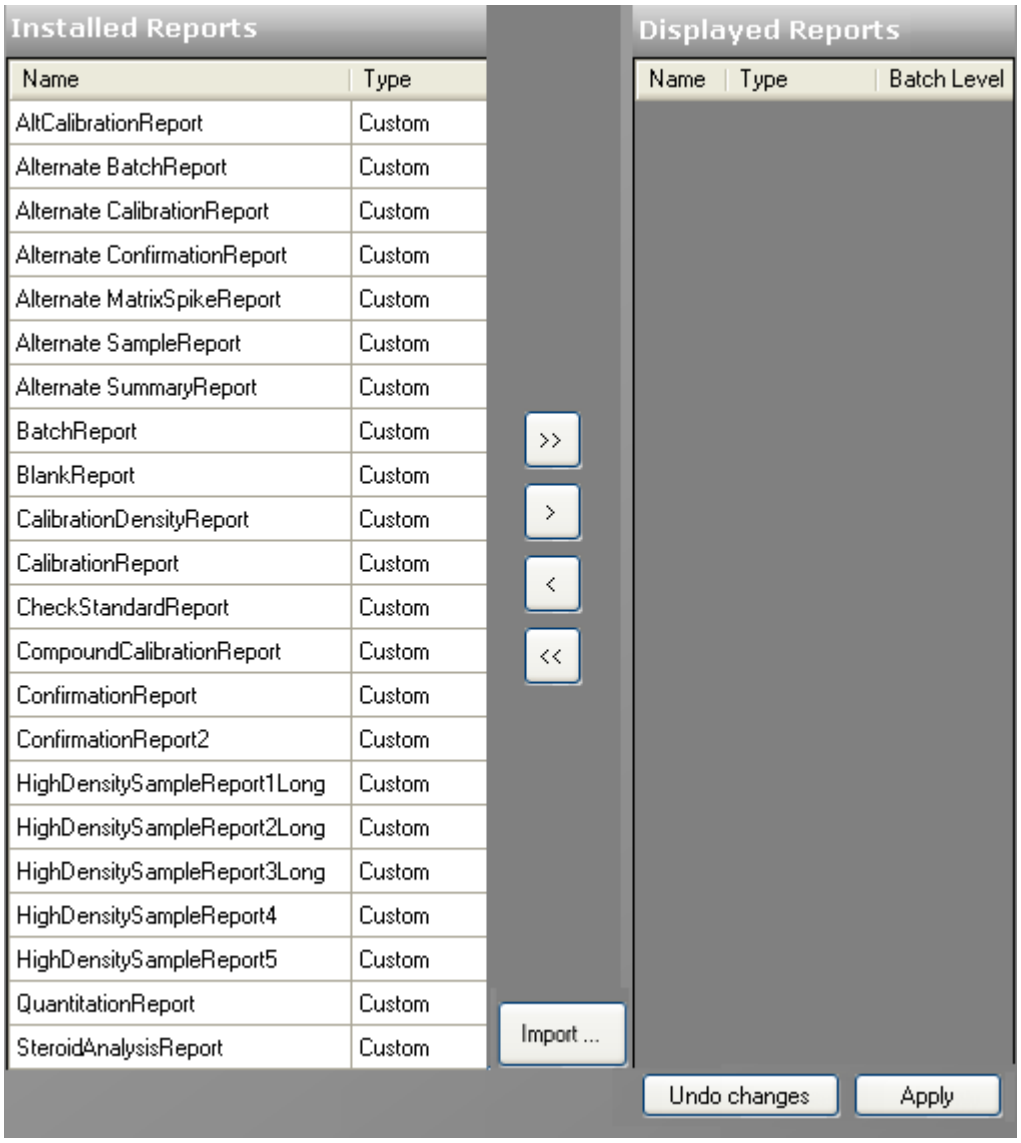
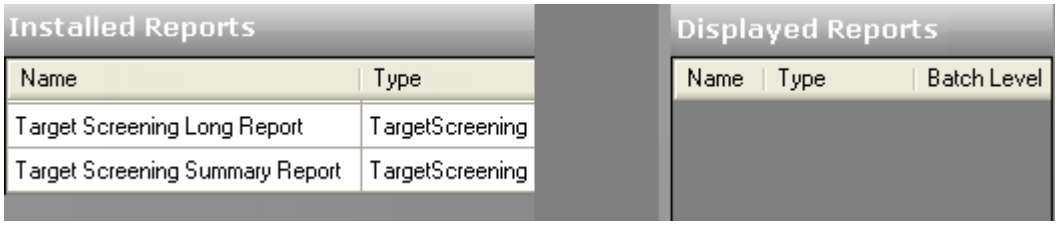


Figure 12. Environmental and Food Safety Reports page showing target screening reports



Note Target Screening reports are available only when you enable target screening. See "Enabling Target Screening" on page 83.

Table 11. Environmental and Food Safety Reports page parameters

Parameter	Description
Installed reports	All reports listed in the Installed Reports pane are potentially available but are not selected for use in the application.
Displayed reports	All reports listed in the Displayed Reports pane are selected for use in the application.
>>	Moves all reports from the Installed Reports list to the Displayed Reports list.
>	Moves the selected reports from the Installed Reports list to the Displayed Reports list.
<	Moves the selected reports from the Displayed Reports list to the Installed Reports list.
<<	Moves all reports from the Displayed Reports list to the Installed Reports list.
Import	Opens a browser where you can select a report file to add to the Installed 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 TraceFinder application before a user can access the reports you selected for the Method Development, Data Review, and Acquisition modes.

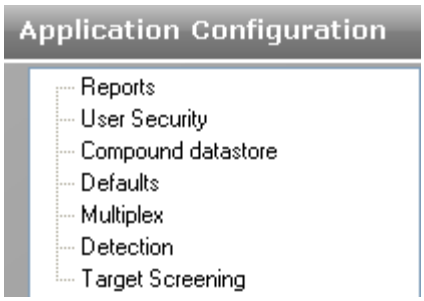
Specifying User Security

In the LabDirector or ITAdmin role, you can enable user security.

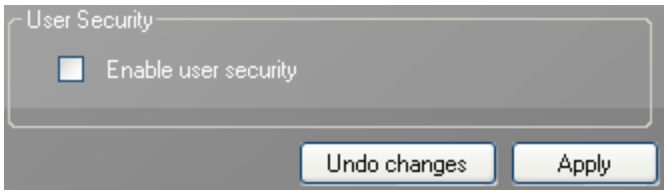
When user security is enabled, all users must log on to the TraceFinder application for access to only those modes assigned to their user role. See "Choosing User Roles" on page 36.

❖ To open the User Security page

In the Application Configuration view, click **User Security**.



The User Security page of the Application Configuration view opens.



❖ To enable user security

1. In the User Security area, select the **Enable User Security** check box.

   When this check box is selected, all users must log on to the TraceFinder application for access to the modes assigned to their user role. See "Choosing User Roles" on page 36.

   When this check box is cleared, users are not required to log on to the TraceFinder application. When they start the application, the dashboard is the first screen that users see and all modes are available to them. Only the User Administration view in Configuration mode is hidden and cannot be edited.

   Note By default, user security is not enabled.

   IMPORTANT If you are the administrator logging on with user security enabled, you can use **Administrator/Password** as the username/password.

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

   A message reminds you that you must restart the TraceFinder application before the user security setting is enabled.

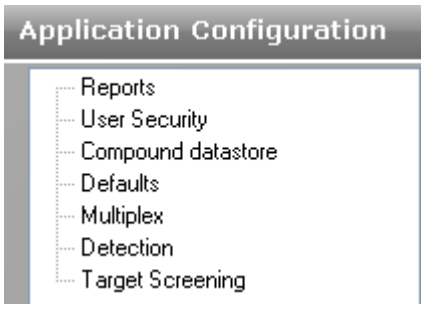
3. When you are prompted to restart the application, click **Yes**.

Enabling a Compound Datastore

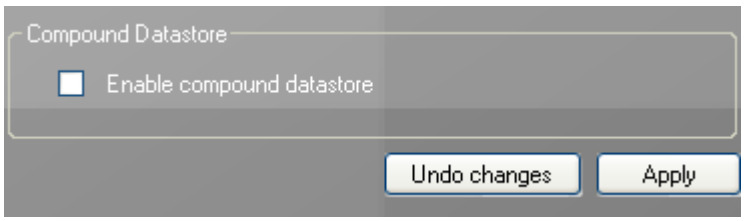
In the LabDirector or ITAdmin role, you can enable the compound datastore.

❖ To open the Compound Datastore page

1. In the Application Configuration view, click **Compound Datastore**.



   The Compound Datastore page of the Application Configuration view opens.



2. In the Compound Datastore Selection area, select the **Enable Compound Datastore** check box.

   Note By default, the Enable Compound Datastore option is not selected.

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

4. When prompted to restart the application, click **Yes**.

   After restarting, the application implements the following changes:

   - Displays the Acquisition List page on the Compounds page in the Master Method View. See "Editing the Compounds Page" on page 114.
   - Displays the Compound Datastore task pane on the Configuration mode navigation pane. See "Compound Datastore" on page 44.
   - Enables the Export SRM Data command in the Method Development mode. See "Exporting SRM Data" on page 199.

Specifying Configuration Defaults

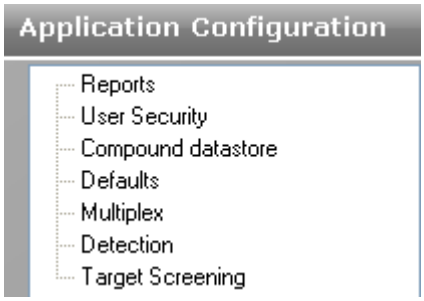
In the Application Configuration view of the Configuration mode, as a user in the LabDirector or ITAdmin role, you can specify the default laboratory and instrument names, mass precision, and intensity scale to use for reporting.

Use the following procedures:

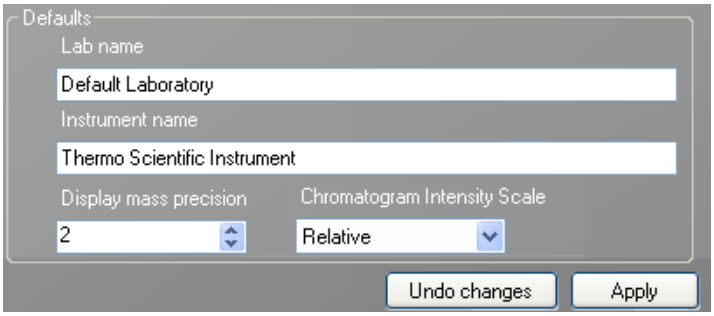
- To open the Defaults page
- To specify a default laboratory name and instrument name
- To specify default mass precision and the intensity scale

❖ To open the Defaults page

In the Application Configuration view, click **Defaults**.



The Defaults page of the Application Configuration view opens.



❖ To specify a default laboratory name and instrument name

1. Type the name of your laboratory in the Lab Name box.

   When you create a method, the application uses this default laboratory name for the Laboratory Name value on the General page of the Master Method View. The application uses this laboratory name in the report headings.

   Note This default laboratory name is not applied to previously created methods. By default, the laboratory name is Default Laboratory.

2. Type the name of your instrument in the Instrument Name box.

   When you create a batch, the application uses this default instrument name for the Instrument Name value. The application uses this instrument name in the report headings.

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

   Note This default instrument name is not applied to previously created batches. By default, the instrument name is Thermo Scientific Instrument.

4. When prompted to restart the application, click **Yes**.

❖ To specify default mass precision and the intensity scale

1. In the Display Mass Precision box, set the mass precision decimal places value to an integer from 0 to 5, inclusive.

   The default mass precision is 2. The TraceFinder application uses this mass precision value in the following locations:

   - Reports:
     - Blank Report
     - Confirmation Report (data spectra, library spectra, quan ion display, and qual ion display)
     - All High Density reports (*m/z* values)
     - Ion Ratio Failure Report (quan ion and qual ion)
     - Manual Integration Report (*m/z* value)
     - Qualitative Summary Report (all *m/z* values)
     - Quantitation Report (QIon)
   - All peaks on the Detection pages in the Method Development mode
   - The spectrum display in the Data Review mode
   - The spectrum display in the Method Forge dialog box

2. Select **Relative** or **Absolute** from the Chromatogram Intensity Scale list.

   This sets the default display type for both quan and qual chromatograms displayed in data review and reports.

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

4. When prompted to restart the application, click **Yes**.

Specifying Multiplexing Parameters

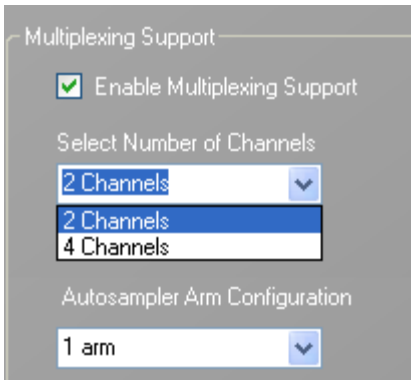
In the LabDirector or ITAdmin role, you can enable multiplexing and specify the maximum number of channels to use.

A user in the LabDirector, Supervisor, or Technician role can choose which channels to use for acquisition before submitting a batch from the Acquisition mode.

❖ To enable multiplexing

1. In the Application Configuration view, click **Multiplex**.

   The Multiplexing Support page opens.



2. Select the **Enable Multiplexing Support** check box.
3. In the Select Number of Channels list, select **2 Channels** or **4 Channels**.
4. When you select 2 channels, select a 1- or 2-arm autosampler configuration.

   The **1 arm** configuration enables channels 1 and 3; the **2 arm** configuration enables channels 1 and 2.

   When you use a 4-arm configuration, autosampler 1 uses channels 1 and 3 and autosampler 2 uses channels 2 and 4.

5. To apply the multiplexing settings, do the following:
   a. In the Application Configuration view, click **Apply**.

      A message reminds you that you must restart the TraceFinder application before the multiplexing selections are reflected in the Acquisition mode.

   b. To restart the TraceFinder application now, click **Yes,** or to remain on the Multiplexing Support page, click **No**.

Specifying Detection Parameters

In the LabDirector or ITAdmin role, you can specify detection parameters for Genesis, ICIS, or Avalon detection algorithms. Use the Peak Detection Defaults page to specify a peak detection algorithm and its options and to determine the area under a curve.

This section includes procedures for specifying the following detection algorithms:

- Genesis Detection Method
- ICIS Detection Method
- Avalon Detection Method

❖ To specify common detection parameters

1. In the Application Configuration view, click **Detection**.

   The Peak Detection Defaults page opens. See "Common peak detection areas" on page 72.

2. In the Detector Type list, select a detector type.
3. In the Mass Tolerance area, do the following:
   a. Select the units of measure you want to use.
   b. In the Value box, specify the number of millimass units or parts per million to use as the upper limit.

   The application applies this mass tolerance to the extracted chromatograms. The default is 500 MMU.
4. In the Retention Time area, do the following:
   a. In the Window box, specify the width of the window (in seconds) to indicate how far around the expected retention time the system will look for a peak apex.
   b. In the View Width box, specify the viewable size (in minutes) of the ion chromatogram display.
5. In the Ion Ratio Parameters area, do the following:
   a. In the Window Type box, select **Absolute** or **Relative** as the calculation approach for determining the acceptable ion ratio range.
   b. In the Window (+/-%) box, select the acceptable ion ratio range.
   c. In the Ion Coelution box, select the maximum difference in retention time between a confirming ion peak and the quantification ion peak.
6. In the Peak Detection Parameters area, select one of the detection algorithms: **Genesis**, **ICIS**, or **Avalon**.

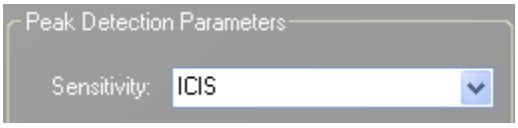


Figure 13. Common peak detection areas

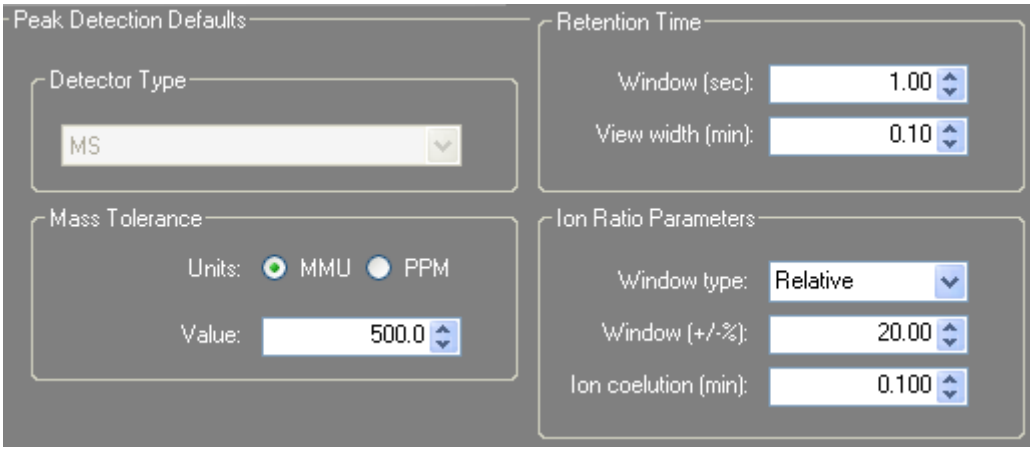


Table 12. Common peak detection parameters

Parameter	Description
Detector Type	
Mass Tolerance	
Units	• (Default) MMU (millimass units) MMU is a static calculation to the extracted mass. • PPM (parts per million) PPM is a variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.
Value	Upper limit of MMU or PPM. Default: 500 Range: 0.1 through 50 000
Retention Time	
Window (sec)	Width of the window (in seconds) to indicate how far around the expected retention time the system will look for a peak apex.
View width (min)	Viewable size (in minutes) 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.
Ion Ratio Parameters	
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.

Genesis Detection Method

The TraceFinder application provides the Genesis peak detection algorithm for backward compatibility with Xcalibur 1.0 studies.

Figure 14. Genesis peak detection page

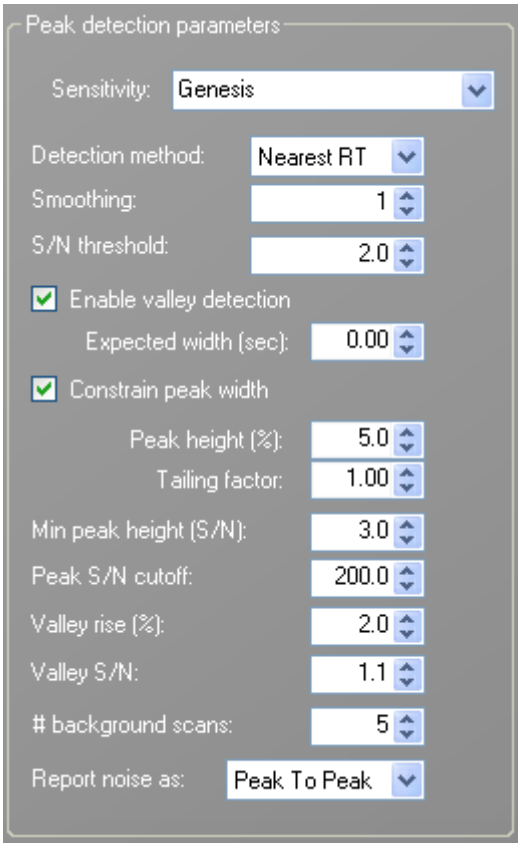


Table 13. Genesis peak detection page parameters (Sheet 1 of 3)

Parameter	Description
Sensitivity	Specifies the 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

Table 13. Genesis peak detection page parameters (Sheet 2 of 3)

Parameter	Description
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 parameter 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 TraceFinder application terminates the peak at that point. The 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.
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 you select the Constrain Peak Width check box. 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 you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

Table 13. Genesis peak detection page parameters (Sheet 3 of 3)

Parameter	Description
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 TraceFinder 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
Valley rise (%)	The peak trace can rise above the baseline by this percentage after passing through a minimum (before or after the peak). This criteria is useful for integrating peaks with long tails. 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. 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 TraceFinder 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.

ICIS Detection Method

The ICIS peak detection algorithm is designed for MS data and has superior peak detection efficiency at low MS signal levels.

Figure 15. ICIS peak detection page

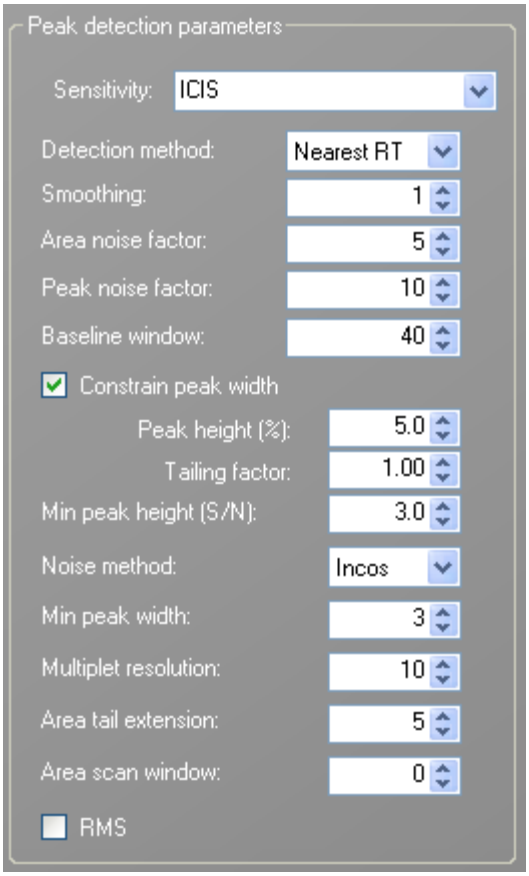


Table 14. ICIS peak detection page parameters (Sheet 1 of 3)

Parameter	Description
Sensitivity	Specifies the 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

Table 14. ICIS peak detection page parameters (Sheet 2 of 3)

Parameter	Description
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 you select the Constrain Peak Width check box. 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 you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

Table 14. ICIS peak detection page parameters (Sheet 3 of 3)

Parameter	Description
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 the analysis 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
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.

Avalon Detection Method

The Avalon peak detection algorithm is designed for UV data. The Avalon peak detection algorithm also supports negative peaks.

Figure 16. Avalon peak detection page

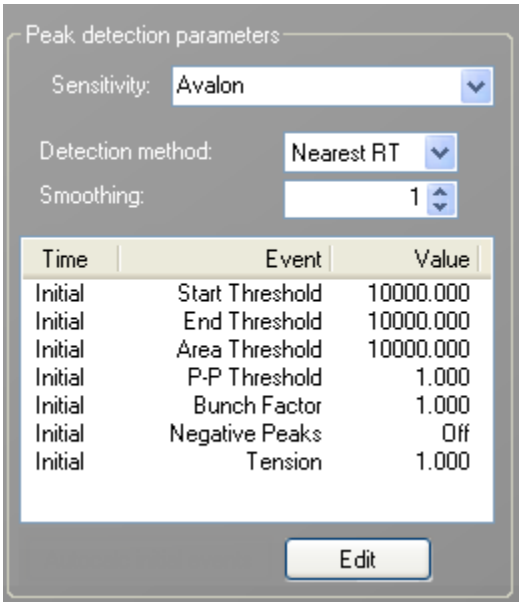


Table 15. Avalon peak detection page parameters

Parameter	Description
Sensitivity	Specifies the Avalon 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
Time/Event/Value	Displays the events specified in the Avalon Event List dialog box. Initially displays only the default events that cannot be edited or deleted.
Edit	Opens the Avalon Event List dialog box where you can edit the Time/Event/Value parameters. See "Avalon Event List" on page 80.

Avalon Event List

The event list includes both user-defined and noneditable default events. The application displays the default events when you choose Avalon sensitivity. You cannot delete these events or change their time or values. For a detailed list of events and value ranges, see "Event types" on page 81.

Figure 17. Avalon Event List dialog box

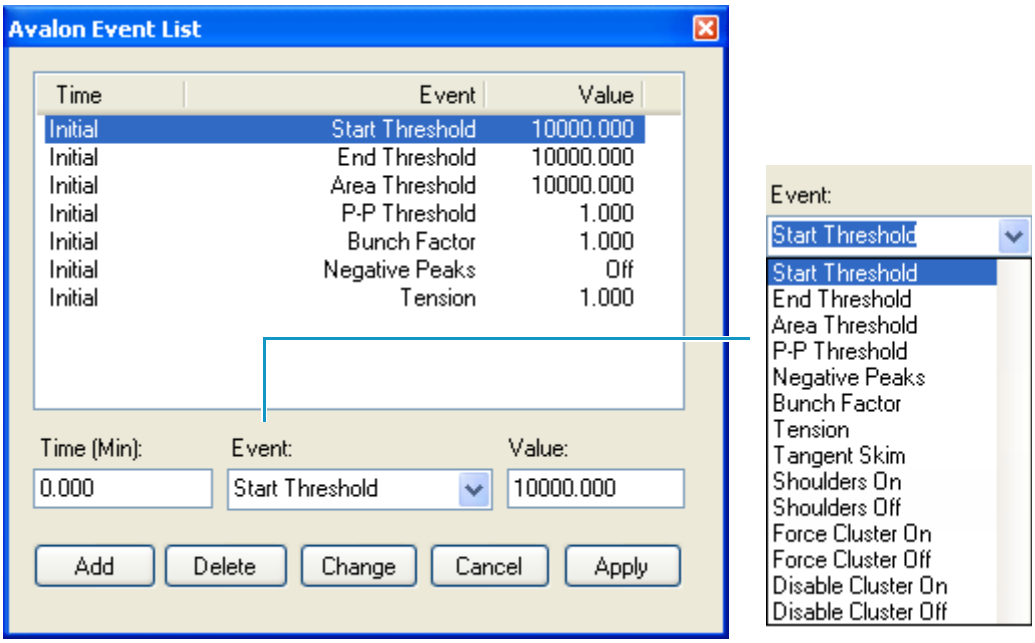


Table 16. Avalon Event List dialog box parameters

Parameter	Description
Time (Min)	Specifies the start time of the event.
Event	Specifies the type of event. For a detailed list of events and value ranges, see "Event types" on page 81.
Value	Specifies the value of the event.
Add	Adds a new event to the list with the current Time/Event/Value parameters.
Delete	Removes the selected Time/Event/Value parameter from the event list.
Change	Applies the current parameter values.
Cancel	Closes the dialog box without making any changes. Any additions, deletions, or changes revert to their original state.
Apply	Closes the dialog box.

Figure 18. Event types

Table 17. Event type definitions (Sheet 1 of 2)

Parameter	Description
Start Threshold	Specifies the threshold at the start of a peak. The Start Threshold is directly related to the RMS noise in the chromatogram. Range: 0 to 999 999 999
End Threshold	Specifies the threshold at the end of a peak. The End Threshold is directly related to the RMS noise in the chromatogram. Range: 0 to 999 999 999
Area Threshold	Controls the area cutoff. Any peaks with a final area less than the area threshold will not be detected. This control is in units of area for the data. Range: 0 to 999 999 999
P-P Threshold	The peak-to-peak resolution threshold controls how much peak overlap must be present before two or more adjacent peaks create a peak cluster. Peak clusters have a baseline drop instead of valley-to-valley baselines. Specified as a percent of peak height overlap. Range: 0.1 to 99.99
Negative Peaks	Permits detection of a negative going peak. Automatically resets after finding a negative peak. Valid values: On or Off
Bunch Factor	Specifies the number of points grouped together during peak detection. This event controls the bunching of chromatographic points during integration and does not affect the final area calculation of the peak. A high bunch factor groups peaks into clusters. Range: 0 to 999

Table 17. Event type definitions (Sheet 2 of 2)

Parameter	Description
Tension	Controls how closely the baseline should follow the overall shape of the chromatogram. A lower tension traces the baseline to more closely follow changes in the chromatogram. A high baseline tension follows the baseline less closely, over longer time intervals. Range: 0 to 999.99 minutes
Tangent Skim	Using this event, you can tangent skim any peak clusters. By default, it chooses the tallest peak in a cluster as the parent. You can also identify which peak in the cluster is the parent. Tangent skim peaks are detected on either side (or both sides) of the parent peak. Tangent skim automatically resets at the end of the peak cluster. Range: 0 to 1
Shoulders On	Allows peak shoulders to be detected (peaks which are separated by an inflection rather than a valley) Sets a threshold for the derivative.
Shoulders Off	Disables peak shoulder detection. Range: 0 to 50
Force Cluster On	Force the following peaks to be treated as a cluster (single peak).
Force Cluster Off	End the forced clustering of peaks.
Disable Cluster On	Prevent any peaks from being clustered.
Disable Cluster Off	Permit clusters to occur again.

Enabling Target Screening

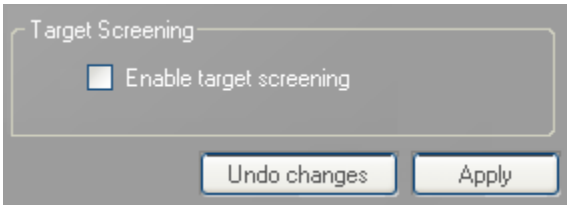
In the Application Configuration view of the Configuration mode, you can enable target screening features.

Note You must have the ToxID application installed on your computer before you can generate Target Screening reports.

❖ To enable target screening

1. In the Application Configuration view, click **Target Screening**.

   The Target Screening page of the Application Configuration view opens.



2. In the Target Screening area, select the **Enable Target Screening** check box.
3. In the Application Configuration view, click **Apply**.

   A message reminds you that you must restart the TraceFinder application before the target screening feature is enabled.

4. When prompted to restart the application, click **Yes**.

Using the Method Development Mode

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

Contents

- Working with Master Methods
- Working with Instrument Methods
- Working with Development Batches

From the Method Development mode, you can create a master method, an instrument method, or a simple development batch to test your instrument method.

❖ To access the Method Development mode

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

The Method Development navigation pane opens. For a detailed description of all the features on the Method Development navigation pane, see "Method Development navigation pane" on page 86.

Figure 19. Method Development navigation pane

Table 18. Method Development navigation pane functions (Sheet 1 of 2)

Function	Description
Method View	See "Working with Master Methods" on page 88.
Create method	Opens the Create Master Method dialog box where you can choose the process you want to use to begin your master method.
Open method	Opens the Open Master Method dialog box where you can choose a master method to open.

Table 18. Method Development navigation pane functions (Sheet 2 of 2)

Function	Description
Import Published Method	
Export SRM data	Writes the selected reaction monitoring (SRM) table to the following file: …\Thermo\TraceFinder\1.1\Methods*methodname*.xml You can use the data in this file in the instrument method editor when you open the TSQ 2.1 application. This command is available only when you have selected the Enable Compound Datastore option on the Compound Datastore page of the Application Configuration view. See "Application Configuration" on page 56. The compounds in the Acquisition List must contain at least one SRM experiment type.
Recent Files	Displays recently saved master methods.
Instrument View	See "Working with Instrument Methods" on page 200.
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 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.
Development Batch	See "Working with Development Batches" on page 207.
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 Thermo Xcalibur Qual Browser where you can view the acquired raw data files.

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.

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

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. 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 data processing and information reporting for batches 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 the TraceFinder application saves all of your commonly used method settings in a template, such as number of confirming ions or use of data-dependent data.

This section includes instructions for the following tasks:

- Creating a New Master Method
- Editing a Master Method
- Creating a Method Template
- Importing Published Master Methods
- Exporting SRM Data

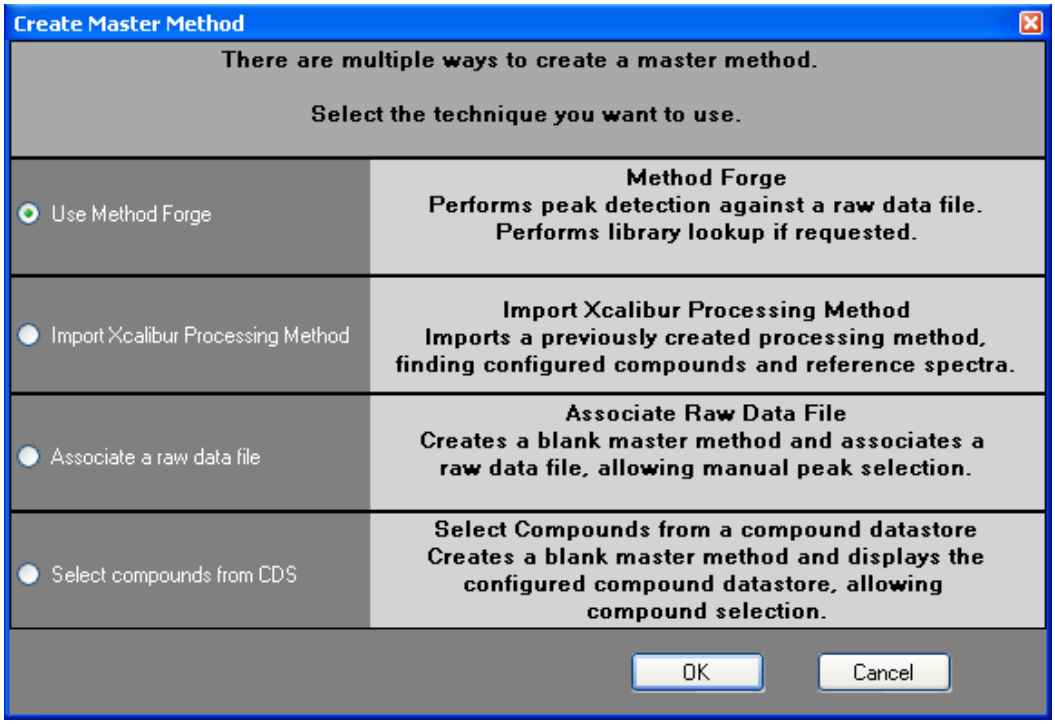
Creating a New Master Method

To begin a master method, follow any of four different procedures:

- Creating a New Method with Method Forge
- Importing an Xcalibur Master Method
- Associating a Raw Data File
- Selecting Compounds from the Compound Datastore

With each procedure, you begin the method in a specific way and then use the common features of the Master Method View to complete and save your master method.

Figure 20. Create Master Method dialog box



Creating a New Method with Method Forge

With Method Forge, you can create a new master method by manually selecting peaks, selecting multiple compounds, renaming peaks, or comparing mass spectra from the library searches. You can also choose to let the TraceFinder application automatically create a master method for you. For a detailed description of all the Method Forge parameters, see "Method Forge dialog box parameters" on page 96.

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

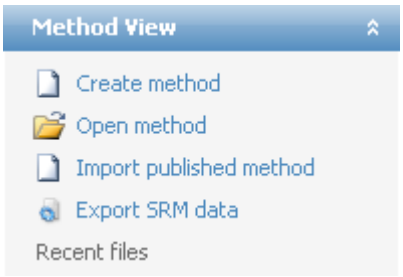
- Reviews your raw data file and identifies compounds that are present in your sample.
- Uses your mass spectral reference libraries to assign compound names and CAS numbers.
- Uses mass spectral information to select potential quantification and confirming ions and a reference mass spectrum for the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

Use the following procedures:

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

❖ To automatically select compounds to create a new method

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



   The Create Master Method dialog box opens.

2. In the Create Master Method dialog box, select the **Use Method Forge** option and click **OK**.

   The Method Forge dialog box opens. For a detailed description of all the features on the Method Forge dialog box, see "Method Forge dialog box" on page 95.

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

3. 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 188.

4. 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 application names the method for the raw data file used to create the method.

5. Select the **Automatically Create the Master Method** check box.

6. 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.

   c. Go to step 8.

   –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 TraceFinder application will write the raw data file.

   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.

7. If you chose to acquire a new raw data file, do one of the following:

   Choose **Manual Injection**.

   –Or–

   Do the following:

   a. Choose **Use Autosampler**.

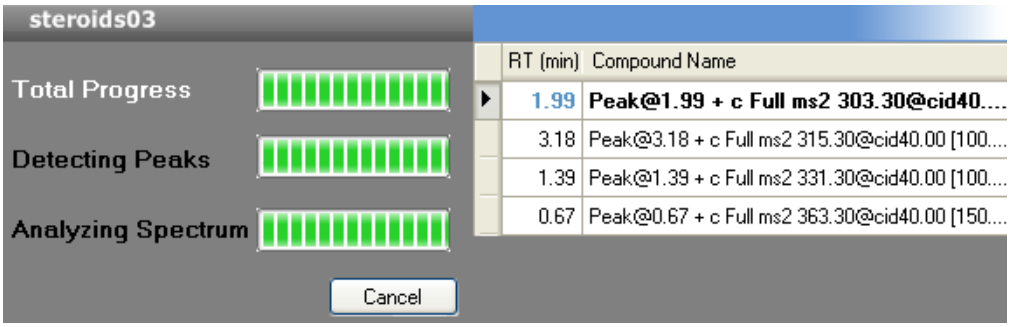
   b. In the Vial Position box, type a vial position.

   c. In the Injection Volume box, type an injection volume.

      The minimum injection volume allowed is 0.1µL; the maximum injection volume allowed is 5000µL.

8. To automatically create the master method, click **OK** (or **Overwrite**).

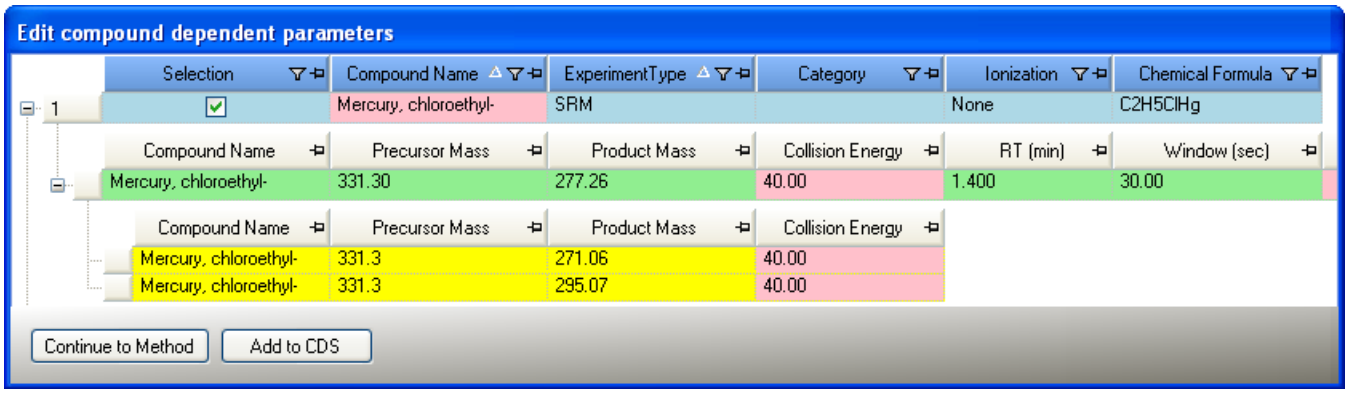
   As the Method Forge creates the method, it displays the following status:



Note The Method Forge process searches the NIST library and displays the identified compound names instead of peak times.

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

If the compounds in the raw data file you used to create the method are not in the current compound datastore, the TraceFinder application displays the compounds in the Edit Compound Dependent Parameters dialog box.



9. (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 You must use the Add to CDS command before you continue to the method.

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

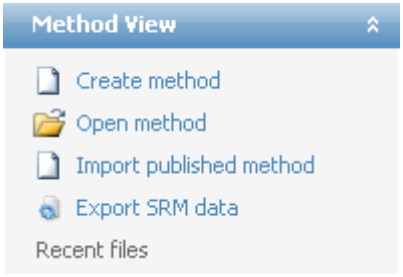
    The TraceFinder application uses all compounds found in the raw data file in your method and displays the General page of the Master Method View. For a detailed description of all the features on the General page, see "General page" on page 111.

11. From the Instrument Method list on the General page, select an instrument method.
12. From the Qualitative Peak Processing Template list, select a method template for performing peak detection on quantitative samples following target compound analysis.
13. From the Background Subtraction Range Option list, select how you want the background subtraction range determined from one of these options:
    - **Before Peak**: Averages and subtracts a specified number of scans before the apex of the peak.
    - **After Peak**: Subtracts a specified number of scans following the apex of the peak.
    - **Both Sides of Peak**: Subtracts a specified number of scans from each side of the apex of the peak.
14. To save the new method, choose **File > Save** from the main menu.

    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 104.

❖ To manually select compounds to create a new method

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



   The Create Master Method dialog box opens.

2. In the Create Master Method dialog box, select **Use Method Forge** and click **OK**.

   The Method Forge dialog box opens. For a detailed description of all the features on the Method Forge dialog box, see "Importing an Xcalibur Master Method" on page 97.

3. 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 188.

4. 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 data file used to create the method.

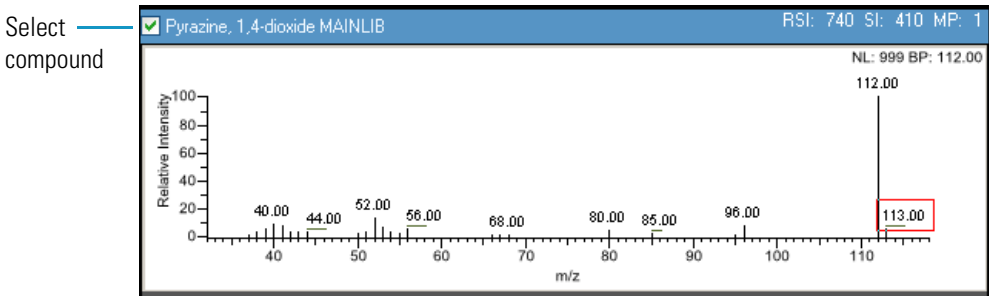
5. Ensure that the **Automatically Create the Master Method** check box is not selected.

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

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

   The Master Method View displays a list of possible matches in the Library Results pane. The TraceFinder application displays the best match in the Compound Name list and displays the peak spectrum for that compound.

8. To use a compound other than the compound chosen by the TraceFinder application, scroll to the spectrum for that compound and select the compound name in the header of the spectrum pane.



9. After you manually select your compound, click **Create** to create the master method.

   All compounds found in the raw data file are used in your method. The TraceFinder application displays the General page of the Master Method View. For a detailed description of all the features on the General page, see "General page" on page 111.

10. From the Instrument Method list on the General page, select an instrument method.

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

    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 104.

Figure 21. Method Forge dialog box

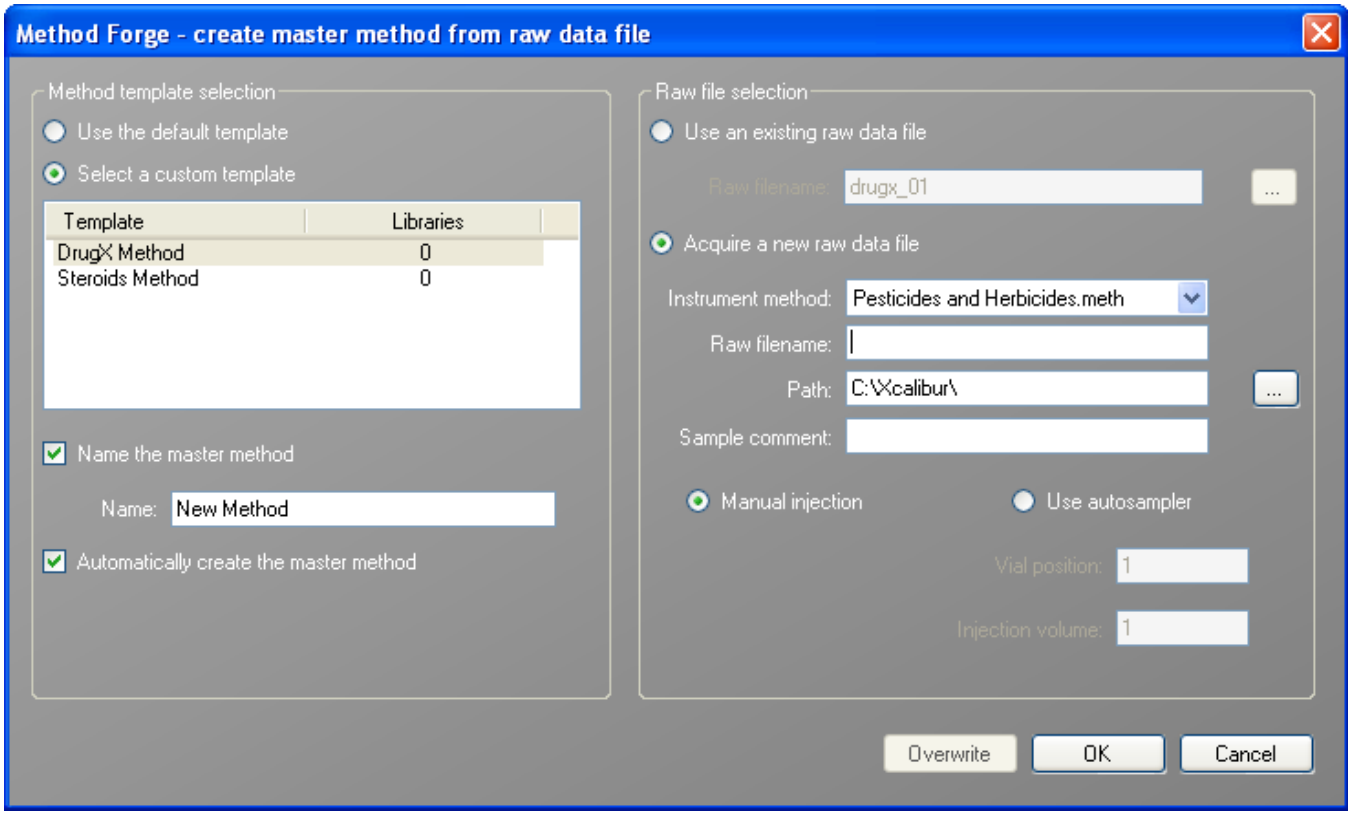


Table 19. Method Forge dialog box parameters

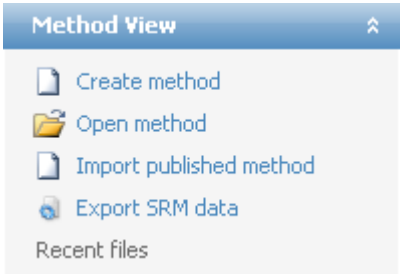
Parameter	Description
Method template selection	
Use the default template	Creates a new method with the default template.
Select a custom template	Lists all the available method templates. For detailed instructions about creating a custom method template, see "Creating a Method Template" on page 188.
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, library searching, and characteristic ion and reference spectrum identification. This information is loaded into a new master method. This process occurs immediately when you specify an existing raw data 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 data file to use to create the master method.
Instrument method	The saved method (.meth) file to use for acquiring the data.
Raw filename	The file name where the TraceFinder application writes the raw data.
Path	The location where the TraceFinder application saves the 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 button	
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 Master Method

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

❖ To import an Xcalibur master method

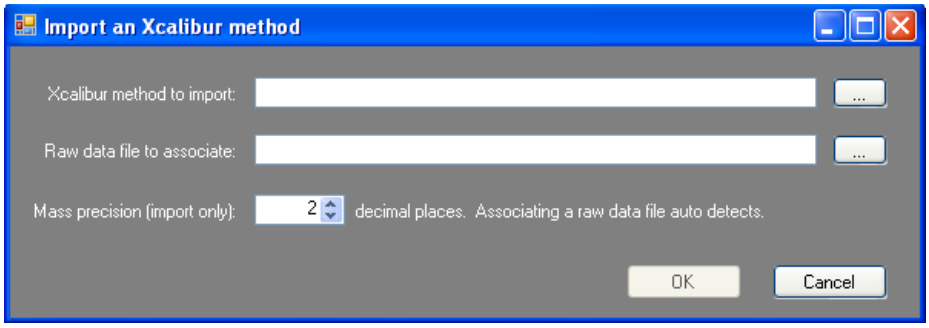
1. From the Method View task pane, click **Create Method**.



   The Create Master Method dialog box opens.

2. In the Create Master Method dialog box, select **Import Xcalibur Processing Method** and click **OK**.

   The Import an Xcalibur Method dialog box opens.



3. Click the browse button for the Xcalibur Method to Import box, browse to the Xcalibur processing method file, and open the file.

   The TraceFinder application imports the compound information from the Xcalibur method file.

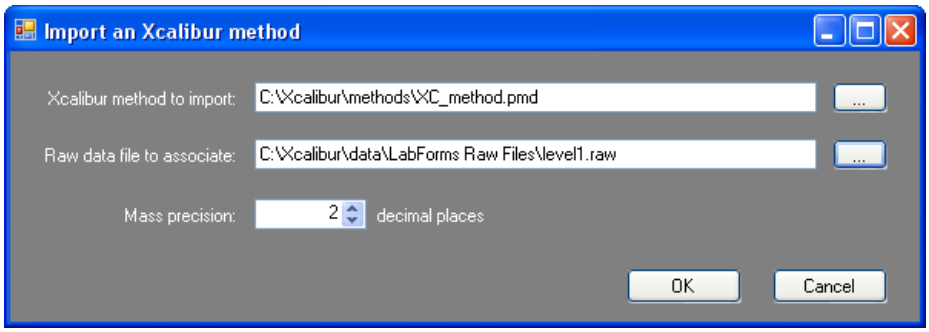
4. (Optional) Click the browse button for the Raw Data File to Associate box, browse to the raw data file, and open the file.

5. (Optional) Change the number of decimal places in the Mass Precision box.

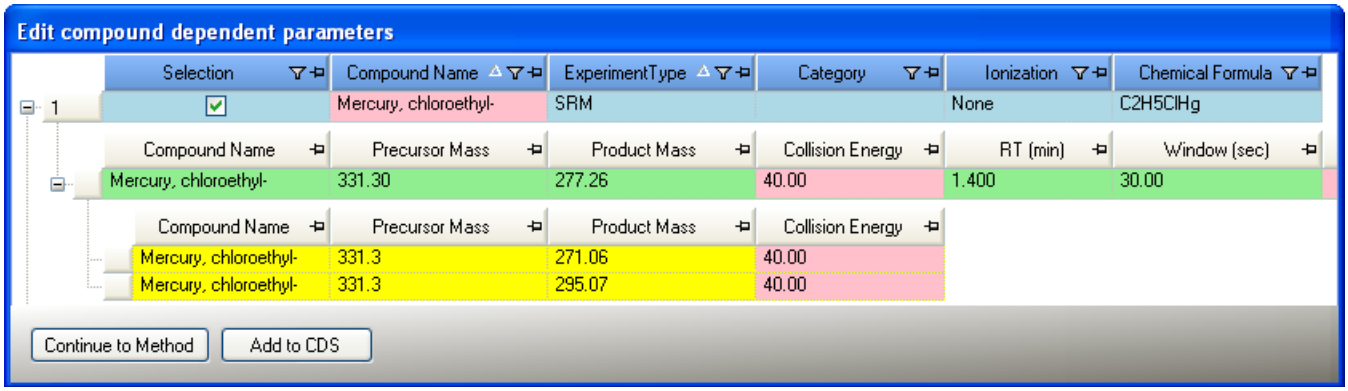
   You can set the mass precision decimal places to any integer between 0 and 5, inclusive.

> **Note** When you associate a raw data file, the application read the mass precision from the file and this parameter is unavailable.

6. Click **OK**.



If the compounds in the imported Xcalibur method file are not in the Compound Datastore, the TraceFinder application displays the compounds in the Edit Compound Dependent Parameters dialog box.



7. (Optional) Select the compounds 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 the Add to CDS command before you continue to the method. When you click Continue to Method, the Edit Compound Dependent Parameters dialog box closes and you cannot return to add the compounds.

8. To add these compounds to your method and close the dialog box, click **Continue to Method**.

   The TraceFinder application adds all compounds found in the imported Xcalibur method and displays the General page of the Master Method View. For a detailed description of all the features on the General page, see "General page" on page 111.

9. From the Instrument Method list on the General page, select an instrument method.

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

    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 104.

Associating a Raw Data File

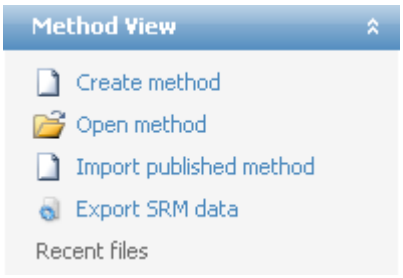
You can use the compounds in a previously acquired raw data file to create a new master method.

Use the following procedures:

- To associate a raw data file with the method
- To add compounds to the method

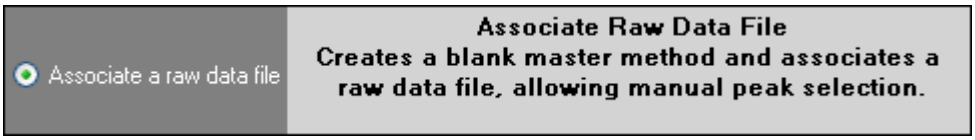
❖ To associate a raw data file with the method

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

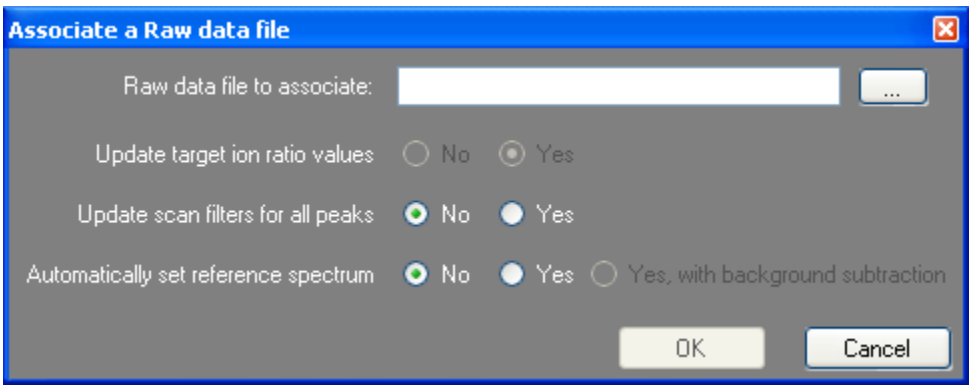


The Create Master Method dialog box opens.

2. In the Create Master Method dialog box, select **Associate a Raw Data File** and click **OK**.



The Associate a Raw Data File dialog box opens.



3. Click the browse button and locate a raw data file to associate with the method.

4. To set a reference spectrum, do one of the following:

   Click **Yes**.

   –Or–

   Click **Yes, with Background Subtraction.**

   This feature is available only when you have set background subtraction values on the General page of the Master Method View. See "Editing the General Page" on page 106.

   The TraceFinder application adds all compounds found in the raw data file to your method and displays the General page of the Master Method View. For a detailed description of all the features on the General page, see "General page" on page 111.

5. From the Instrument Method list on the General page, select an instrument method.

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

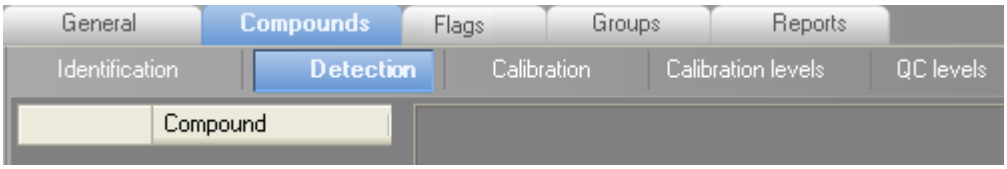
   If the compounds in the associated raw data file are not found in the Compound Datastore, you cannot save the method. Follow the instructions "To add compounds to the method" on page 100.

   For a detailed description of how to modify a master method, see "Editing a Master Method" on page 104.

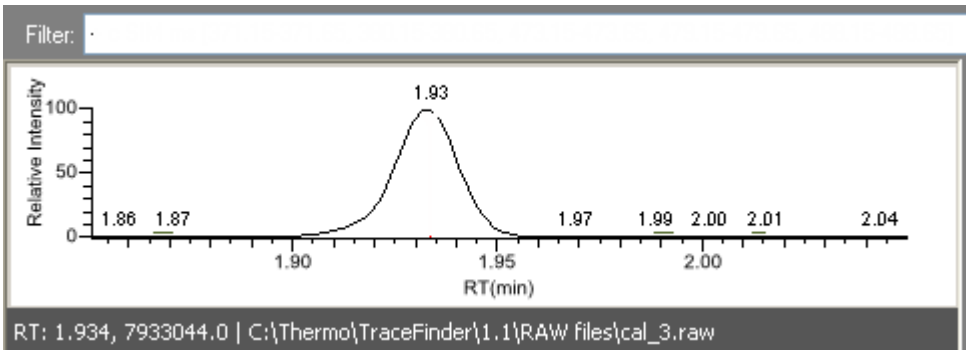
❖ To add compounds to the method

1. Click the **Compounds** tab.

   The Detection page is selected by default.

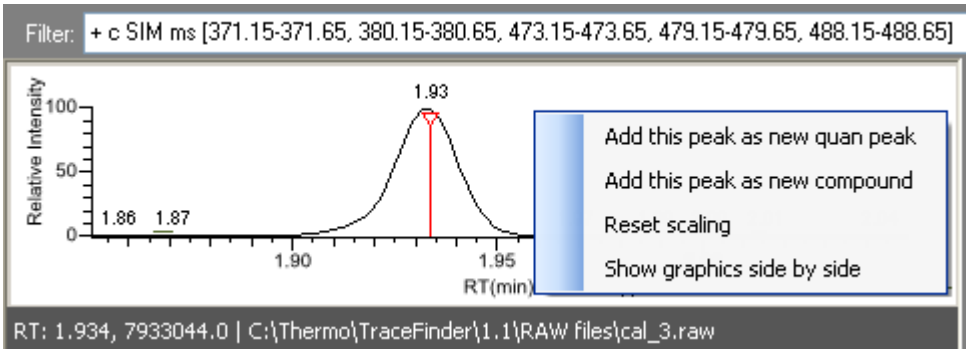


   The Detection page shows an empty Compound list and displays the chromatographic data for the compounds in the raw data file.



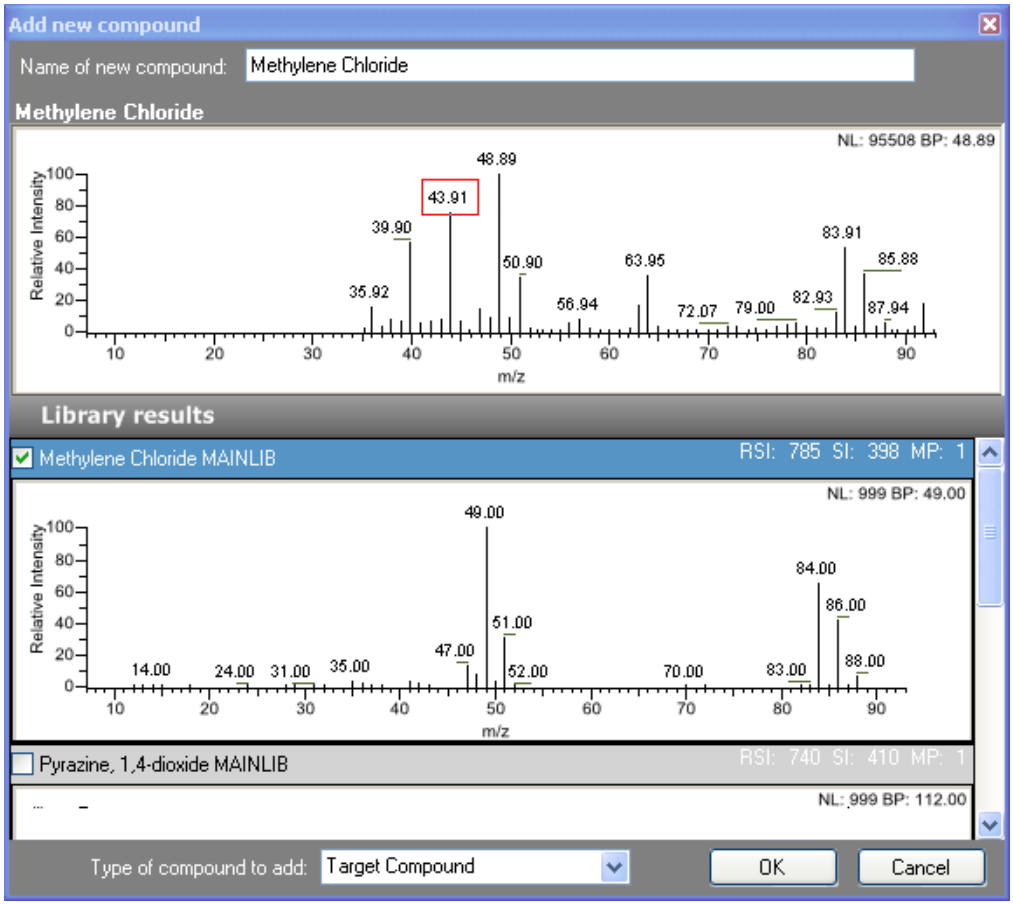
2. Select a filter from the Filter list.

3. Click the peak in the chromatogram that represents the compound you want to add to the method.
4. Right-click and choose **Add This Peak as New Compound** from the shortcut menu.

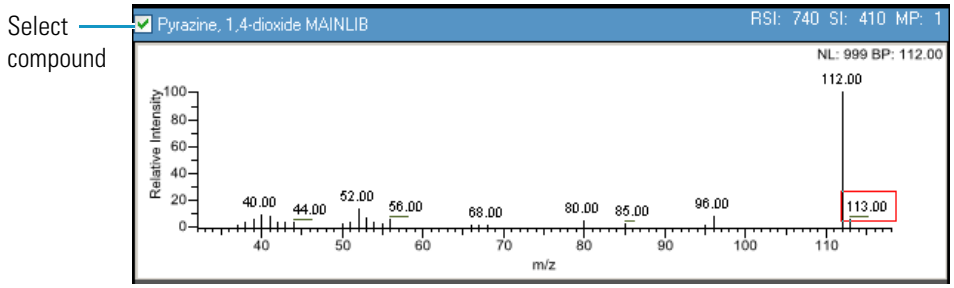


The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quan peak, and the second and third largest ions as the confirming ions.

If the name of the first match is already in the library, the Add New Compound dialog box opens.



5. (Optional) In the Add New Compound dialog box, do the following:
   a. To use a compound other than the compound already in the library, scroll to the spectrum for that compound and select the compound name in the title bar of the spectrum pane.



   b. In the Type of Compound to Add list, select a compound type.
   c. Click **OK**.
6. Repeat this procedure for each compound you want to add to the method.

   For a detailed description of all the features on the Detection page, see "Editing the Compounds Page" on page 114.

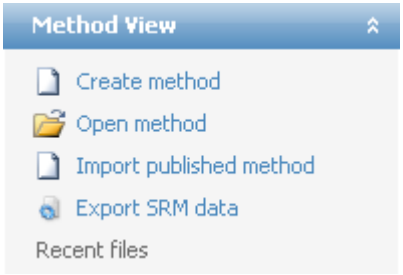
   For a detailed description of how to modify a master method, see "Editing a Master Method" on page 104.

Selecting Compounds from the Compound Datastore

You can select compounds from the compound datastore to create a new master method. This method for creating a master method is available only when the compound datastore is enabled. See "Enabling a Compound Datastore" on page 67.

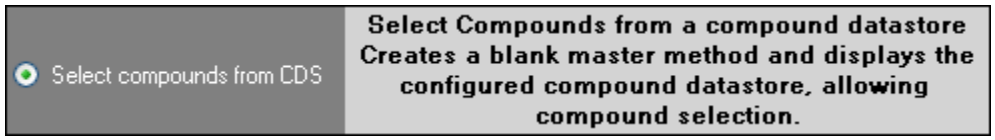
❖ To select compounds from the datastore

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

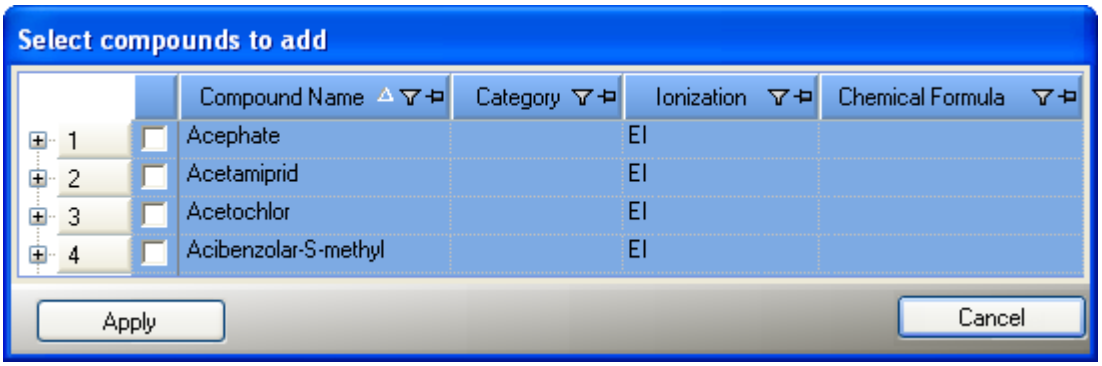


   The Create Master Method dialog box opens.

2. In the Create Master Method dialog box, select **Select Compounds from CDS** and click **OK**.



The Select Compounds to Add dialog box opens, listing all the compounds defined in the compound datastore.



3. Select the check box for each of the compounds you want to add to the method.
4. To quickly select multiple compounds, right-click and use any of the commands on the shortcut menu.

Table 20. Select Compounds to Add shortcut menu

Command	Description
Select All	Selects all compounds in the compound datastore.
Deselect All	Clears all compounds in the compound datastore.
Copy Down	Copies the state (checked or cleared) of the currently selected compound to all compounds below it in the compound list.

5. Click **Apply**.

The TraceFinder application adds the selected compounds to the method.

Note After you add a compound to a method, the compound is no longer enabled in the Select Compounds to Add dialog box. You cannot remove the applied compounds from the method by returning to this dialog box. To remove a compound from a method, see "Acquisition List" on page 114.

6. From the Instrument Method list on the General page, select an instrument method.
7. To save the new method, choose **File > Save** from the main menu.

For a detailed description of how to modify a master method, see "Editing a Master Method" on page 104.

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 Compounds Page
- Editing the Flags Page
- Editing the Groups Page
- Editing the Reports Page

Opening a Master Method

Use the TraceFinder application to open a master method that was created and saved in the current TraceFinder application or imported from TraceFinder version 1.0.1.

Use the following procedures:

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

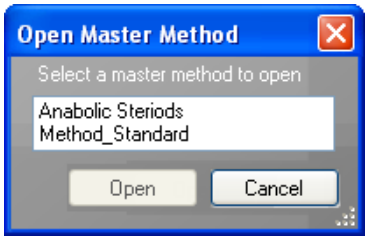
❖ To open a saved master method

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

   The Method Development navigation pane opens.

2. In the Method View task pane, click **Open Method,** or choose **File > Open > Master Method** from the main menu.

   The Open Master Method dialog box opens.



   The Open Master Method dialog box displays all available methods. The list of TraceFinder methods can include any method created with TraceFinder 1.0.1 or greater.

3. Select a master method and click **Open**.

   The General page for the selected method opens in the Method View. For a detailed description of all the features on the General page, see "General page" on page 111.

   When you open a TraceFinder 1.0.1 method, the TraceFinder application copies all components of the selected method including its associated instrument method.

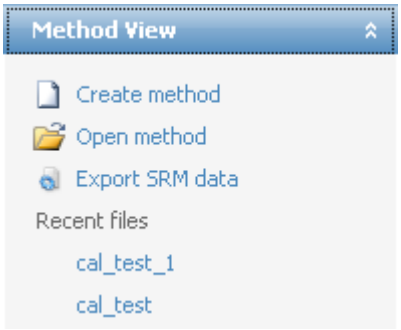
   - If the TraceFinder 1.0.1 master method does not have an associated instrument method, the Master Method View for the imported method indicates that you must select an instrument method.
   - If you open a TraceFinder 1.0.1 master method that uses an instrument method name already used in your Xcalibur\methods folder, you are prompted to overwrite the instrument method or use the method with the same name already in your methods folder.

❖ To open a saved master method from the Recent Files list

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

   The Method Development navigation pane opens.

   When you save a method, the application adds it 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.

   The General page for the selected method opens in the Method View. For a detailed description of all the features on the General page, see "General page" on page 111.

Editing the General Page

The General page defines basic information about the master method. For a detailed description of all the features on the General page, see "General page" on page 111.

Use the following procedures:

- To specify general information for a master method
- To edit the instrument method parameters
- To set automated background subtraction options
- To specify a chromatogram reference sample
- To specify mass tolerance

❖ 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.

   The default name is Default Laboratory.

2. In the Assay Type box, type the assay type to be targeted by the method.

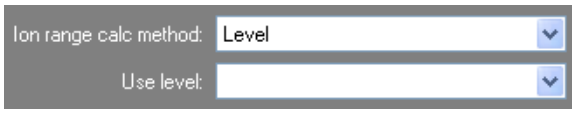
3. From the Injection Volume box, select the injection volume (in µL) to be used for sample injection.

   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.

   IMPORTANT The TraceFinder application uses this injection volume in the master method, not the injection volume from the instrument method.

4. From the Ion Range Calc Method list, select a method for calculating the ion ratio range windows.

   When you select Level, the TraceFinder application displays an Use Level list where you can choose a calibration level. To define the calibration levels on the Compounds page, see "Editing the Compounds Page" on page 114.

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

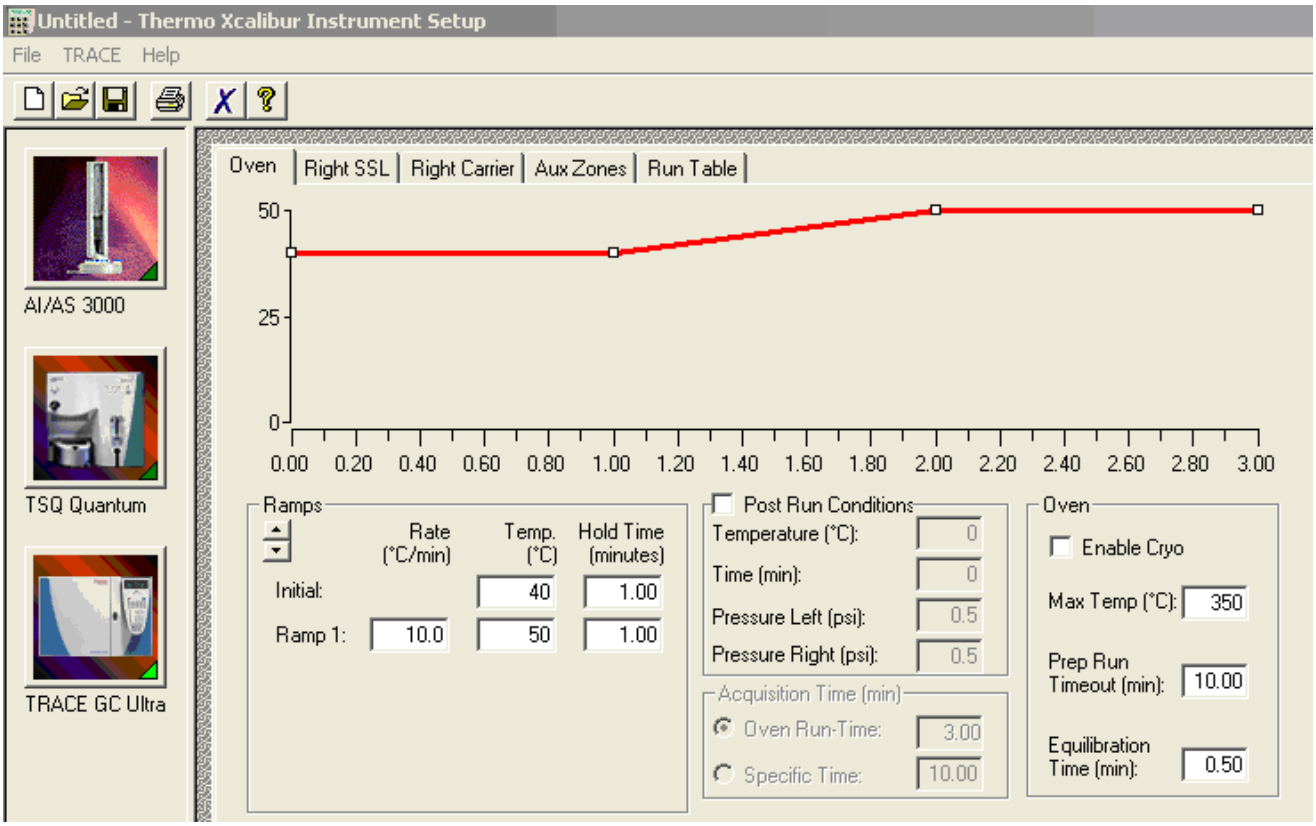
❖ To edit the instrument method parameters

1. From the Instrument Method list on the General page, select an instrument method.

   For a detailed description of all the features on the General page, see "General page" on page 111.

2. To edit the instrument method for this master method, click **Edit**.

   The Thermo Xcalibur Instrument Setup dialog box opens. This example instrument setup shows multiple configured instruments.



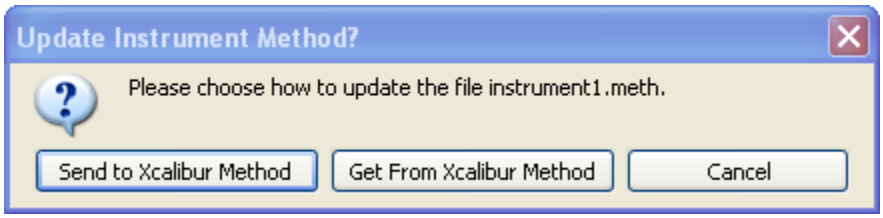
3. Edit the values on the instrument page for your instrument.

4. From the main menu on the Thermo Xcalibur Instrument Setup dialog box, choose **File > Save** and then choose **File > Exit**.

   The TraceFinder application returns you to the General page.

5. To update any changes that were made to the instrument method after you created this master method, click **Update**.

   The Update Instrument Method? dialog box opens.



6. Choose one of the following options:

   - **Send to Xcalibur Method**: Overwrites the Xcalibur method with the current instrument method.
   - **Get From Xcalibur Method**: Overwrites the current instrument method with the Xcalibur method.
   - **Cancel**: Make no changes to the instrument method in the current master method.

❖ To set automated background subtraction options

1. In the Background Subtraction Range Option list, select how you want the subtraction range determined from the following options:

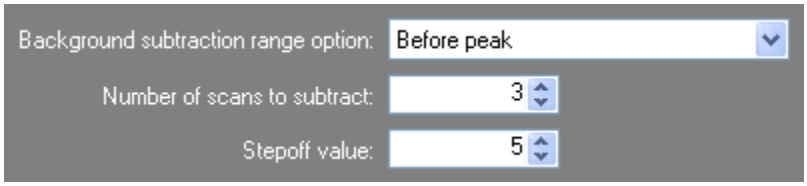
   - **Before Peak**: Averages and subtracts a specified number of scans before the apex of the peak.
   - **After Peak**: Subtracts a specified number of scans following the apex of the peak.
   - **Both Sides of Peak**: Subtracts a specified number of scans from each side of the apex of the peak.

2. In the **Number of Scans to Subtract** box, enter a number.

   This is the number of scans that the TraceFinder application subtracts from the background after averaging. If you specified to subtract scans from both sides of the peak, the application subtracts this number of scans from **each** side of the peak.

3. In the **Stepoff Value** box, enter a number.

   The TraceFinder application uses this offset value to average and subtract scans that are not adjacent to the apex of the peak. For example:

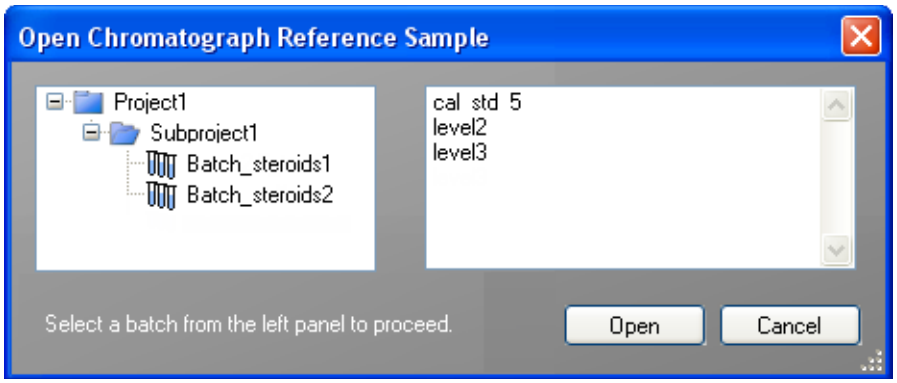


   If you specified to subtract 3 scans before the peak and the stepoff value is 5, the TraceFinder application ignores the first 5 scans to the left of the peak and applies the averaging and subtraction to the 6th, 7th, and 8th scans to the left of the peak.

❖ To specify a chromatogram reference sample

1. In the **Set Chromatogram Reference Sample** list, select **External**.
2. Click **Select**.

   The Open Chromatograph Reference Sample dialog box opens.



Note If you are creating a new method, you will not see any reference samples here. You must first create and save a batch using this method to see the reference samples in this list.

3. Select a project from the list of projects.
4. Select a subproject from the list of subprojects.
5. Select a batch from the list of batches.

   The TraceFinder application displays only batches that were created using the current master method.

6. Select a sample from the list of processed samples.

   The TraceFinder application displays all the processed samples in the selected batch. To use a sample as a reference sample, it must have been processed with the current master method.

7. Click **Open**.

   The selected sample is displayed as the chromatogram reference sample in the Master Method View.

Tip To clear the reference sample from the master method, select **None** in the **Set Chromatogram Reference Sample** list.

❖ To specify mass tolerance

1. Select the units of measure you want to use.
2. Specify the number of millimass units or parts per million to use as the *m/z* ± tolerance value.

   The application applies this mass tolerance to the extracted chromatograms.

Figure 22. General page

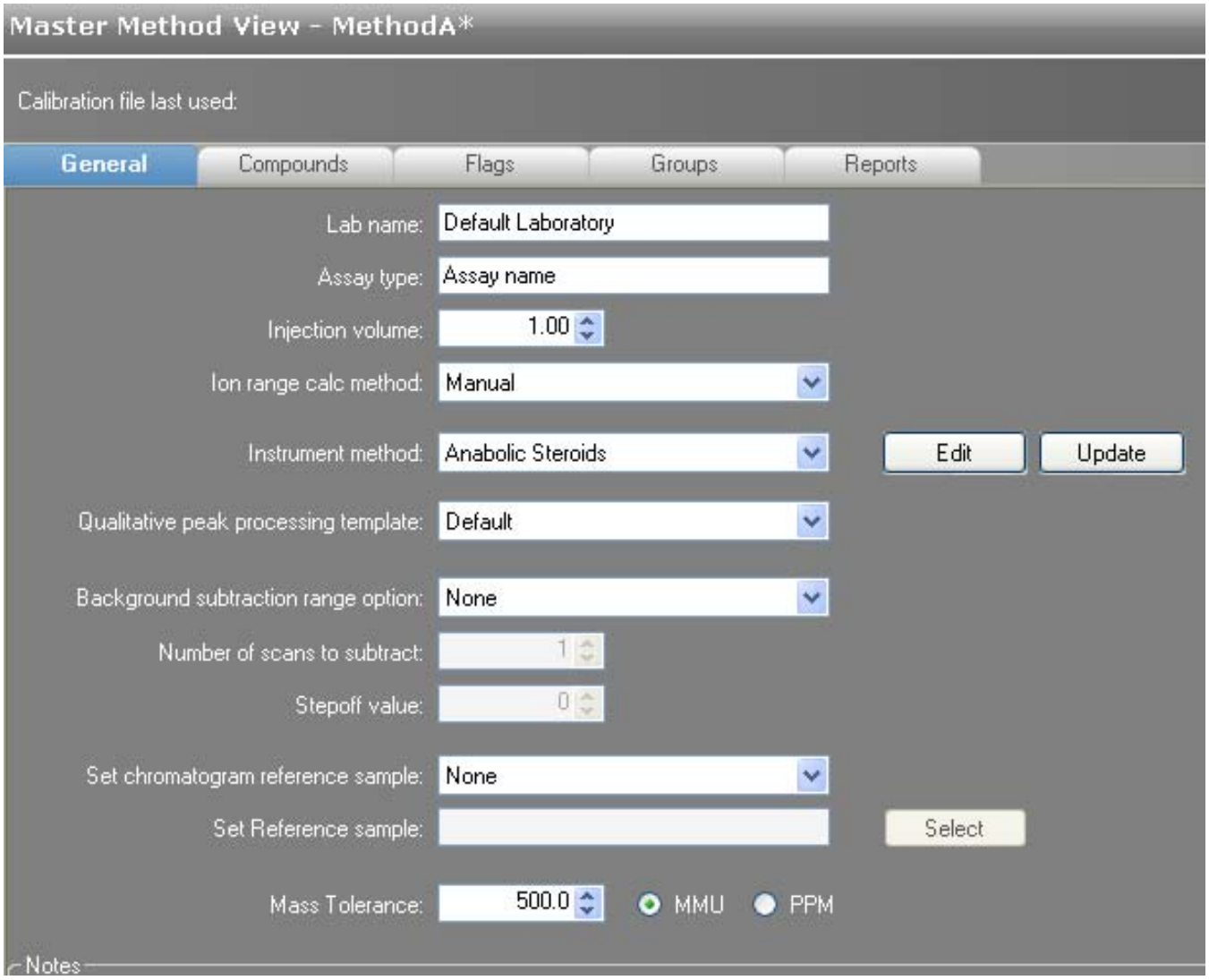


Table 21. General page parameters (Sheet 1 of 3)

Parameter	Description
Lab name	The laboratory name to be displayed on the top of each printed, saved, or exported report. Default: Default Laboratory To specify this default laboratory name, see "Specifying Configuration Defaults" on page 68.
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, you might use an assay type of PAH for the analysis of Polynuclear Aromatic Hydrocarbons). The TraceFinder application uses this assay type in the method template.

Table 21. General page parameters (Sheet 2 of 3)

Parameter	Description
Injection volume	The system uses the injection volume (in µL) for sample injection. For a more detailed explanation, refer to the documentation for the autosampler. The injection volume in the master method overrides the injection volume in the instrument method. The injection volume in the batch overrides the injection volume in the master method. Range: 0.1 through 5000µL
Ion range calc method	The TraceFinder application uses the selected 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 is displayed where you can select a calibration level amount. To define these calibration levels on the Compounds page, see "Editing the Compounds Page" on page 114.
Instrument method	Instrument method used for acquiring samples.
Edit	Opens the Thermo Xcalibur Instrument Setup dialog box where you can edit the instrument method.
Update	Choose one of the following: • **Send to Xcalibur Method**: Overwrites the Xcalibur method with the current instrument method. • **Get From Xcalibur Method**: Overwrites the current instrument method with the Xcalibur method.
Qualitative peak processing template	The TraceFinder application uses the qualitative peak processing template to perform peak detection on quantitative samples following compound analysis.
Background subtraction range option	Valid values: None, Before Peak, After Peak, Both Sides of Peak Default: None
Number of scans to subtract	Valid values: Even numbered integers Default: 0
Stepoff value	Offset from the selected peak to the first subtracted peak.
Set chromatogram reference sample	Valid values: None, External Default: None
Set Reference sample	This parameter is enabled only when Set Chromatogram Reference Sample is set to External. Click the Select button to choose a reference sample from the project folders.

Table 21. General page parameters (Sheet 3 of 3)

Parameter	Description
Mass Tolerance	Upper limit of MMU or PPM. Default: 500 Range: 0.1 through 50 000 • (Default) MMU (millimass units): MMU is a static calculation to the extracted mass. • PPM (parts per million): PPM is a variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.
Notes	Notes you add about the method.

Editing the Compounds Page

Use the Compounds page to set 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:

- Acquisition List
- Identification
- Detection
- Calibration
- Calibration Levels
- QC Levels
- Real Time Viewer
- Using the Shortcut Menu Commands

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. For a detailed description of all the features on the Acquisition List page, see "Acquisition List page" on page 116.

The Acquisition List page is displayed only when you select the Enable Compound Datastore option on the Compound Datastore page in the Application Configuration view. For a detailed description of all the features on the Application Configuration view., see "Application Configuration" on page 56.

Use the following procedures:

- To filter the compound list
- To delete a compound from the list
- To add a compound to the list

❖ To filter the compound list

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

   The application displays a list of filterable criteria. In all lists, 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.

   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. Click the **Remove Compound** icon, , or right-click and choose **Remove Compound** from the shortcut menu.

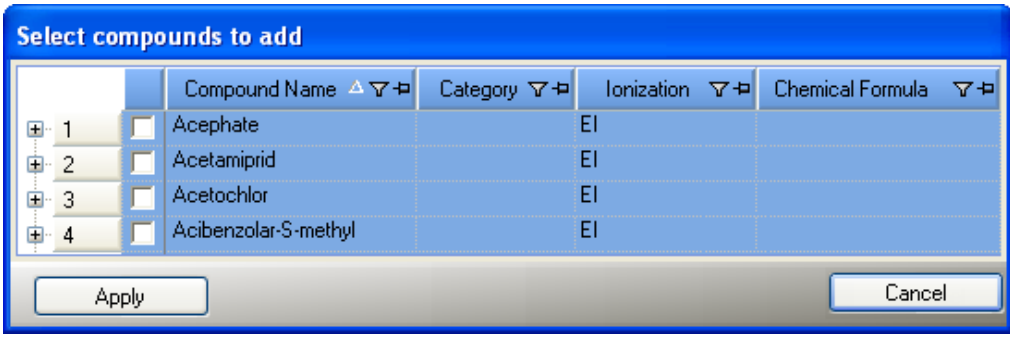
   A confirmation dialog box opens, listing the compound to be removed.
3. To confirm the deletion, click **Yes**.

   The selected compound is removed from the acquisition list, which has no effect on the compound datastore.

❖ To add a compound to the list

1. Click the **Add Compound** icon, , or right-click and choose **Add Compound** from the shortcut menu.

   The Select Compounds to Add dialog box opens, listing all the compounds defined in the compound datastore.



2. Select the check box for each of the compounds you want to add to the method.
3. To quickly select multiple compounds, right-click and use any of the commands on the shortcut menu.

   Table 22. Select Compounds to Add shortcut menu

Command	Description
Select All	Selects all compounds in the compound datastore.
Deselect All	Clears all compounds in the compound datastore.
Copy Down	Copies the state (checked or cleared) of the currently selected compound to all compounds below it in the compound list.

4. Click **Apply**.

   The TraceFinder application adds the compounds to the Acquisition List and Compounds pages of the Master Method View.

Figure 23. Acquisition List page

Table 23. Acquisition List page parameters (Sheet 1 of 3)

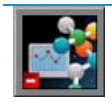
Parameter	Description
Function Icons	
	Opens the Select Compounds to Add dialog box that lists all the compounds defined in the compound datastore.
	Deletes the selected compound. The icon is unavailable when no row is selected. If you used the filters to display a subset of compounds, the selected compound might not be visible on the Acquisition List page.
Compound parameter	
Compound Name	Alphanumeric name assigned to the compound.
Experiment Type	Experiment type: SRM, XIC, or SIM.
Category	(Optional) Alphanumeric identifier.
Ionization	(Optional) Alphanumeric identifier. Valid values: ESI, APCI, EI, CI, APPI
Chemical Formula	(Optional) Alphanumeric chemical identifier.
Quan peak parameters	
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. Available only for SRM experiments. 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. Available only for SRM experiments. Range: 10.000 to 2999.999

Table 23. Acquisition List page parameters (Sheet 2 of 3)

Parameter	Description
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. Available only for XIC and SIM experiments. 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. The time after injection when the compound elutes. The total time that the compound is retained on the column. The TraceFinder application uses the 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 TraceFinder application uses the 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	Available only for SRM experiments. Range: 0.00 to 200.00
Confirming ion parameters	
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. Available as a read-only field for SRM experiments only. 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. Available only for SRM experiments. Range: 10.000 to 2999.999

Table 23. Acquisition List page parameters (Sheet 3 of 3)

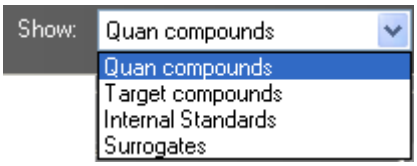
Parameter	Description
Mass	The mass-to-charge ratio of the quan ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (*m/z*) units. Available only for XIC and SIM experiments. Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00

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, select the type of compounds you want to display in the compounds list.



Compound type	Description
Quan compounds	Displays only quan compounds, such as target compounds, internal standards, and surrogates.
Target compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.
Surrogates	Displays only surrogate compounds.

Figure 24. Identification page

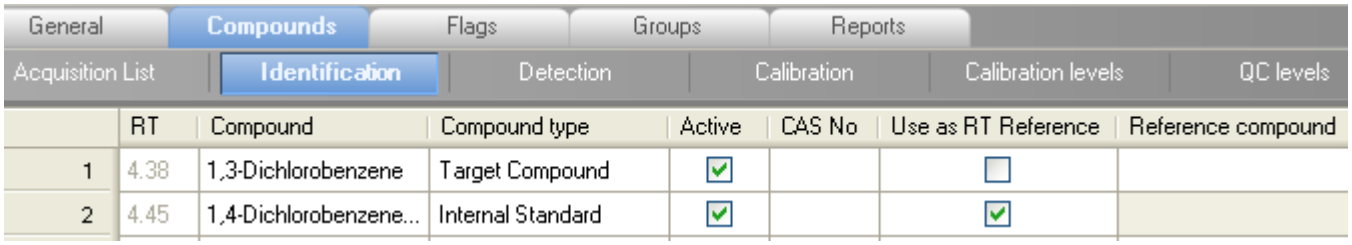


Table 24. Identification page parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column. The TraceFinder application uses the 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
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.

Table 24. Identification page parameters (Sheet 2 of 2)

Parameter	Description
Compound type	Compound types are Quan Compound, Target Compound, Internal Standard, and Surrogate. The TraceFinder application uses target compounds, internal standards, and surrogates in quantitative analysis.
Active	Identifies each compound to be included in data review and reporting. By default, all added compounds are set to active. This active or inactive setting populates to the Batch View and Data Review view in the Data Review mode.
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	When performing peak detection with retention time standards, the TraceFinder 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	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.

From the Detection page, you can access the following pages:

- Times
- Signal
- Detect
- Spectrum
- Ratios

On the Detection page (see "Detection page" on page 129), 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.

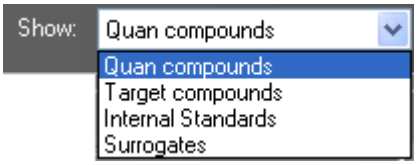
You can change the parameters used to identify a quantification peak, mass range, or confirming ion. The TraceFinder application automatically uses the first match it finds as the compound name, the base peak of the mass spectrum as the quan peak, and the second and third largest ions as the confirming ions.

Use the following procedures:

- To filter the displayed compounds
- To add compounds to the method
- To change the compound reference spectrum
- To replace a quan mass
- To add a mass to the existing quan mass ranges
- To add a quan peak
- To add a mass as a new compound
- To replace a confirming ion
- To add a mass as a new confirming ion
- To save the new method

❖ To filter the displayed compounds

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

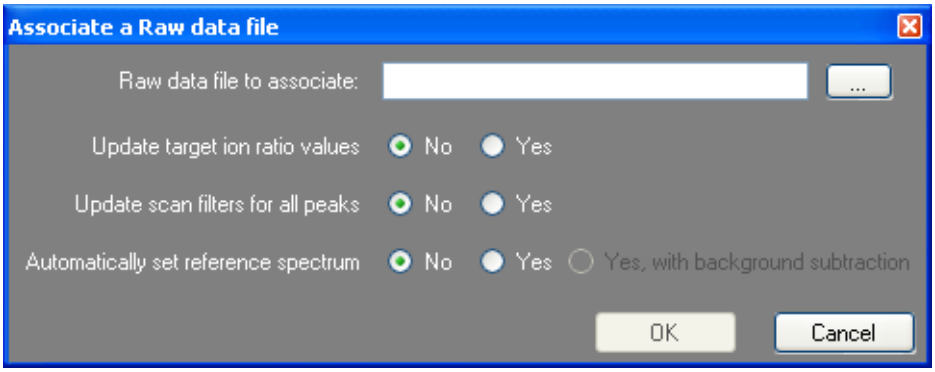


Compound Type	Description
Quan compounds	Displays all quan compounds, such as target compounds, internal standards, and surrogates.
Target compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.
Surrogates	Displays only surrogate compounds.

❖ To add compounds to the method

1. From the main menu, choose **Master Method > Associate a Raw Data File**.

   The Associate a Raw Data File dialog box opens.



2. Browse to a raw data file to associate with the method and open the file.
3. To update the target ion ratio values when you associate this raw data file, select the **Yes** option.
4. To update the scan filters when you associate this raw data file, select the **Yes** option.
5. To set a reference spectrum, do one of the following:

   Select the **Yes** option.

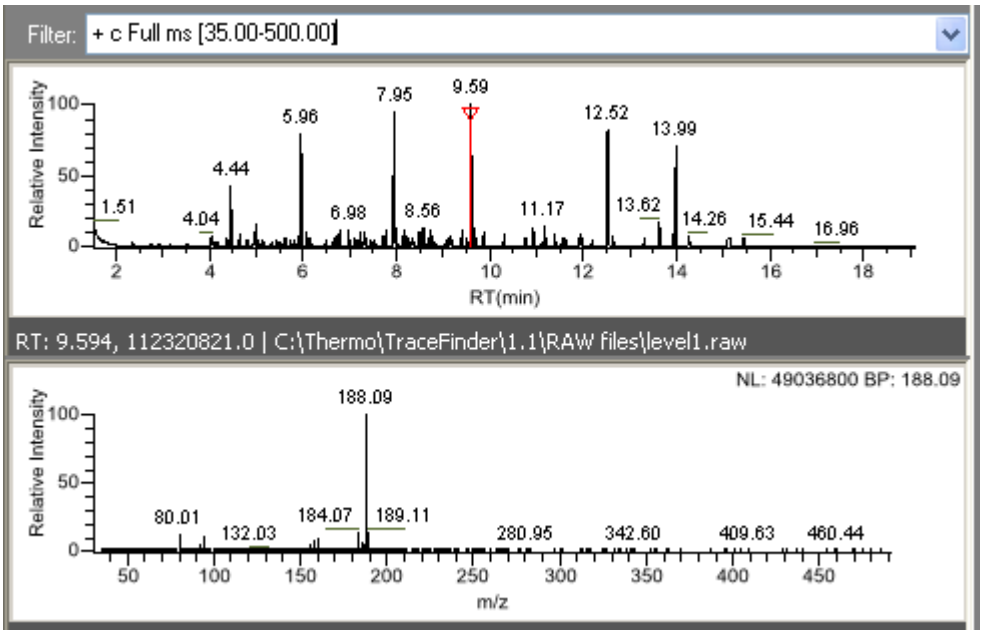
   –Or–

   Select the **Yes, with Background Subtraction** option.

   This feature is available only when you have set background subtraction values on the General page of the Master Method View. See "Editing the General Page" on page 106.

6. Click **OK**.

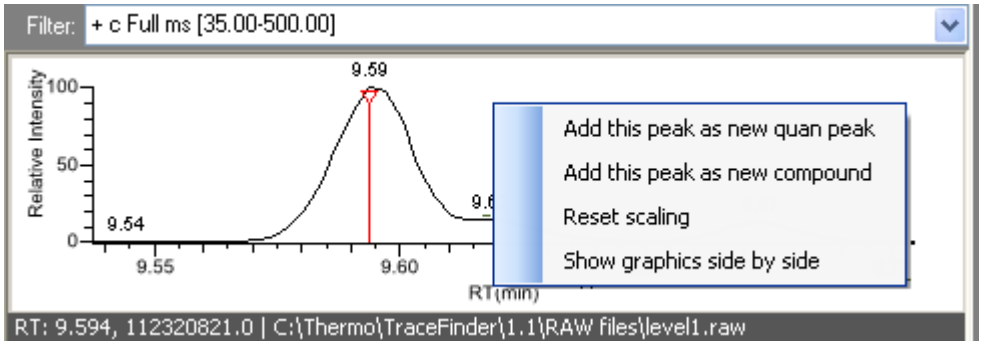
   The TraceFinder application displays the chromatographic and spectrum data for the compounds in the selected raw data file.



7. Select a filter from the Filter list.

8. Click to select the peak in the chromatogram that represents the compound you want to add to the method.

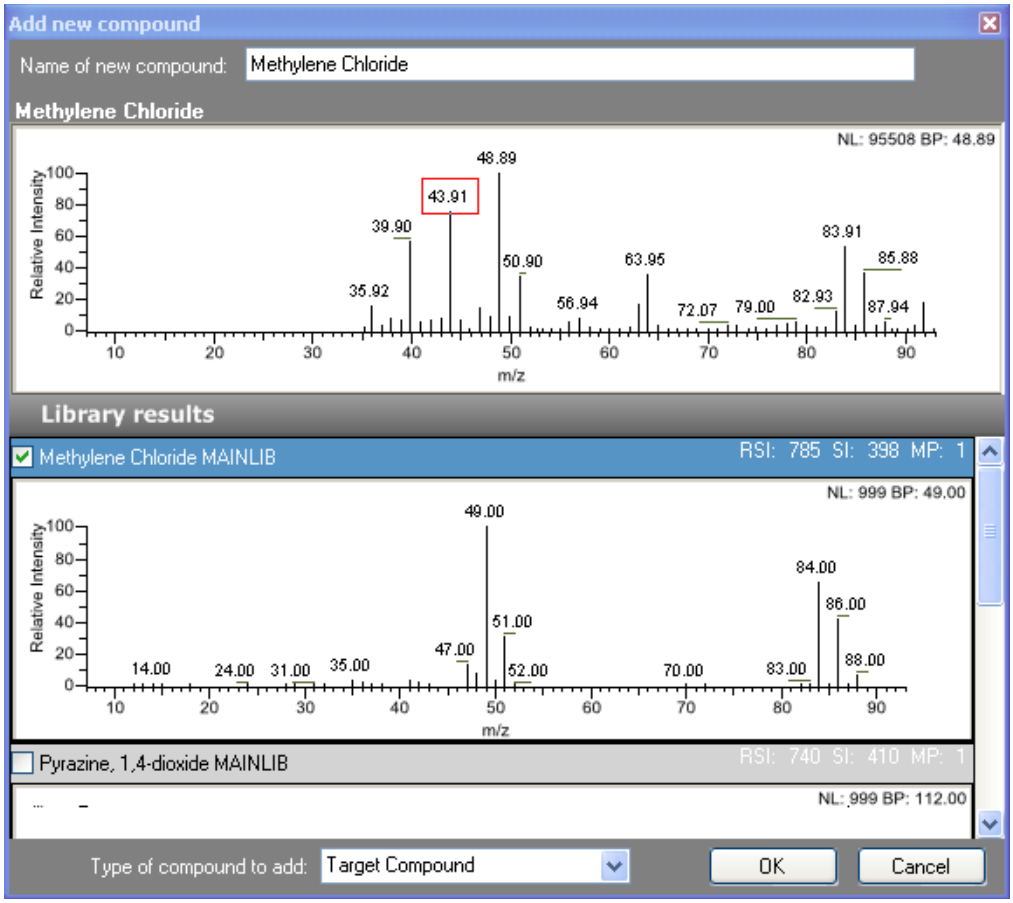
9. Right-click and choose **Add This Peak as New Compound** from the shortcut menu.



   The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quan peak, and the second and third largest ions as the confirming ions.

   If the name of the first match is already in the library, the Add New Compound dialog box opens.

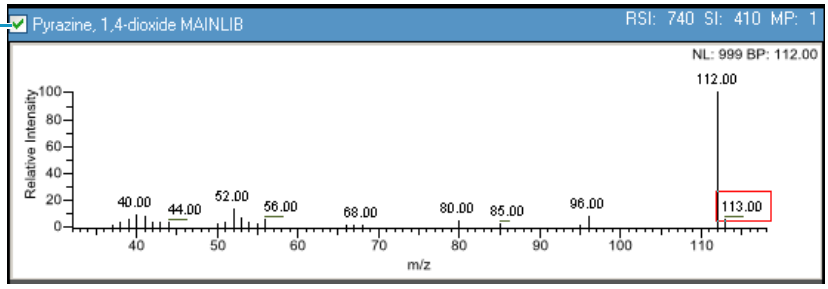
Figure 25. Add New Compound dialog box



10. (Optional) In the Add New Compound dialog box, do the following:

    a. (Optional) To use a compound other than the compound already in the library, scroll to the spectrum for that compound and select the compound name in the title bar of the spectrum pane.

    Selected compound



    b. In the Type of Compound to Add list, select a compound type.

    c. Click **OK**.

11. Repeat this procedure for each compound you want to add to the method.

❖ To change the compound reference spectrum

1. In the raw data file chromatogram pane, click a peak.

   The TraceFinder application displays the spectrum for the selected peak in the spectrum pane.

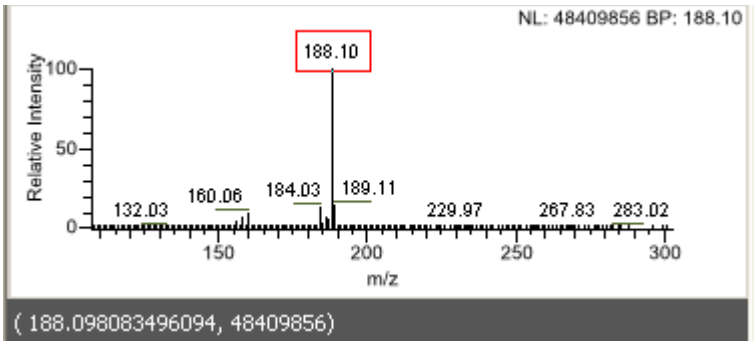
2. In the raw data file spectrum pane, right-click and choose **Use This Spectrum for Compound Reference Spectrum** from the shortcut menu.

   The TraceFinder application replaces the spectrum on the Spectrum page of the quan peak pane with this spectrum.

❖ To replace a quan mass

1. Click the pane for the quan mass that you want to replace.
2. In the raw data file spectrum pane, hold the cursor over a peak.

   The red box indicates the selected peak.



3. Right-click and choose **Set This Mass as Quan Mass** from the shortcut menu.
4. Choose either **Don't Update Ion Ratios** or **Update Ion Ratios Using This Spectrum**.

   You can see the updated ion ratios on the Ratios page for the confirming ions. See "Ratios" on page 149.

❖ To add a mass to the existing quan mass ranges

1. In the raw data file spectrum pane, hold the cursor over a peak.

   The red box indicates the selected peak.

2. Right-click and choose **Add This Mass to Existing Quan Mass Ranges** from the shortcut menu.
3. Choose either **Don't Update Ion Ratios** or **Update Ion Ratios Using This Spectrum**.

   The TraceFinder application adds the selected mass to the existing quan mass ranges to increase the signal.

   If you chose to update the ion ratios, you can see the updated ion ratios on the Ratios page for the confirming ions. See "Ratios" on page 149.

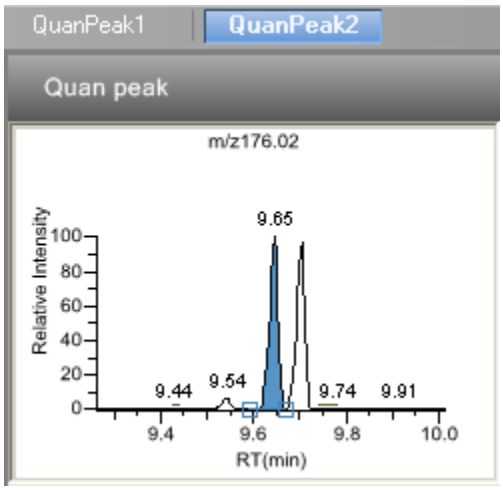
❖ To add a quan peak

1. In the raw data file spectrum pane, hold the cursor over a peak.

   The red box indicates the selected peak.

2. Right-click and choose **Add This Mass as New Quan Peak** from the shortcut menu.

   The application adds a new quan peak to the compound.



   You can use the shortcut menu on the spectrum pane for this new quan peak to perform any of the tasks you could perform on the original quan peak.

❖ To add a mass as a new compound

1. In the raw data file spectrum pane, hold the cursor over a peak.

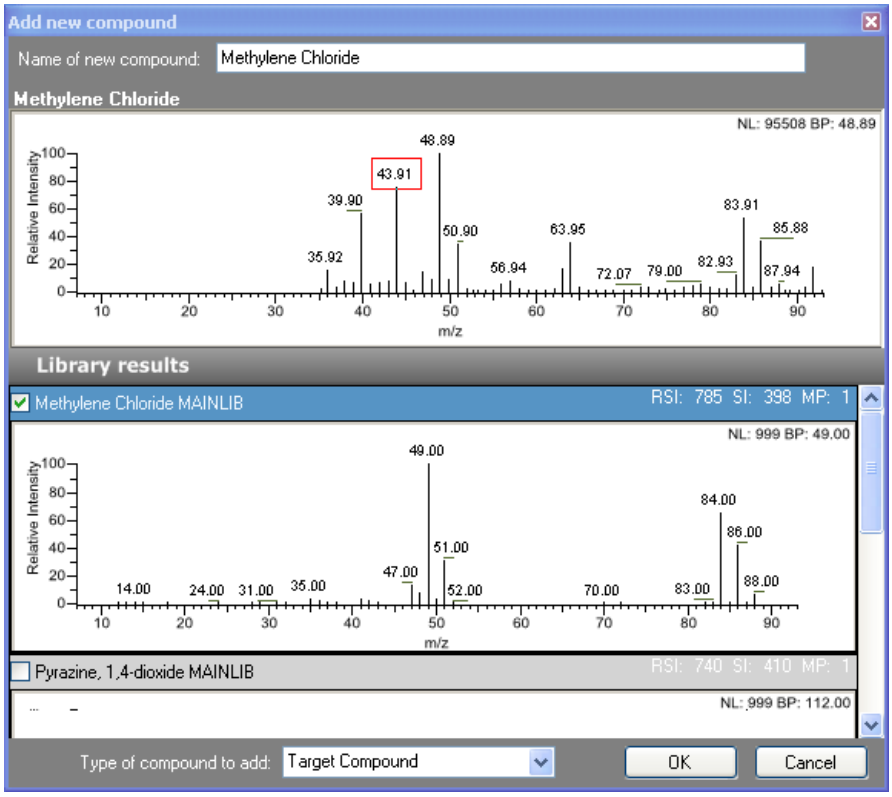
   The red box indicates the selected peak.

2. Right-click and choose **Add This Mass as New Compound** from the shortcut menu.

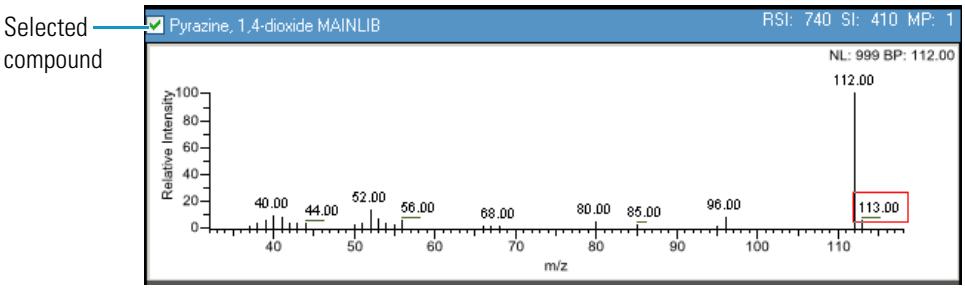
   The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quan peak, and the second and third largest ions as the confirming ions.

   If the name of the first match is already in the library, the Add New Compound dialog box opens with the matching compound selected.

Figure 26. Add New Compound dialog box



3. (Optional) In the Add New Compound dialog box, make any of the following changes:
   a. Change the name for the compound in the Name of New Compound box.
   b. Use a compound other than the compound chosen by the TraceFinder application by scrolling to the spectrum for that compound and selecting the compound name in the title bar of the spectrum pane.



   c. In the Type of Compound to Add list, select a compound type.
4. Click **OK**.

❖ To replace a confirming ion

1. Click the pane for the confirming ion that you want to replace.
2. In the raw data file spectrum pane, hold the cursor over a peak.

   The red box indicates the selected peak.
3. Right-click and choose **Set this Mass as Confirming Ion** from the shortcut menu.

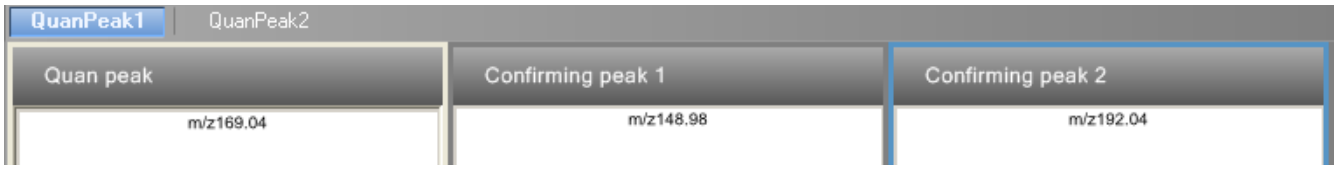
   The TraceFinder application replaces the confirming ion with the selected mass.

❖ To add a mass as a new confirming ion

1. In the raw data file spectrum pane, hold the cursor over a peak.

   The red box indicates the selected peak.
2. Right-click and choose **Add this Mass as New Confirming Ion** from the shortcut menu.

   The TraceFinder application adds the confirming ion to the quan peak.



You can use the shortcut menu on the spectrum pane for this new confirming ion to perform any of the tasks you could perform on the original confirming ions.

❖ 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\1.1\Methods

Figure 27. Detection page

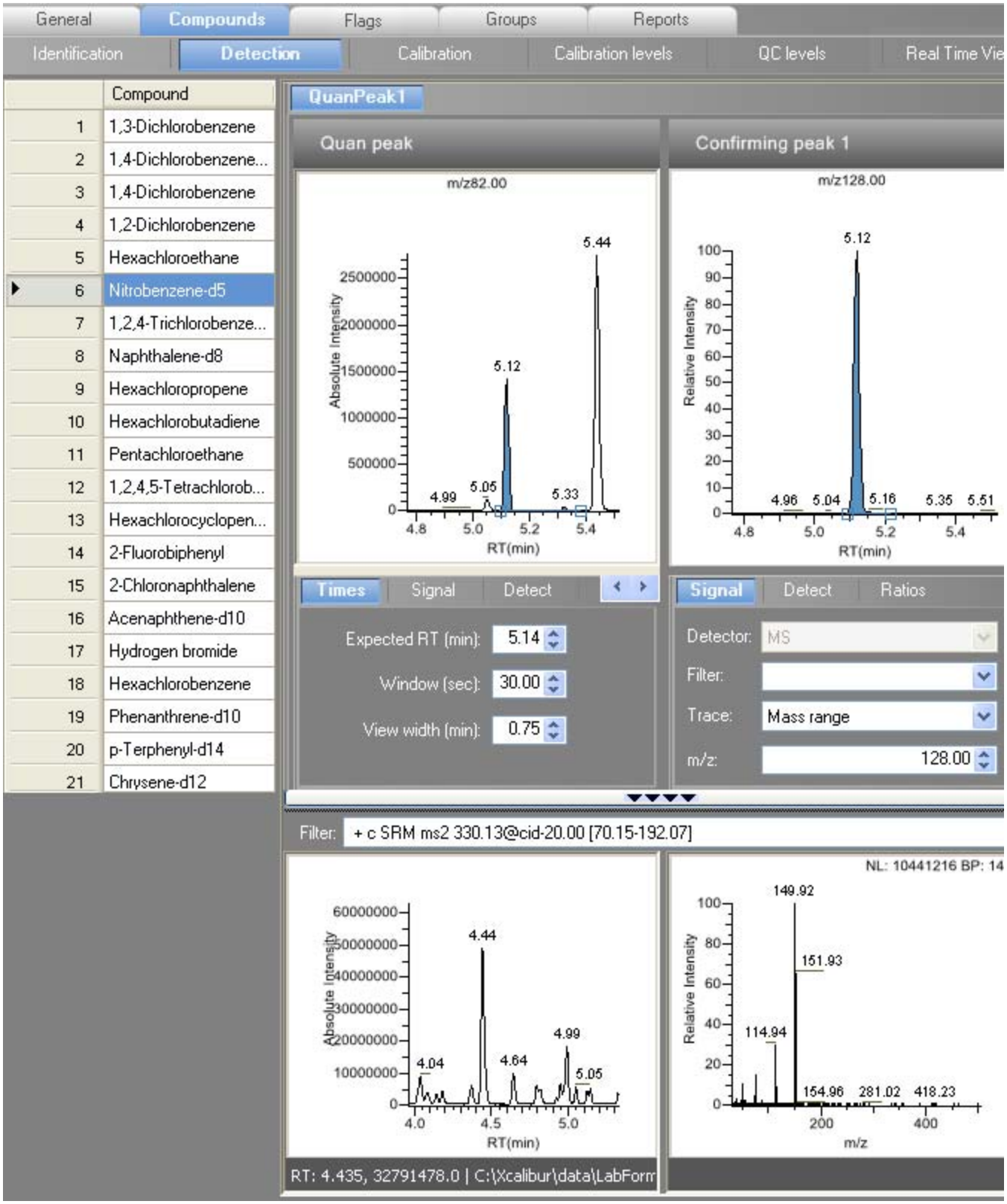


Table 25. Detection page parameters

Parameter	Description
Compound list	Lists all compounds in the master method.
Quan peak	Displays a chromatogram for the quan peak and its confirming ions. The quan peak and confirming ion panes include additional pages for retention time, signal, detection, spectrum, and ratio parameters.
Filter	Displays the filter used for the raw data file.
Reference chromatogram and spectra	Displays a reference chromatogram and spectra for the raw data file.
Additional pages	
Times	Defines the retention time and window for a quan peak. See "Times" on page 131.
Signal	Defines the detector and its parameters used to display each chromatogram trace. See "Signal" on page 132.
Detect	Defines the peak detection algorithm and its options. See "Detect" on page 135.
Spectrum	Defines a reference mass spectrum for a quan peak or compound. See "Spectrum" on page 144.
Ratios	Defines the criteria for evaluating, confirming, or qualifying ions. See "Ratios" on page 149.

Times

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

Figure 28. Times page

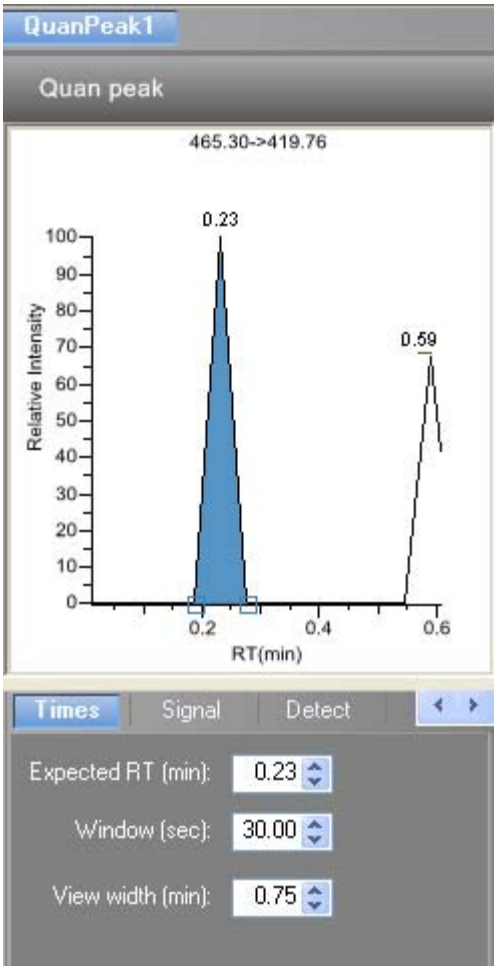


Table 26. Times page parameters

Parameter	Description
Expected RT (min)	Expected retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Window (sec)	Width of the window (in seconds) to indicate how far around the expected retention time the system looks 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

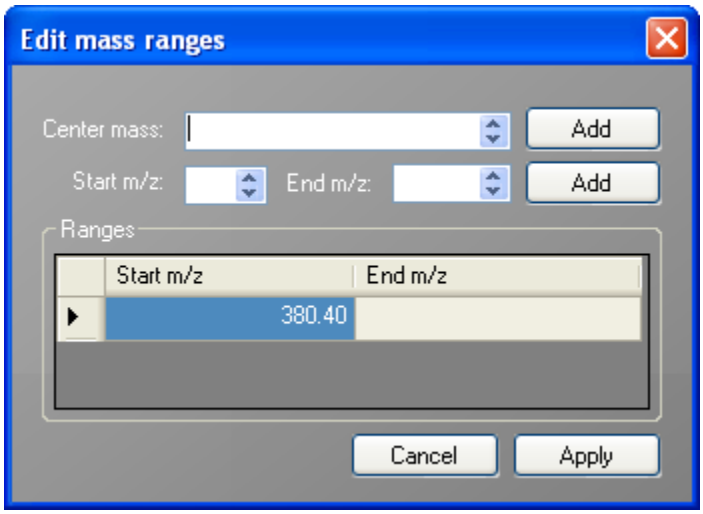
Use the Signal page to define the detector and its parameters as you display each chromatogram trace. For a detailed description of all the features on the Signal page, see "Signal page parameters" on page 133.

❖ To specify ranges of ions for detection and integration

1. In the Ranges area, click **Edit**.

   The Edit Mass Ranges dialog box opens where you can enter rows using a center of mass or a range.

   Figure 29. Edit Mass Ranges dialog box

2. Enter a value in the Center Mass box and click **Add**.

   The application adds a row with this value to the ranges grid. Center mass values are listed in the Start *m/z* column. The application uses a range of one amu centered on this value.

3. Enter values in the Start *m/z* and End *m/z* columns and click **Add**.

   The application adds a row with these start and end values.

4. Add as many ranges as you want.

   When you process a batch with this method, the application sums the multiple ions specified by these ranges.

5. Click **Apply**.

   When you are editing a master method, the application applies the entries to the list of ranges.

Figure 30. Signal page

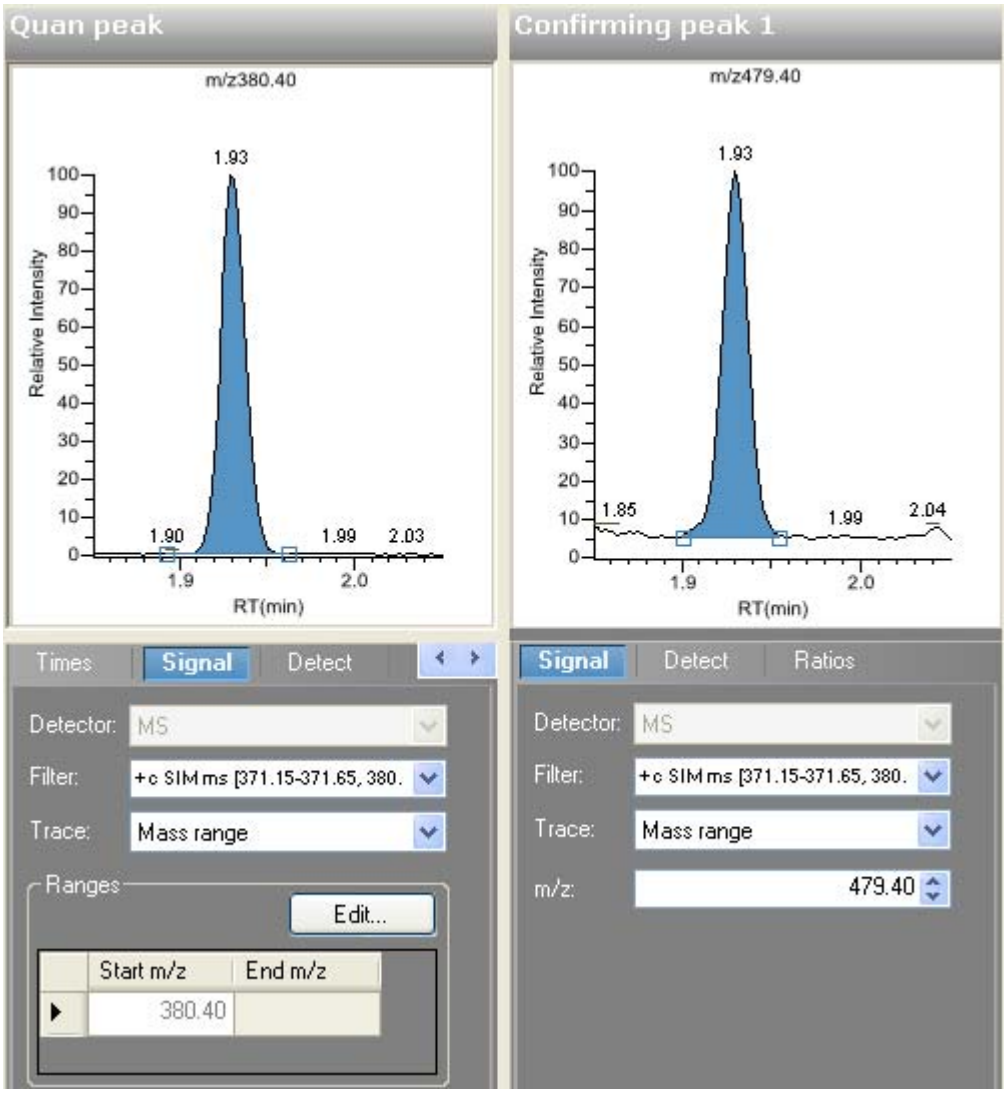


Table 27. Signal page parameters (Sheet 1 of 2)

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 data file.
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.
Trace	Represents a specific range of the data. In conjunction with the filter, the TraceFinder application uses the trace to identify the characteristic ions for a compound. The options are: Mass Range, TIC, or Base Peak.

Table 27. Signal page parameters (Sheet 2 of 2)

Parameter	Description
Ranges	
Edit	Opens the Edit Mass Ranges dialog box where you can specify a range of ions for detection and integration. See "Edit Mass Ranges dialog box" on page 132.
Start m/z End m/z	Specifies ranges of ions for detection and integration. The application sums the multiple ions specified by these ranges. Ranges specified by a center mass value are listed as a single value in the Start *m/z* column. The application uses a range of one amu centered on this value.

Detect

Use the Detect page to define the peak detection algorithm (sensitivity) and its options and to determine the area under a curve. There are three sensitivity modes: Genesis, ICIS, and Avalon. On this page, you can specify how you want each mode to run.

For a detailed description of all the features on the Detect page for Genesis sensitivity, see "Detect page parameters for Genesis" on page 137.

For a detailed description of all the features on the Detect page for ICIS sensitivity, see "Detect page parameters for ICIS" on page 140.

For a detailed description of all the features on the Detect page for Avalon sensitivity, see "Detect page parameters for Avalon" on page 142.

❖ To apply current peak detection settings to all peaks

1. Edit the parameters for either the Quan peak or a Confirming peak.
2. Right-click the Detect page and choose **Apply to All Peaks in Method** from the shortcut menu.

   The application updates all compounds in the method with the current settings on the Detect page. These updates apply to both quan and confirming ions.

❖ To apply current peak detection settings to all peaks that use the same detection mode

1. Edit the parameters for either the Quan peak or a Confirming peak.
2. Right-click the Detect page and choose Apply to All Peaks with Like Sensitivity Setting from the shortcut menu.

   The application uses the current settings on the Detect page to update all compounds in the method that use the same sensitivity mode (Genesis, ICIS, or Avalon). These updates apply to both quan and confirming ions that use the same sensitivity mode.

Figure 31. Detect page for Genesis

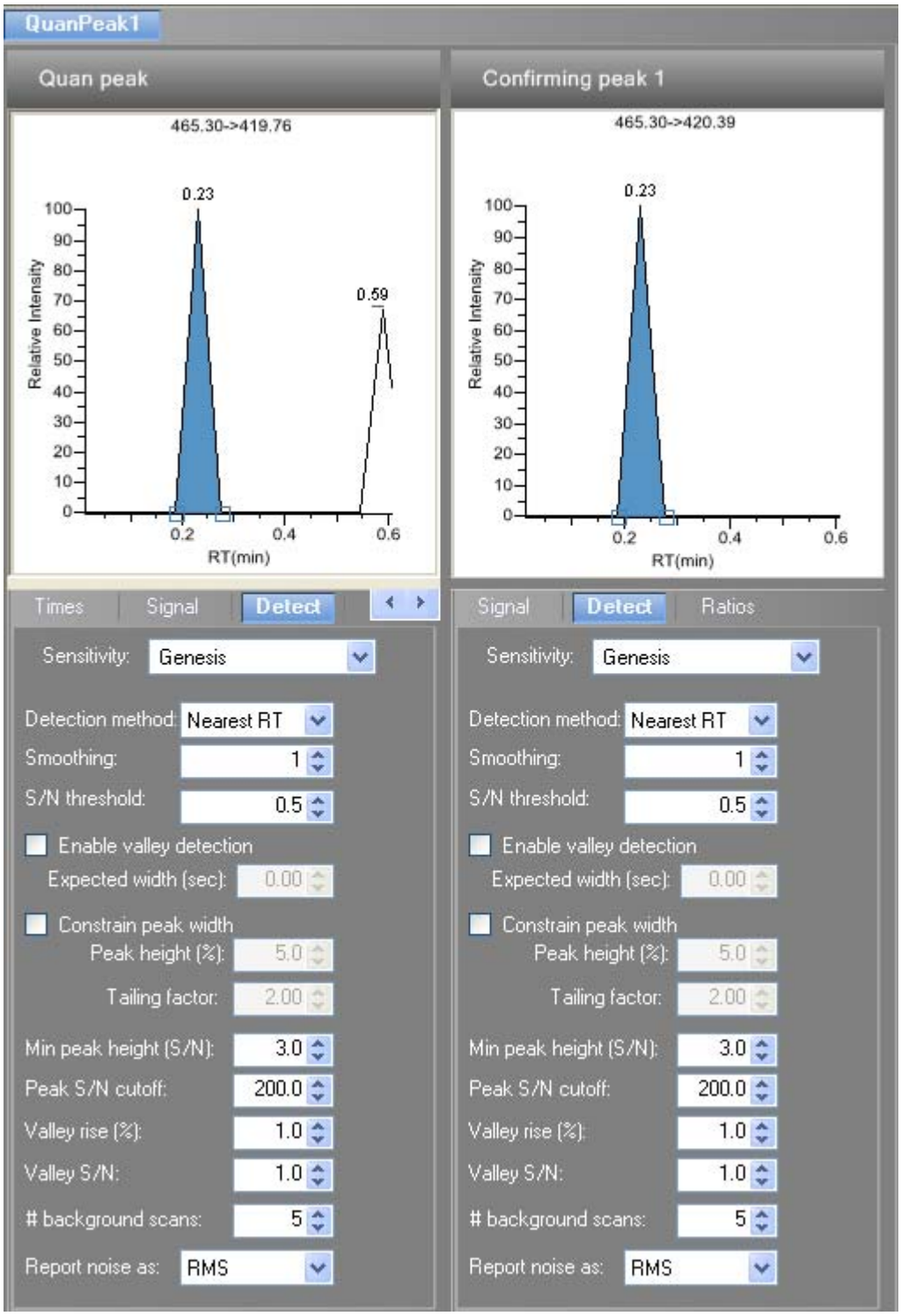


Table 28. Detect page parameters for Genesis (Sheet 1 of 2)

Parameter	Description
Sensitivity	Specifies the 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. 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 parameter 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 TraceFinder application terminates the peak at that point. The 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.
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 you select the Constrain Peak Width check box. Range: 0.0 to 100.0%

Table 28. Detect page parameters for Genesis (Sheet 2 of 2)

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 you select the Constrain the Peak Width check box. 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 identifies 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 TraceFinder 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
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. The TraceFinder application applies this test 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 TraceFinder application.
Report noise as	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or a peak-to-peak resolution threshold. Options are RMS or Peak to Peak.

Figure 32. Detect page for ICIS

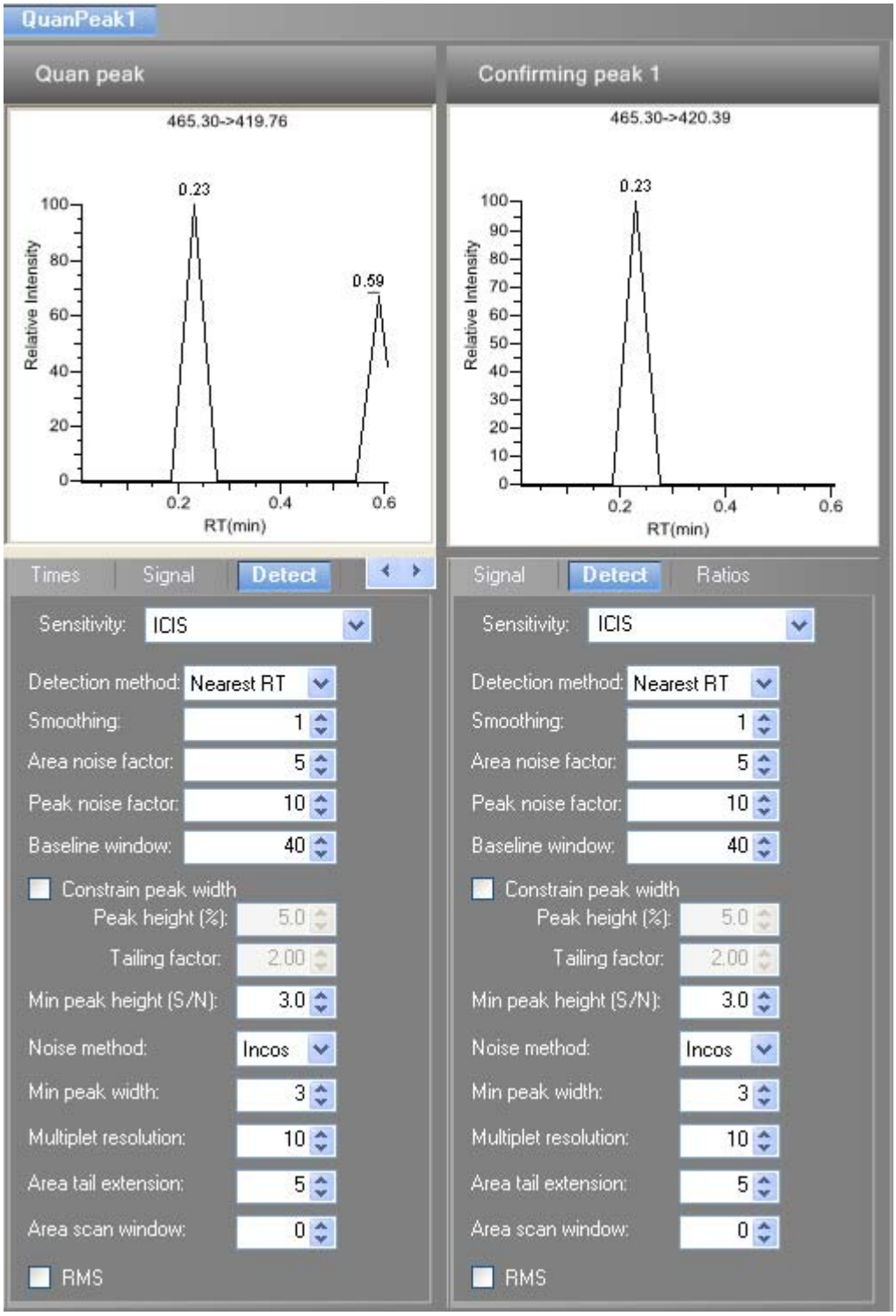


Table 29. Detect page parameters for ICIS (Sheet 1 of 2)

Parameter	Description
Sensitivity	Specifies the 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. 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. Range: 1 through 500 Default: 5
Peak noise factor	The noise level multiplier used to determine the potential peak signal threshold. Range: 1 through 1000 Default: 10
Baseline window	The TraceFinder application looks for a local minima over this number of scans. 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 you select the Constrain Peak Width check box. 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 you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

Table 29. Detect page parameters for ICIS (Sheet 2 of 2)

Parameter	Description
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. Repetitive: Uses a multiple pass algorithm to determine the noise level. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but the analysis takes longer.
Min peak width	The minimum number of scans required in a peak. Range: 0 to 100 scans Default: 3
Multiplet resolution	The minimum separation in scans between the apexes of two potential peaks. This is a criterion to determine if two peaks are resolved. Range: 1 to 500 scans Default: 10
Area tail extension	The number of scans past the peak endpoint to use in averaging the intensity. Range: 0 to 100 scans Default: 5
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.

Figure 33. Detect page for Avalon

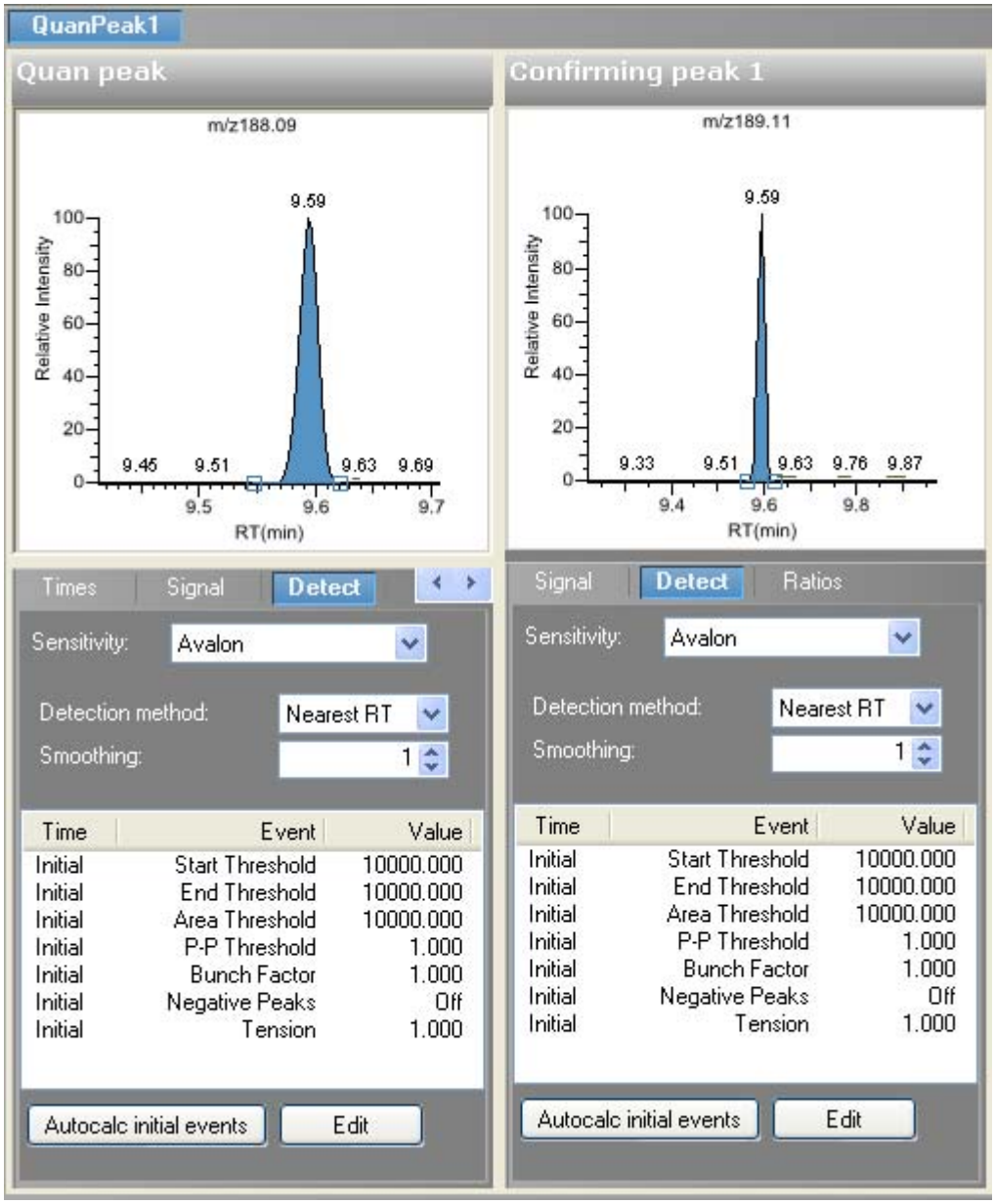


Table 30. Detect page parameters for Avalon (Sheet 1 of 2)

Parameter	Description
Sensitivity	Specifies the Avalon 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.

Table 30. Detect page parameters for Avalon (Sheet 2 of 2)

Parameter	Description
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Range: Any odd integer from 1 through 15 points Default: 1
Autocalc Initial Events	Automatically calculates the events in the Event list.
Edit	Opens the Avalon Event List dialog box. See "Avalon Event List" on page 80.

Spectrum

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

For a detailed description of all the shortcut menu commands on the Spectrum page, see "Spectrum shortcut menu functions" on page 148.

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 on the chromatogram or spectrum displays

❖ To update confirming ion ratios

1. Click a peak in the quan peak 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, hold the cursor over the *m/z* value for an ion.

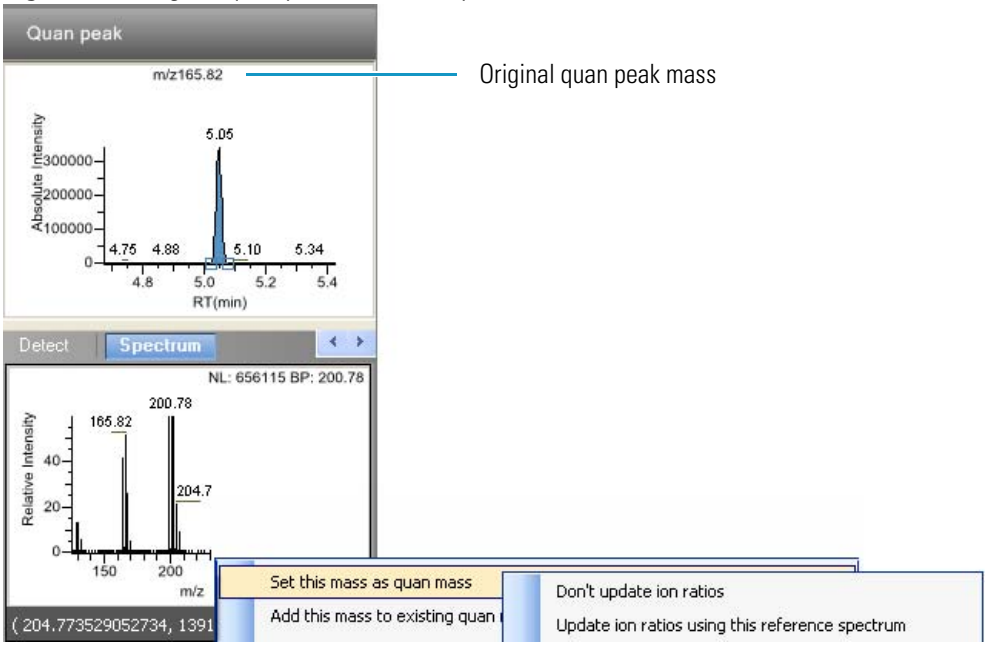
   A red box around the ion's *m/z* value indicates that the ion is selected.

3. Right-click and choose one of the following commands from the shortcut menu:

   - Set This Mass as Quan Mass > Don't Update Ion Ratios
   - Set This Mass as Quan Mass > Update Ion Ratios Using This Reference Spectrum

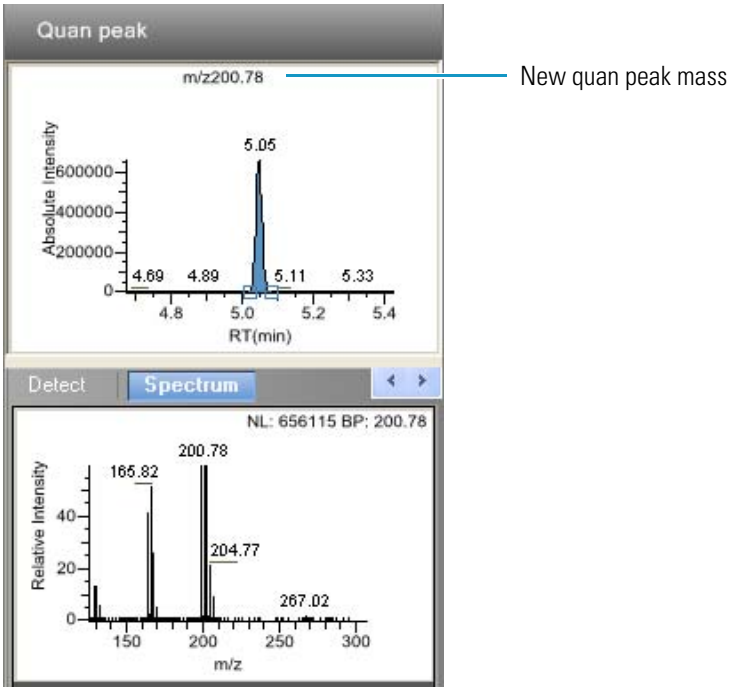
The following examples show an original quan peak and a quan peak with an updated quan mass.

Figure 34. Original quan peak mass example



The TraceFinder application replaces the original quan mass with the selected mass.

Figure 35. Updated quan peak mass example



❖ To add ions together to get an accumulated signal

1. Hold the cursor over the *m/z* value for an ion in the Spectrum pane.

   A red box around the ion's *m/z* 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.

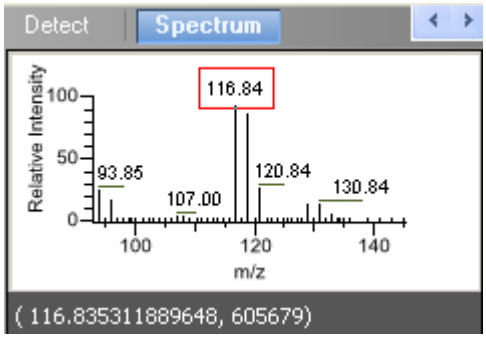
❖ To add a quan peak to an existing compound

1. Click the peak in the Quan Peak chromatogram pane.

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

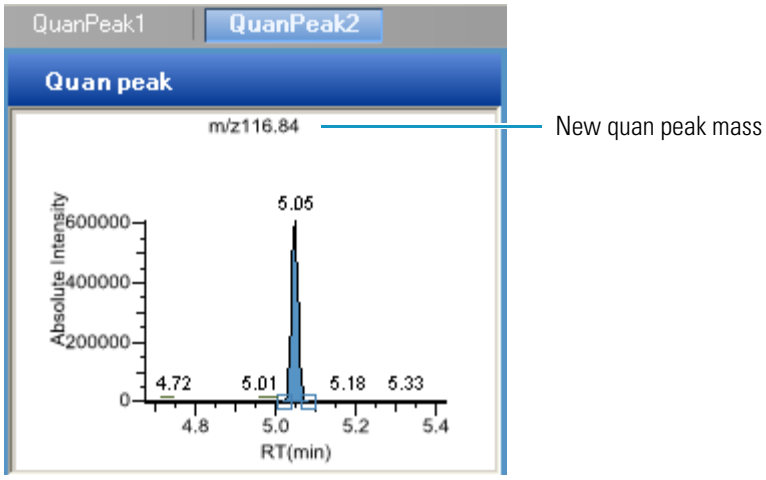
2. In the Spectrum pane, hold the cursor over the *m/z* value for an ion.

   A red box around the ion's *m/z* value indicates that the ion is selected.



3. Right-click and choose **Set This Mass as New Quan Peak** from the shortcut menu.

   The TraceFinder application adds this ion as a new quan peak.



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

1. Click the peak in the chromatogram pane.

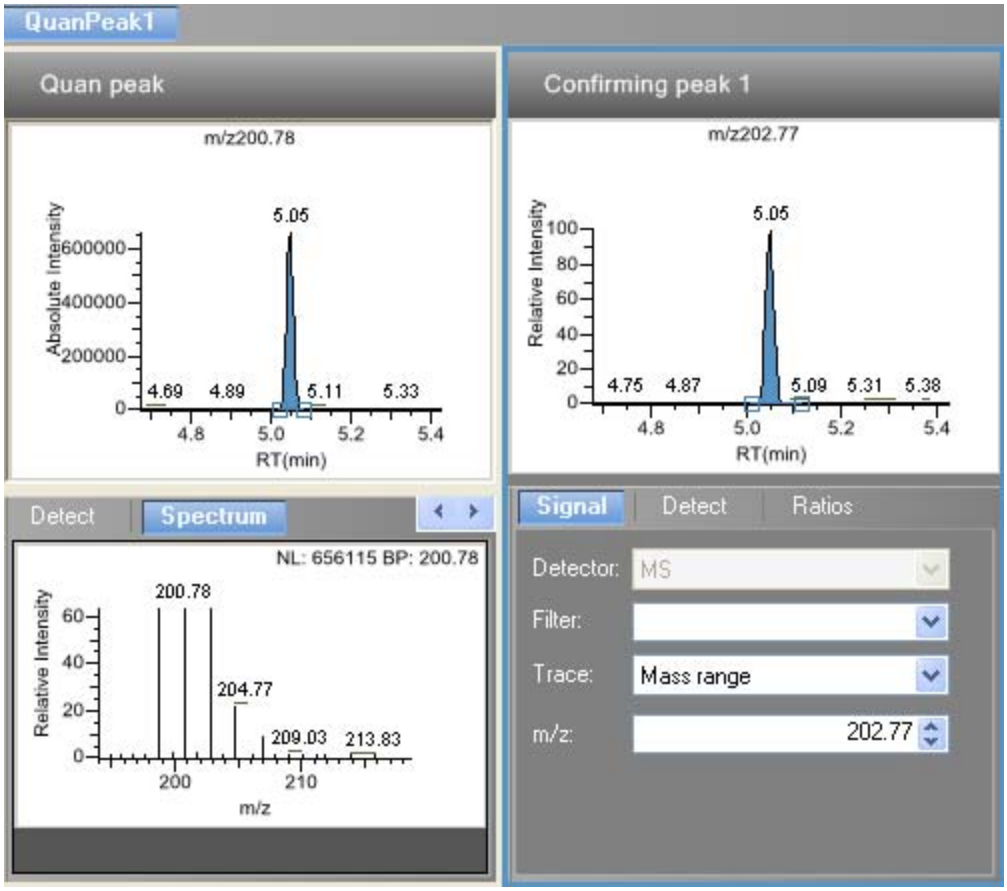
   The mass spectrum for the peak is displayed in the Spectrum pane.

2. In the Spectrum pane, hold the cursor over the *m/z* value for an ion.

   A red box around the ion's *m/z* value indicates that the ion is selected.

3. Right-click and choose to **Add This Mass as New Confirming Ion** from the shortcut menu.

   The TraceFinder application adds the selected mass as a confirming peak for this quan peak.



❖ To zoom in on the chromatogram or spectrum displays

1. Drag the cursor to delineate a rectangle.

   The display zooms in on the specified rectangle.

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

Figure 36. Spectrum page

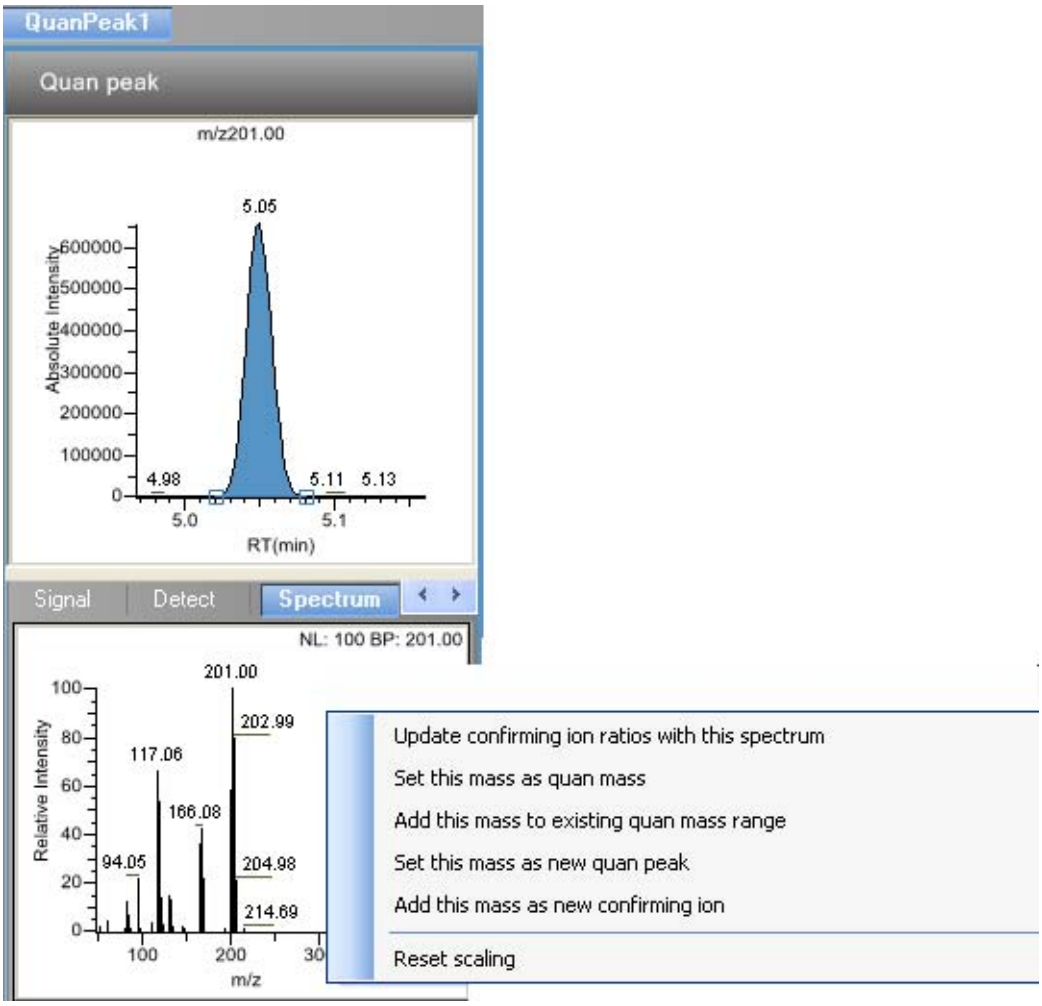


Table 31. Spectrum shortcut menu functions

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. You can choose to update the ion ratios or not update the ion ratios using this reference spectrum.
Add this mass to existing quan mass range	Adds the selected mass to your existing quan mass range. You can choose to update the ion ratios to adjust the confirming ion comparisons to the new summed quan peak signal.
Set this mass as new quan peak	Adds a new quan peak to an existing compound.
Add this 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

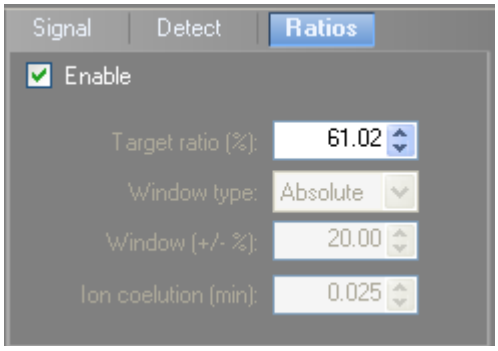
Use the Ratios page to define the criteria for evaluating the confirming or qualifying ions. The TraceFinder application detects compounds that have confirming ion values outside their acceptable window and flags them in the Acquisition mode and on reports.

For a detailed description of all the features on the Ratios page, see "Ratios page parameters" on page 150.

❖ To specify ion ratio criteria

1. Select the **Enable** check box to enable the 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 list, 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 is Relative, the plus or minus value is 20% of 61.02% (or 12.20%), so the acceptable window for this confirming ion is 48.82 to 73.22%.

Figure 37. Ratios page

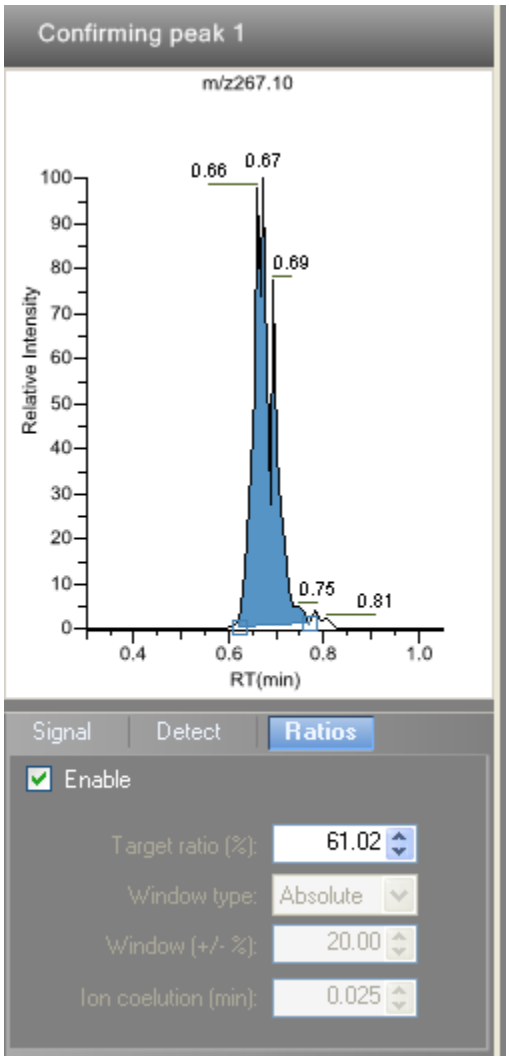


Table 32. Ratios page parameters

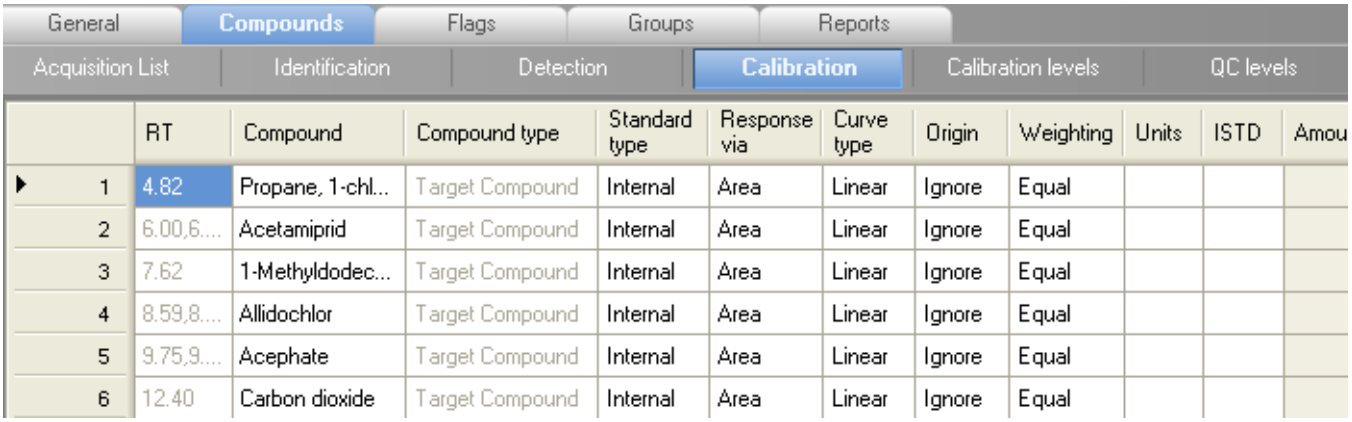
Parameter	Description
Enable	Makes the ion ratio criteria available.
Target ratio (%)	The theoretical ratio of the confirming ion's response to the quantification ion's response.
Window type	The absolute or relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	The 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 Acquisition mode when you view the results of an actual calibration batch.

Figure 38. Calibration page



	RT	Compound	Compound type	Standard type	Response via	Curve type	Origin	Weighting	Units	ISTD	Amou
1	4.82	Propane, 1-chl...	Target Compound	Internal	Area	Linear	Ignore	Equal			
2	6.00,6....	Acetamiprid	Target Compound	Internal	Area	Linear	Ignore	Equal			
3	7.62	1-Methyldodec...	Target Compound	Internal	Area	Linear	Ignore	Equal			
4	8.59,8....	Allidochlor	Target Compound	Internal	Area	Linear	Ignore	Equal			
5	9.75,9....	Acephate	Target Compound	Internal	Area	Linear	Ignore	Equal			
6	12.40	Carbon dioxide	Target Compound	Internal	Area	Linear	Ignore	Equal			

Table 33. Calibration page parameters

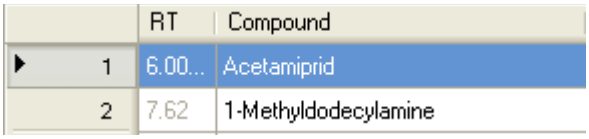
Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Compound type	Displays the compound type as an internal standard, an external standard, or a target compound.
Standard type	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.

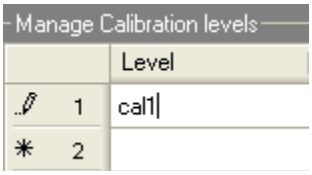
❖ To specify calibration levels and concentrations

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

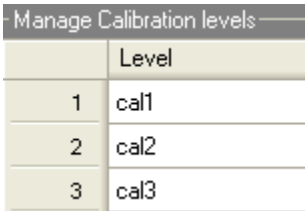


2. In the Manage Calibration Levels area, type a value for the first calibration level.

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



3. Continue adding calibration levels.



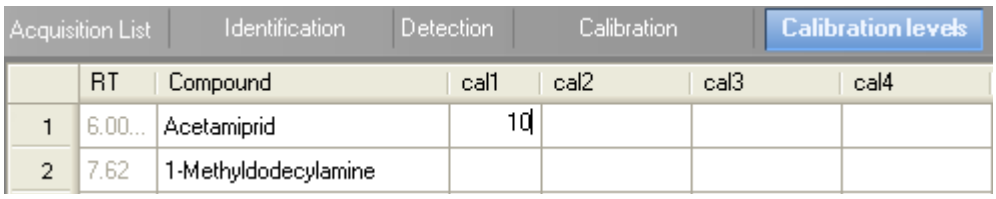
   When you finish adding calibration levels, you can specify the concentrations for each level for each compound.

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.

Figure 39. Calibration Levels page

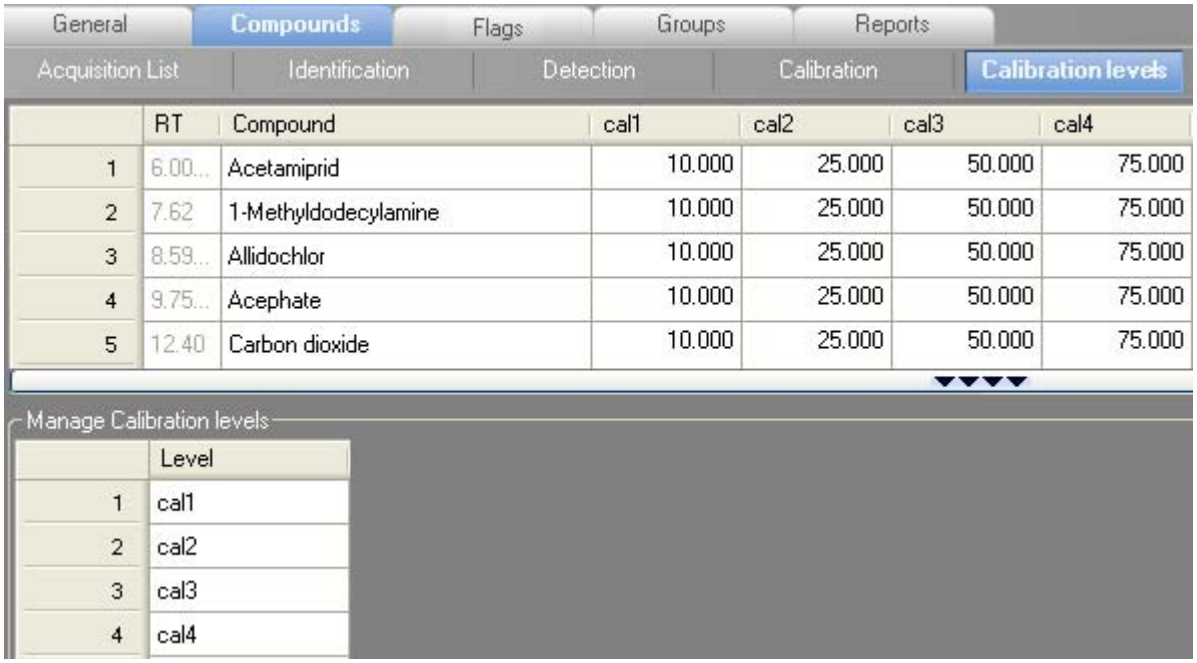


Table 34. Calibration levels page parameters

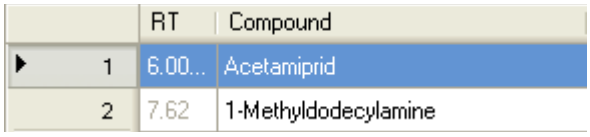
Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
cal1-cal*n*	User-defined calibration levels for the compound.
Manage Calibration levels	Defines values for each of the calibration level values for the selected compound.

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. For a detailed description of all the features on the QC Levels page, see "QC levels page parameters" on page 155.

❖ To specify QC levels and concentrations

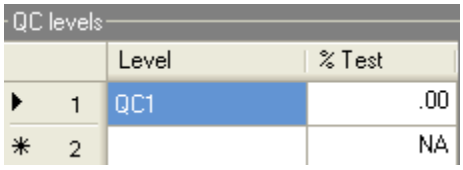
1. Select the compound whose QC levels, percentage test values, and concentrations you want to define.



	RT	Compound
▶ 1	6.00...	Acetamiprid
2	7.62	1-Methyldodecylamine

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

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

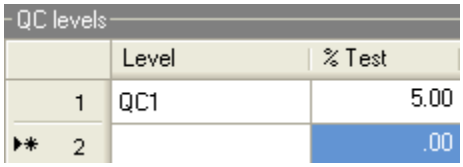


QC levels

	Level	% Test
▶ 1	QC1	.00
✳ 2		NA

3. Type a value for the % Test.

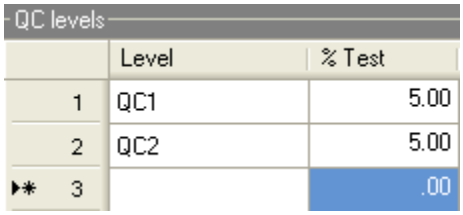
   The % Test is the acceptable difference (as a percentage) between the known amount and the calculated (measured) amount of each QC level.



QC levels

	Level	% Test
1	QC1	5.00
▶✳ 2		.00

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



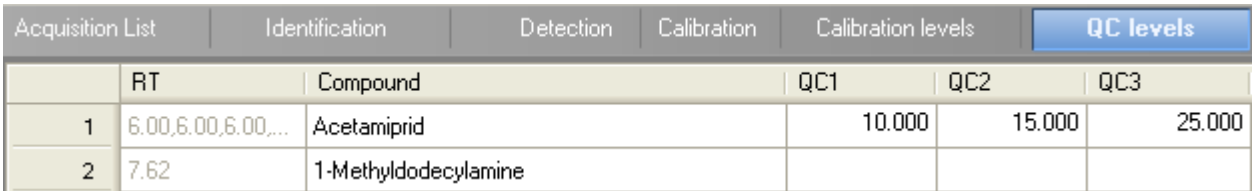
QC levels

	Level	% Test
1	QC1	5.00
2	QC2	5.00
▶✳ 3		.00

   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.



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.

Figure 40. QC Levels page

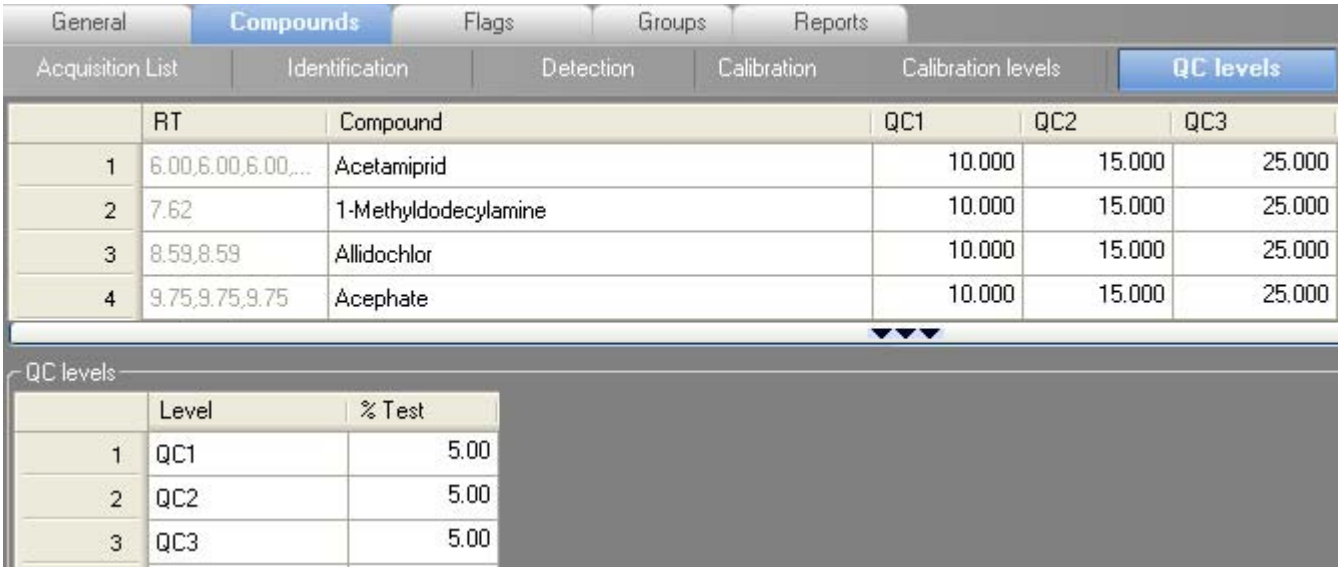


Table 35. QC levels page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
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.

Real Time Viewer

Use the Real Time Viewer page to specify which traces display in the real-time status pane when you perform acquisition in the Acquisition mode or when you acquire a development batch in the Method Development mode. See "Real-time Display" on page 246.

Figure 41. Real Time Viewer page

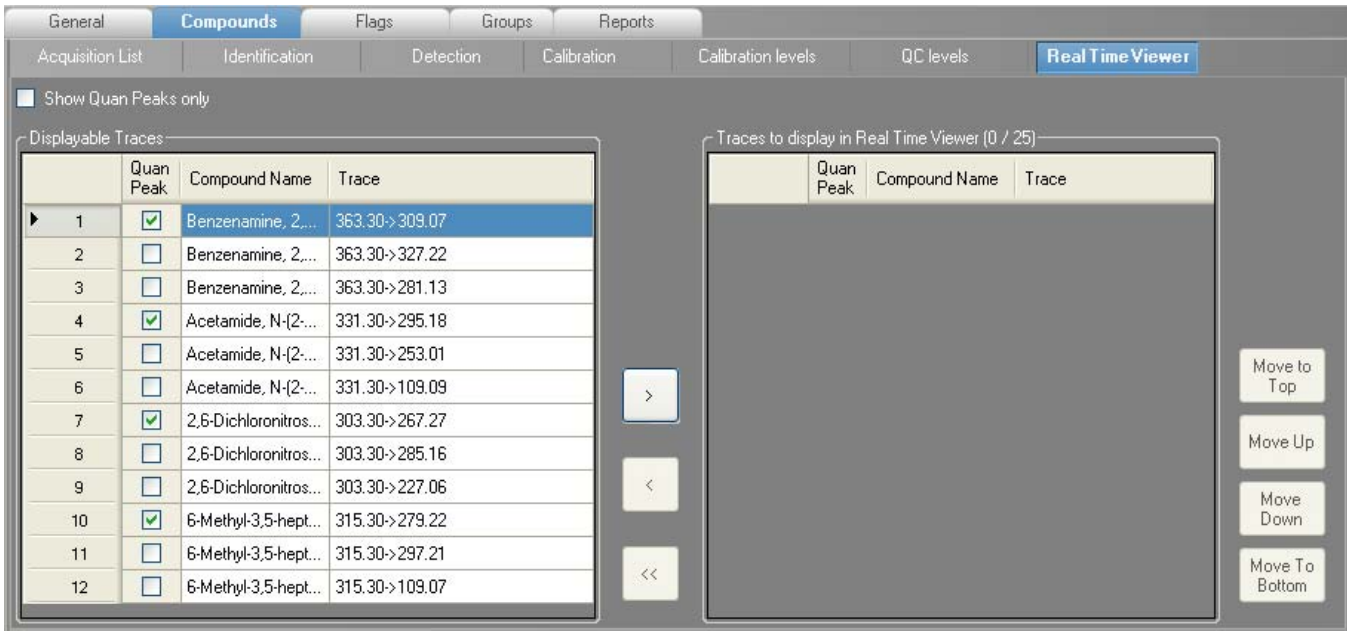


Table 36. Real Time Viewer page parameters (Sheet 1 of 2)

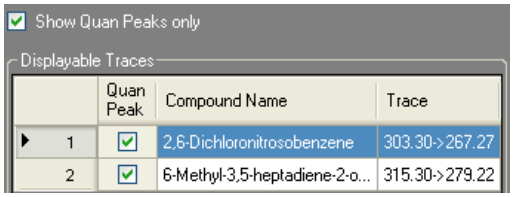
Parameter	Description
Show Quan Peaks Only	Displays only quan peaks in the compounds list. Quan peaks are indicated with a check in the Quan Peak column. 
Displayable Traces	
Quan Peak	Checks indicate quan peak traces. Unchecked traces indicate confirming ions.
Compound Name	Names of all compounds in the method.
Trace	Lists the simple mass or precursor mass for all traces—both quan peak and confirming ion—for each compound.
>	Moves the selected trace to the Traces to Display in Real Time Viewer pane.
<	Moves the selected trace to the Displayable Traces pane.

Table 36. Real Time Viewer page parameters (Sheet 2 of 2)

Parameter	Description
<<	Moves all traces to the Displayable Traces pane. To move multiple traces to the Traces to Display... pane, hold down the SHIFT key, select multiple traces, and then click >.
Traces to Display in Real Time Viewer (0/25)	List the traces to be displayed and the display order in the real-time viewer in the Acquisition mode. Maximum number of traces is 25.
Move to Top	Moves the selected trace to the top of the Traces to Display... list and the second position in the real-time display. The TIC is always the first position in the real-time display.
Move Up	Moves the selected trace up one position in the list.
Move Down	Moves the selected trace down one position in the list.
Move to Bottom	Moves the selected trace to the bottom of the list.

Using the Shortcut Menu Commands

Each page on the Compounds page (except the Acquisition List page) uses right-click shortcut menu commands to display or hide the retention column, remove compounds from the method, copy and paste data, or save the compound list to a .csv file.

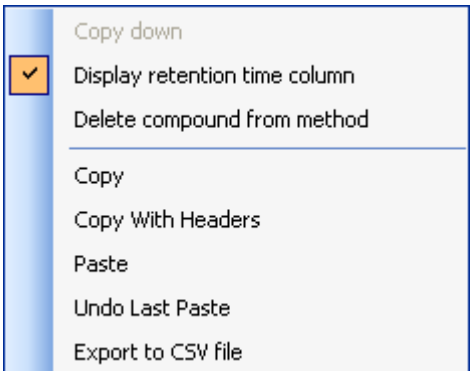
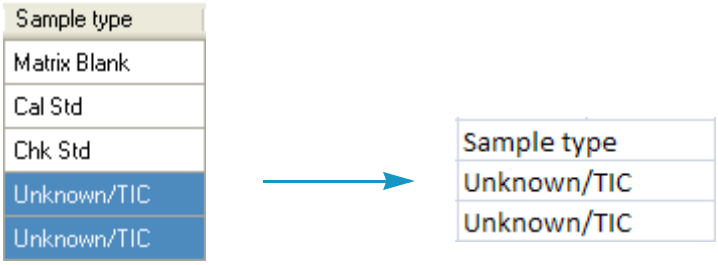


Table 37. Compounds page shortcut menu (Sheet 1 of 2)

Command	Description
Copy down	Copies the value in the selected row to all rows below it. This command is available only when you have selected a value that can be copied down. See Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Table 37. Compounds page shortcut menu (Sheet 2 of 2)

Command	Description
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy compound information to another application, such as an Excel spreadsheet. You cannot paste this data back into the method development compound list, but you can paste this copied data into other areas of the TraceFinder application.
Copy With Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information to another application, such as an Excel spreadsheet. For example:  Copy With Headers from TraceFinder Paste into Excel spreadsheet You cannot paste this data back into the method development compound list.
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column. The pasted data must be valid data for the selected column.
Undo Last Paste	Removes the last pasted item in the method development compound list.
Export to CSV file	Opens the Save As dialog box where you can save the current compound list to a .csv file.

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:

- Limits
- Calibration
- Chk Std
- Matrix Blank
- Solvent Blank
- ISTD
- Surrogate
- Lab Control (Environmental and Food Safety)
- Method Val (Environmental and Food Safety)
- Matrix Spike (Environmental and Food Safety)

Limits

Use the Limits 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.

Figure 42. Limits page

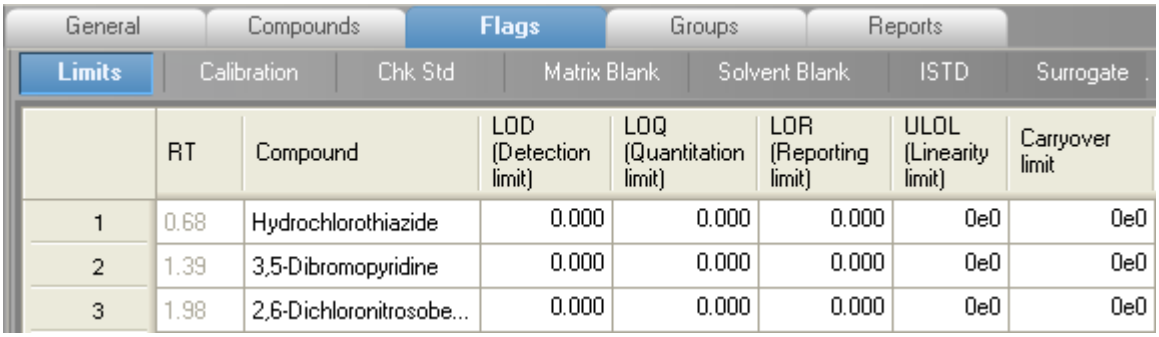


Table 38. Limits page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
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 calibration amount.
LOR (Reporting limit)	Limit of reporting. Also called cutoff in some industries. This is the lowest 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 carryover 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.

Calibration

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.

Figure 43. Calibration page

Table 39. Calibration page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
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).
Min RF	The minimum average response factor (RF) 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).

Chk Std

Use the Chk Std page to review the calibration on an ongoing basis. The TraceFinder application makes the evaluation by comparing the quality 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 TraceFinder 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 Chk Std sample versus the theoretical value is set on the QC levels page of the Compounds page.

Figure 44. Chk Std page

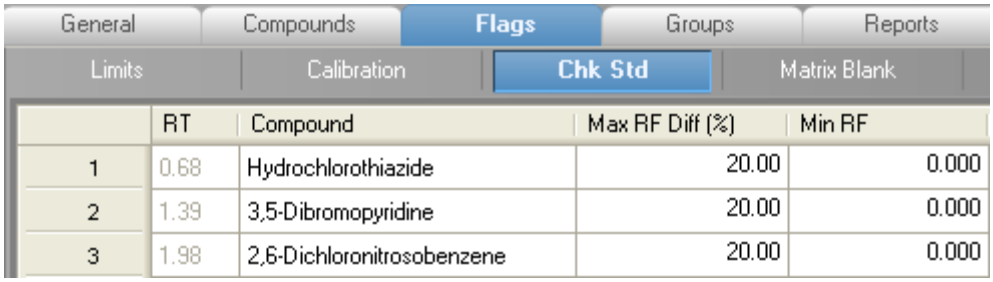


Table 40. Chk Std page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Max RF Diff (%)	The maximum deviation between the response factor (RF) of the Chk Std sample and the average response factor from the calibration (when in average RF mode).
Min RF	The minimum response factor for the Chk Std sample (when in average RF mode).

Matrix Blank

Use the Matrix Blank page to define acceptable levels of target compounds in blank samples. The TraceFinder 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 Matrix Blank report, the application flags the calculated values for target compounds that exceed these limits.

❖ To specify the maximum concentration as a percentage

1. From the Method column list, select one of the following methods:
   - None
   - Concentration
   - % 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, select **Concentration**.
2. In the Max Conc column, type an absolute value.

❖ To specify no maximum concentration

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

Figure 45. Matrix Blank page

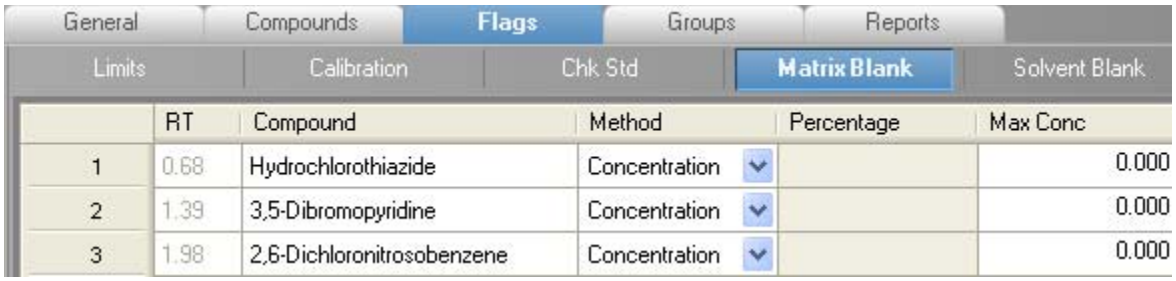


Table 41. Matrix Blank page parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.

Table 41. Matrix Blank page parameters (Sheet 2 of 2)

Parameter	Description
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.
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.

Solvent Blank

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 TraceFinder application flags the calculated values for target compounds that exceed these limits.

Figure 46. Solvent Blank page

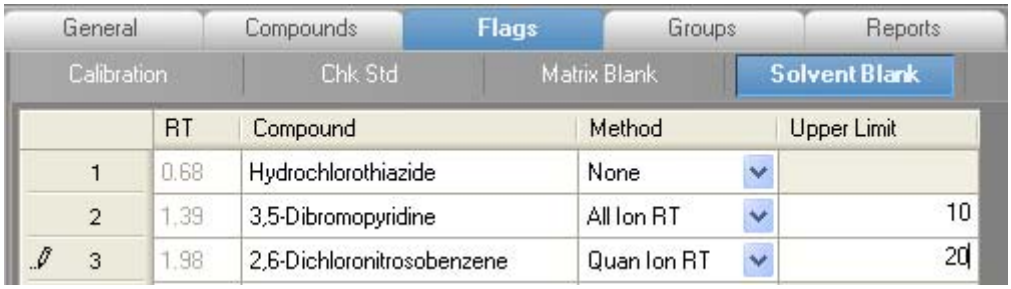


Table 42. Solvent Blank page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Method	The evaluation process to use as 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). To deactivate the solvent blank test for a specific compound, select **None**.
Upper Limit	Specifies an upper limit for each compound in the sample when you select an evaluation process. These values are not concentrations; they are raw response values.

ISTD

Use the ISTD page to review the response and retention time of internal standards (if available). The TraceFinder 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.

Figure 47. ISTD page

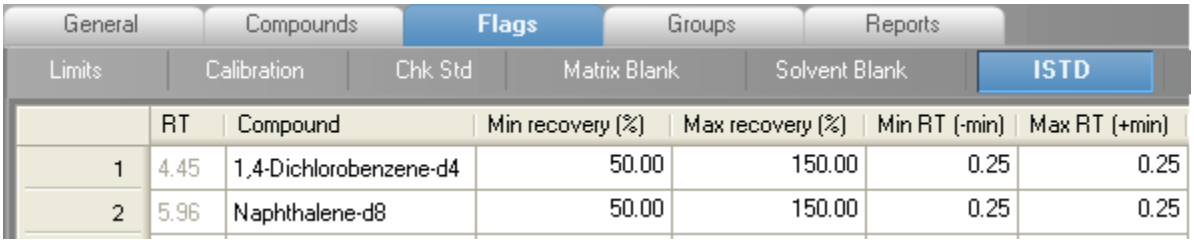


Table 43. ISTD page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
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 (%)	
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 Variance test.

Surrogate

Use the Surrogate page to view or edit values for surrogate recovery 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.

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

Figure 48. Surrogate page

Table 44. Surrogate page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
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.

Lab Control (Environmental and Food Safety)

Use the Lab Control page to view and edit QC values for lab control sample (LCS) and lab control sample duplicate (LCSD) analyses. 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 prepare samples (typically known as clean matrices) as LCS or LCSD. These represent samples where 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.

Figure 49. Lab Control page

Table 45. Lab Control page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
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 LCS or LCSD compound can have its own values for these fields, independent of other LCS or LCSD compounds.
Max recovery (%)	
Max RPD	Specifies a maximum value for relative percent difference (RPD) between two spiked samples.

Method Val (Environmental and Food Safety)

Use the Method 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.

Figure 50. Method Val page

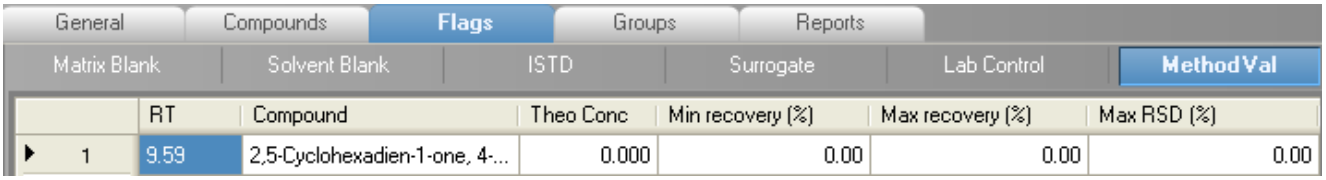


Table 46. Method Val page parameters

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.

Matrix Spike (Environmental and Food Safety)

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 or matrix spike duplicate compounds, prepare samples as MS or MSD. These represent samples where 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.

Figure 51. Matrix Spike page

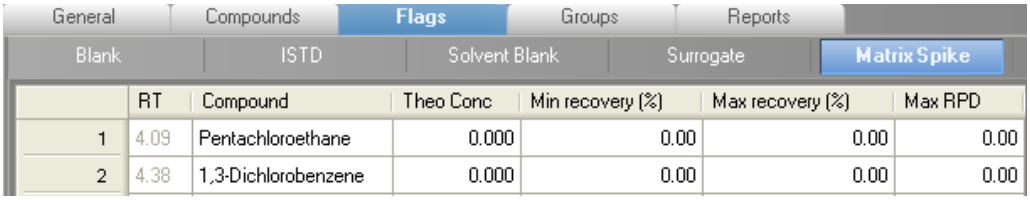


Table 47. Matrix Spike page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Theo Conc	Values for each matrix spike 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 matrix spike concentrations.
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 matrix spike sample can have its own values for these fields, independent of other matrix spike samples.
Max recovery (%)	
Max RPD	Specify a maximum value for relative percent difference (RPD) between two spiked samples.

Editing the Groups Page

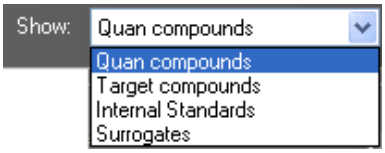
Use the Groups page of the Master Method View to organize compounds into functional or logical groups. You can use these groups for creating a subset of target compounds. For a detailed description of all the features on the Groups page, see "Groups page parameters" on page 172.

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 the Acquisition 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.

You can create multiple groups and include the same compound in more than one group.

❖ To create a group

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



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

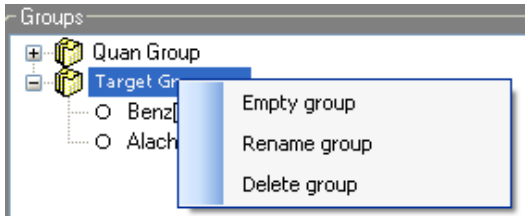
   The Add a New Group dialog box opens.

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, right-click the compound name in the group and choose **Remove from Group** from the shortcut menu.

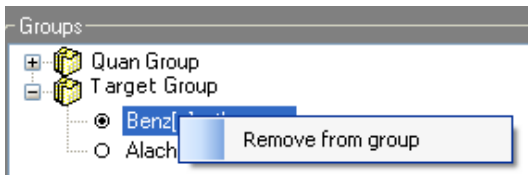


Figure 52. Groups page

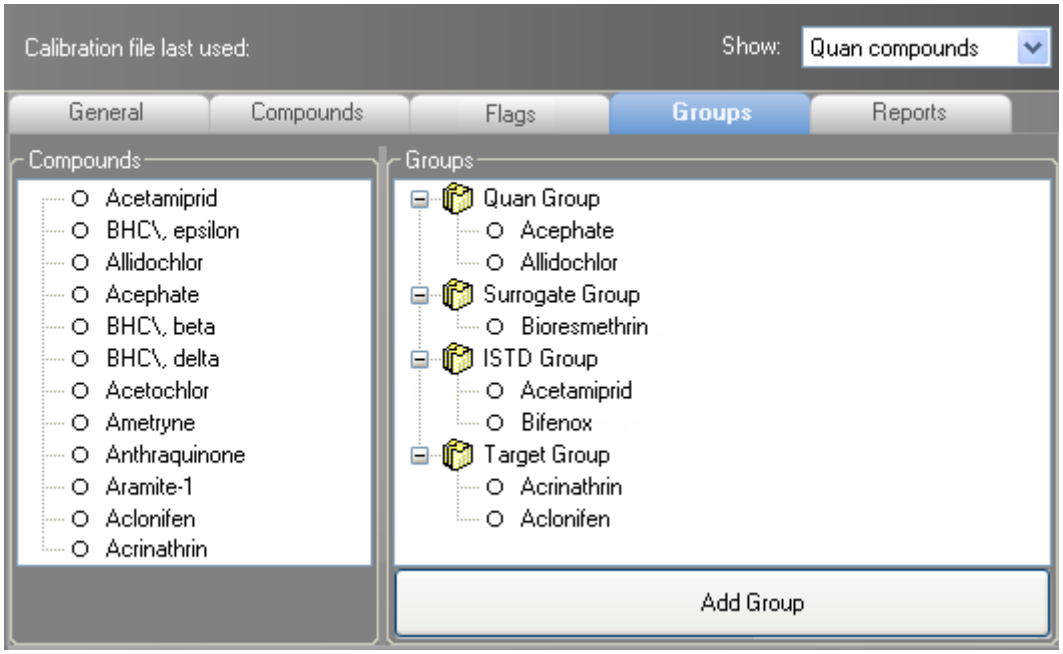


Table 48. Groups page parameters

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 page to specify how you want to save or print your reports. For a detailed description of the features on the Reports page, see "Reports page parameters" on page 176.

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 Quan Report Settings
- Specifying Target Screening Settings

Specifying Report Formats

- For each standard report, you can create a hardcopy printout, a PDF file, or an XML file.
- For each custom report, you can create a hardcopy printout or an Excel Macro-Enabled Workbook (.xlsm) file.
- For each target screening report, you can create a hardcopy printout or a PDF file.

In addition to the report type, you can specify a report description for each of your reports. The default report description is the report name.

❖ To specify standard report types and output formats

1. Click the **Reports** tab.

   The Reports page displays the following columns for all configured reports:

   - The Example icon that opens an example PDF of the report type
   - Report Name, Report Description, and Report Type
   - Options to create a hardcopy, PDF file, or XML file for standard report types
   - Options to create a hardcopy or Excel Macro-Enabled Workbook file for custom report types
   - Options to create a hardcopy or PDF file for target screening report types
   - The Batch Level option that indicates which reports are batch-level reports

General | Compounds | Flags | Groups | **Reports**

	Example	Report Name	Report Description	Report Type	Print	Create PDF	Create XML	Create XLSM	Batch Level
1		Batch Report	Batch Report	Standard	☐	☐	☐	☐	☑
2		Target Screening Summary	Target Screening Summary	TargetScreening	☐	☐	☐	☐	☐
3		Alternate BatchReport	Alternate BatchReport	Custom	☐	☐	☐	☐	☑

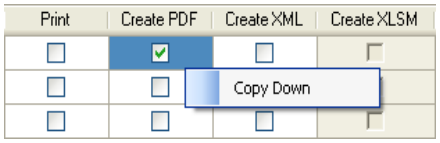
For information about configuring which reports are available when you create a master method or which reports create a batch-level report, see "Specifying the Reports Configuration" on page 58.

2. To edit the Report Description, 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 Description 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. This action applies only to reports where this output format is available.

   By default, all report types are cleared.

Figure 53. Reports page

	Example	Report Name	Report Description	Report Type	Print	Create PDF	Create XML	Create XLSM	Batch Level
1		Batch Report	Batch Report	Standard	☐	☐	☐	☐	☑
2		Batch Report Rev 1	Batch Report Rev 1	Standard	☐	☐	☐	☐	☑
3		Blank Report	Blank Report	Standard	☐	☐	☐	☐	☐
4		Calibration Report	Calibration Report	Standard	☐	☐	☐	☐	☑
5		Check Standard Report	Check Standard Report	Standard	☐	☐	☐	☐	☐
6		Chromatogram Report	Chromatogram Report	Standard	☐	☐	☐	☐	☐
7		Compound Calibration Report	Compound Calibration Re...	Standard	☐	☐	☐	☐	☐
8		Compound Calibration Report - Alternate	Compound Calibration Re...	Standard	☐	☐	☐	☐	☐
9		Confirmation Report	Confirmation Report	Standard	☐	☐	☐	☐	☐
10		Confirmation Report 2	Confirmation Report 2	Standard	☐	☐	☐	☐	☐
11		High Density Calibration Report	High Density Calibration R...	Standard	☐	☐	☐	☐	☑
12		High Density Internal Standard Report	High Density Internal Stan...	Standard	☐	☐	☐	☐	☐
13		High Density Internal Standard Report Long	High Density Internal Stan...	Standard	☐	☐	☐	☐	☐
14		High Density Sample Report 1	High Density Sample Rep...	Standard	☐	☐	☐	☐	☐
15		High Density Sample Report 1 Long	High Density Sample Rep...	Standard	☐	☐	☐	☐	☐
16		High Density Sample Report 2	High Density Sample Rep...	Standard	☐	☐	☐	☐	☐
17		High Density Sample Report 2 Long	High Density Sample Rep...	Standard	☐	☐	☐	☐	☐
18		High Density Sample Report 3	High Density Sample Rep...	Standard	☐	☐	☐	☐	☐
19		High Density Sample Report 3 Long	High Density Sample Rep...	Standard	☐	☐	☐	☐	☐
20		Internal Standard Summary Report	Internal Standard Summar...	Standard	☐	☐	☐	☐	☐
21		Ion Ratio Failure Report	Ion Ratio Failure Report	Standard	☐	☐	☐	☐	☐
22		Manual Integration Report	Manual Integration Report	Standard	☐	☐	☐	☐	☐
23		Method Report	Method Report	Standard	☐	☐	☐	☐	☑
24		Quantitation Report	Quantitation Report	Standard	☐	☐	☐	☐	☐
25		Quantitation Report - 2	Quantitation Report - 2	Standard	☐	☐	☐	☐	☐
26		Solvent Blank Report	Solvent Blank Report	Standard	☐	☐	☐	☐	☐
27		Surrogate Recovery Report	Surrogate Recovery Report	Standard	☐	☐	☐	☐	☐
28		TIC Report	TIC Report	Standard	☐	☐	☐	☐	☐
29		TIC Summary Report	TIC Summary Report	Standard	☐	☐	☐	☐	☐
30		Target Screening Long Report	Target Screening Long R...	TargetScreening	☐	☐	☐	☐	☐
31		Target Screening Summary Report	Target Screening Summar...	TargetScreening	☐	☐	☐	☐	☐
32		AltCalibrationReport	AltCalibrationReport	Custom	☐	☐	☐	☐	☑
33		Alternate BatchReport	Alternate BatchReport	Custom	☐	☐	☐	☐	☑
34		Alternate CalibrationReport	Alternate CalibrationReport	Custom	☐	☐	☐	☐	☑
35		Alternate ConfirmationReport	Alternate ConfirmationRep...	Custom	☐	☐	☐	☐	☐
36		Alternate MatrixSpikeReport	Alternate MatrixSpikeReport	Custom	☐	☐	☐	☐	☐

Figure 54. Reports page, continued

37		Alternate SampleReport	Alternate SampleReport	Custom	☐	☐	☐	☐	☐
38		Alternate SummaryReport	Alternate SummaryReport	Custom	☐	☐	☐	☐	☑
39		BatchReport	BatchReport	Custom	☐	☐	☐	☐	☑
40		BlankReport	BlankReport	Custom	☐	☐	☐	☐	☐
41		CalibrationDensityReport	CalibrationDensityReport	Custom	☐	☐	☐	☐	☑
42		CalibrationReport	CalibrationReport	Custom	☐	☐	☐	☐	☑
43		CheckStandardReport	CheckStandardReport	Custom	☐	☐	☐	☐	☐
44		CompoundCalibrationReport	CompoundCalibrationReport	Custom	☐	☐	☐	☐	☐
45		ConfirmationReport	ConfirmationReport	Custom	☐	☐	☐	☐	☐
46		ConfirmationReport2	ConfirmationReport2	Custom	☐	☐	☐	☐	☐
47		HighDensitySampleReport1Long	HighDensitySampleRepor...	Custom	☐	☐	☐	☐	☐
48		HighDensitySampleReport2Long	HighDensitySampleRepor...	Custom	☐	☐	☐	☐	☐
49		HighDensitySampleReport3Long	HighDensitySampleRepor...	Custom	☐	☐	☐	☐	☐
50		HighDensitySampleReport4	HighDensitySampleReport4	Custom	☐	☐	☐	☐	☐
51		HighDensitySampleReport5	HighDensitySampleReport5	Custom	☐	☐	☐	☐	☐
52		QuantitationReport	QuantitationReport	Custom	☐	☐	☐	☐	☐
53		SteroidAnalysisReport	SteroidAnalysisReport	Custom	☐	☐	☐	☐	☐

Table 49. Reports page parameters

Parameter	Description
Example	Opens a PDF that displays an example of the report type.
Report Name	The name of a report.
Report Description	The user-defined description to be used on a report.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files. Available only for standard reports.
Create XML	Reports to be exported in XML format. Available only for standard reports.
Create XLSM	Reports to be exported in Excel Macro-Enabled Workbook (.xlsm) format. Available only for custom reports.
Batch Level	Rather than creating separate reports for each sample, the application uses a composite of the data from all the samples to create a single report for the entire batch. Batch-level reports are prepended with a **B** to differentiate them. You cannot select this option from the Reports page. You must select the Batch Level option for the report in the report configuration. See "Specifying the Reports Configuration" on page 58.

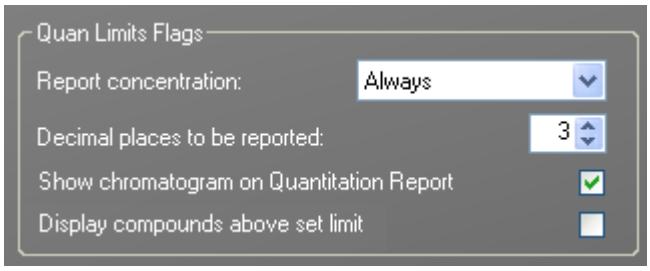
Specifying Quan Report Settings

Use the options on the Quan Report Settings page to choose parameters for flagging values and displaying information in standard report types.

Use the following procedures:

- To specify quantitation limits
- To specify user interface options
- To specify quantitation flag options
- To correct surrogates
- To track the use of the tune file

❖ To specify quantitation limits

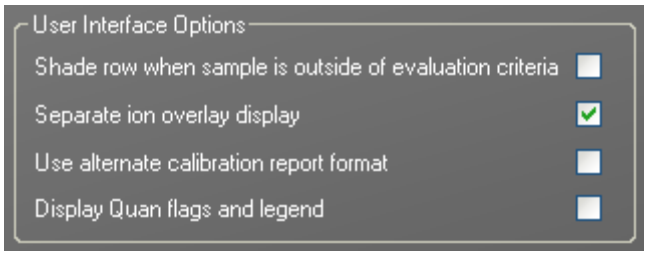


1. To report the calculated concentration at all times or only when the quantified value exceeds LOD, LOQ, or LOR, choose the appropriate value from the Report Concentration list.

   For a description of concentration limits, see "Limits" on page 160.

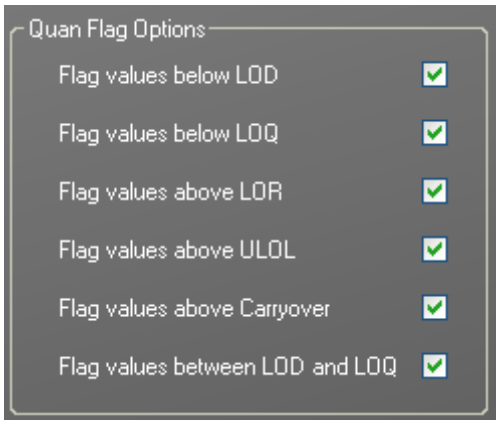
2. To select the number of decimal places to report for calculated concentrations, set the value in the Decimal Places to be Reported box.
3. To include a chromatogram of the sample in the Quantitation Report, select the **Show Chromatogram on Quantitation Report** check box.
4. To display only valid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

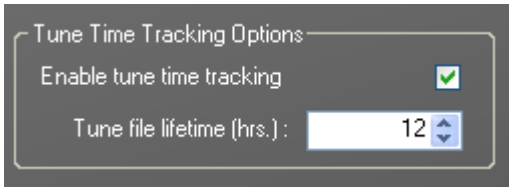
These flags appear on a variety of reports and are defined in the "Quan Report Settings page parameters" on page 180.

❖ To correct surrogates

Select the **Correct Surrogates** check box.

The TraceFinder application 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.

❖ To track the use of the tune file



1. Select the **Enable Tune Time Tracking** check box.

   This option tracks the number of hours between the last instrument tune and each sample acquisition.

2. In the **Tune File Lifetime** box, enter the number of hours you want to allow between the last instrument tune and a sample acquisition.

   Any sample acquired outside this maximum allowable time is flagged on the Batch report.

Figure 55. Quan Report Settings page

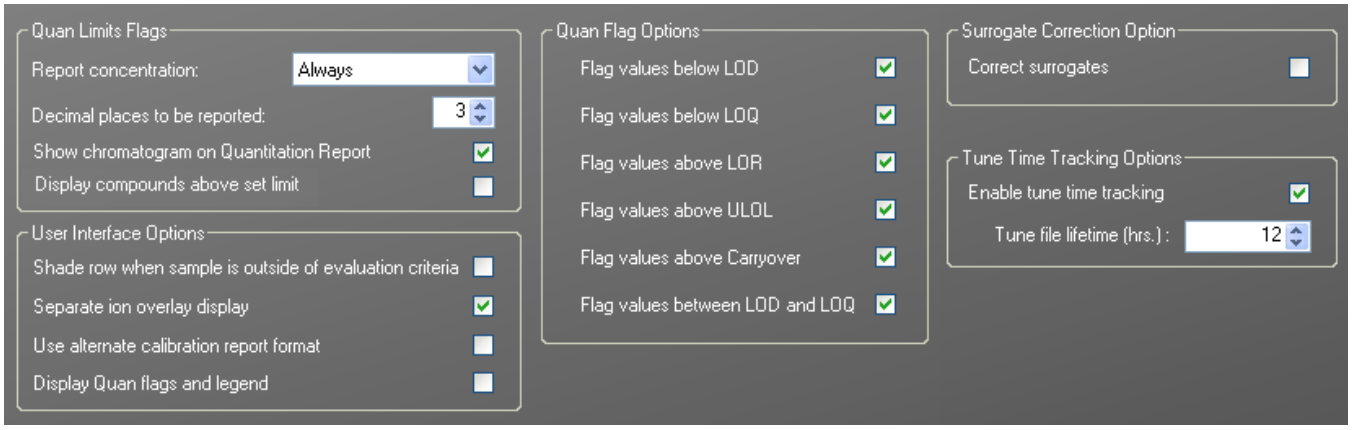


Table 50. Quan Report Settings page parameters (Sheet 1 of 2)

Parameter	Description
Quan Limits Flags	
Report concentration	Reports 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 compounds above set limit	Prints only the positive compounds in a sample. If a compound is above the specified Quan Flag Options limits, the TraceFinder 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.

Table 50. Quan Report Settings page parameters (Sheet 2 of 2)

Parameter	Description
Quan Flag Options	Values that are above or below limits defined on the Limits page. These flags appear on a variety of reports.
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 known as the J flag.
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 TraceFinder application dilutes the surrogates and target compounds and applies 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."
Tune Time Tracking Options	
Enable tune time tracking	Tracks the number of hours between the last instrument tune and each sample acquisition.
Tune file lifetime	Specifies the maximum number of hours between the last instrument tune and a sample acquisition. Any sample acquired outside this maximum allowable time is flagged on the Batch report.

Specifying Target Screening Settings

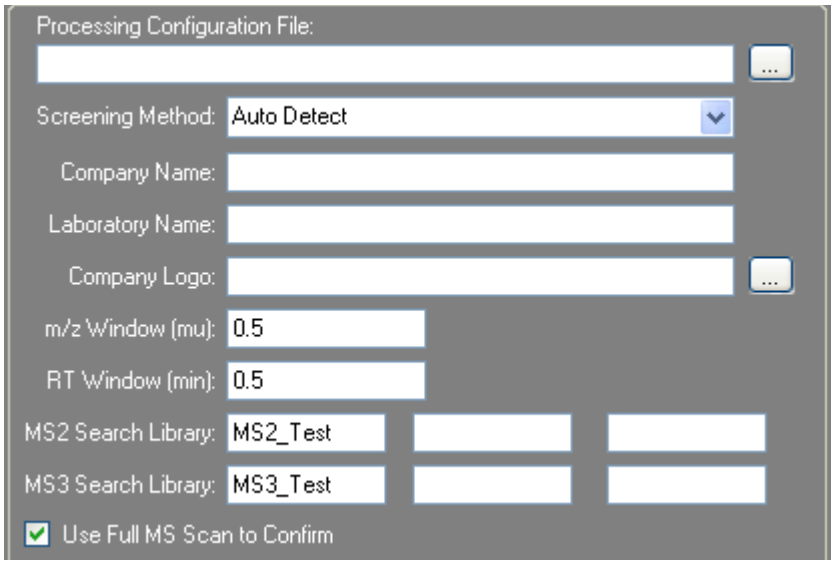
Use the options on the Target Screening Settings page to set the parameters required to produce Target Screening reports. For a detailed description of the features on the Target Screening Settings page, see "Target Screening Settings page parameters" on page 185.

The TraceFinder application use these parameters to process a raw data file and create a report similar to a ToxID report. See "Example Target Screening Summary Report" on page 187.

Use the following procedures:

- To specify the default parameters
- To calculate and report semi-quantitative results
- To specify the ion ratio calculation method
- To specify the exact mass window
- To specify the Exactive parameters

❖ To specify the default parameters



1. Click the Processing Configuration File browse button and select a configuration file (.csv).
2. From the Screening Method list, select one of these compound screening methods.
   •(Default) Auto Detect
   •Based on Full MS2 scans
   •Based on SRM and MS2 scans
   •Based on MS2 and MS3 scans
   •Based on MS3 scans
   •Based on accurate mass scans
   •Based on SRM scans
   •Based on Exactive screening method

3. Type the name of the company to print on the report.
4. Type the name of the laboratory to print on the report.
5. Click the Company Logo browse button and select a graphic file (.jpg, .gif, or .bmp) to print on the report.
6. In the *m/z* Window box, enter a value for the window above and below the m/z value for the compounds.
7. In the RT Window box, enter a value for the window above and below the retention time value for the compounds.
8. In the MS2 Search Library boxes, type the names of as many as three search libraries for searching MS/MS spectra.
9. In the MS3 Search Library boxes, type the names of as many as three search libraries for searching MS^3 spectra.
10. Select the **Use Full MS Scan to Confirm** check box if you want to confirm library search results with parent ion peak detection in the full scan.

    When the application does not detect a peak in the full scan, the compound is not reported as a hit.

❖ To calculate and report semi-quantitative results

1. In the Semi Quantitative area, do the following:
   a. Select the **Report Semi-Quantitative Result** check box.
   b. Type the measurement units.

      The measurement units are used only for labeling purposes.
2. Select either the **Scan Intensity** or **Peak Area** option.
   - Scan Intensity: The application measures the intensity of the MS/MS peak without performing background subtraction.
   - Peak Area: The application measures the peak area of the reconstructed full scan chromatogram peak of the parent ion. When you select Peak Area, the Use Full MS Scan to Confirm check box is automatically selected.

❖ To specify the ion ratio calculation method

1. Select the **Use Scan at Peak Apex** or **Use Average Scan** option.
   - Use Scan at Peak Apex: The application calculates the ion ratio based on the peak apex scan spectrum.
   - Use Average Scan: The application calculates the ion ratio based on the average scan spectrum over the range of the peak's half height. The relative intensity in the configuration file must use the selected scan method.
2. In the Ion Ratio Window (%) box, type the acceptable percentage of the intensity of the qualifier ion to the quan ion.

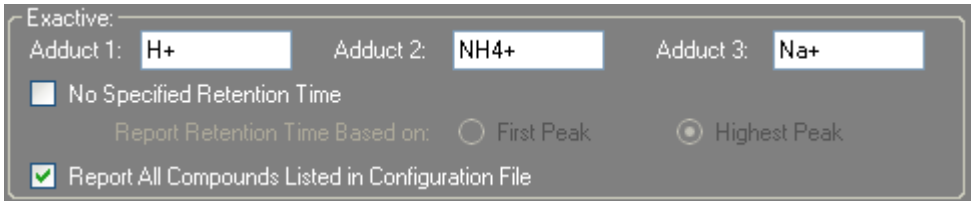
   For example, when the Ion Ratio Window is 20% and the quan ion has an intensity/height of 100, the specified confirming ion/mass must have a height of at least 80 to be considered found.

❖ To specify the exact mass window

Type a total window width value in parts per million for the Exact Mass Window.

For example, when you expect a mass of 50 with a window of 2, the algorithm creates an XIC based on the responses of all masses from 49 to 51.

❖ To specify the Exactive parameters



1. Type values for Adduct 1, Adduct 2, and Adduct 3.

   These values identify the adducts listed in and applied throughout the configuration file. Adducts are polarity sensitive. For negative ionization, enter negative adduct values.

   These values default to H+, NH4+, and Na+, respectively.
2. To search the entire raw data file for the specified peak, do the following:
   a. Select the **No Specified Retention Time** check box.
   b. Select either the **First Peak** or **Highest Peak** option.

      When the search finds more than one *m/z* match in the raw data file, the application uses the specified peak for processing.

3. Select the **Report All Compounds Listed in Configuration File** check box to report all compounds in the configuration file whether or not matches are found for them.

   The default reports on only those compounds where matches are found in the raw data file. This option applies to the Exactive experiment only.

Figure 56. Target Screening Settings page

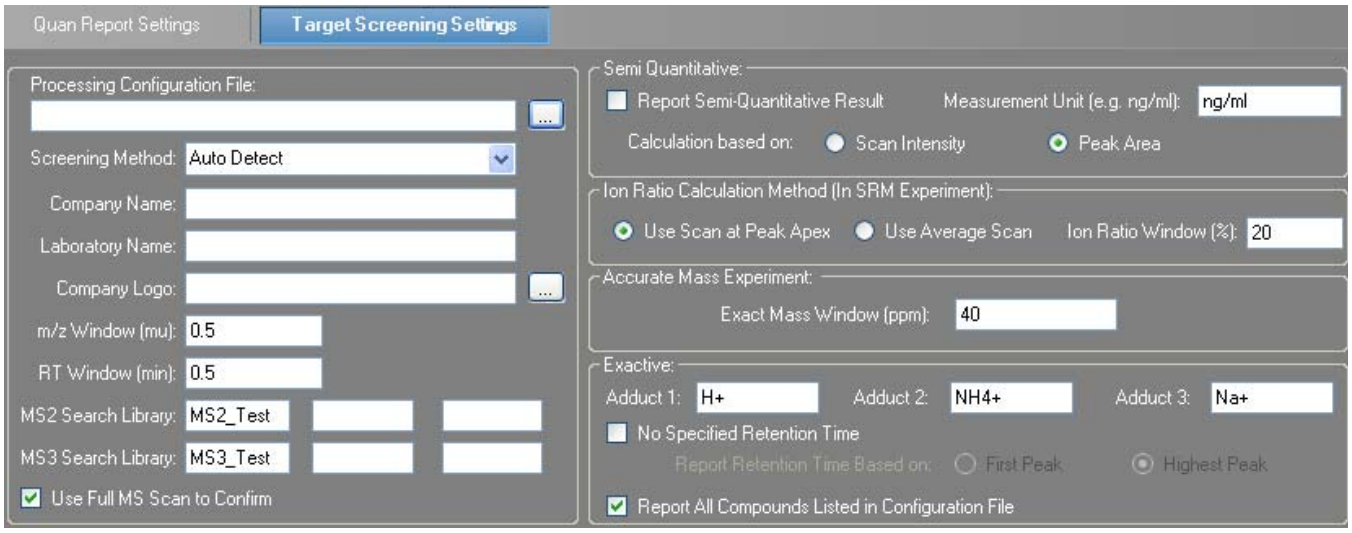


Table 51. Target Screening Settings page parameters (Sheet 1 of 2)

Parameter	Description
Processing Configuration File	Specifies a configuration file (.csv).
Screening Method	Specifies one of the following screening methods: • (Default) Auto Detect • Based on Full MS2 scans • Based on SRM and MS2 scans • Based on MS2 and MS3 scans • Based on MS3 scans • Based on accurate mass scans • Based on SRM scans • Based on Exactive screening method **Note** Using the Auto Detect method, the ToxID application can identify the screening experiment implemented in the acquired data file.
Company Name	Specifies the name of the company to print on the report.
Laboratory Name	Specifies the name of the laboratory to print on the report.
Company Logo	Specifies a graphic file (.jpg, .gif, or .bmp) to print on the report.
m/z Window (mu)	Specifies a value for the window above and below the *m/z* value for the compounds.
RT window (min)	Specifies a value for the window above and below the retention time value for the compounds.

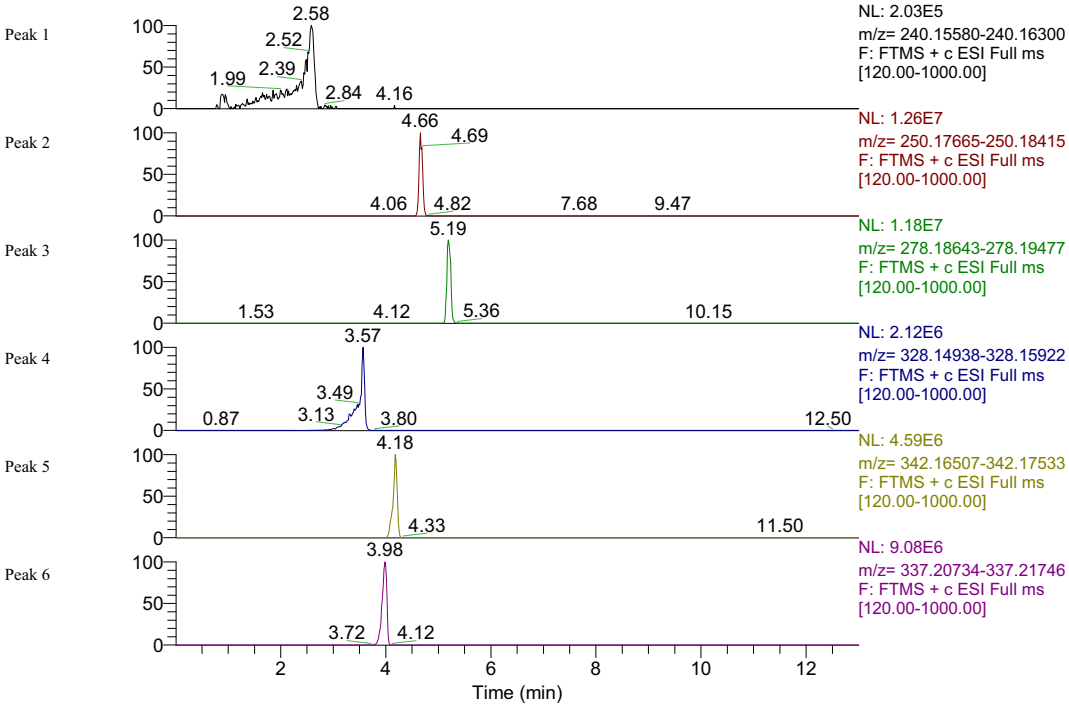
Table 51. Target Screening Settings page parameters (Sheet 2 of 2)

Parameter	Description
MS2 Search Library	Specifies the names of as many as three search libraries for searching MS/MS spectra.
MS3 Search Library	Specifies the names of as many as three search libraries for searching MS^3 spectra.
Use Full MS Scan to Confirm	Specifies that the application confirms library search results with parent ion peak detection in the full scan. When the application does not detect a peak in the full scan, the compound is not reported as a hit.
Semi Quantitative	
Report Semi-Quantitative Result	
Measurement Unit	
Calculation based on	Specifies one of the following calculation methods: • Scan Intensity: Specifies that the application measures the intensity of the MS/MS peak without performing background subtraction. • Peak Area: Specifies that the application measures the peak area of the reconstructed full scan chromatogram peak of the parent ion. When you select Peak Area, the Use Full MS Scan to Confirm check box is automatically selected.
Ion Ratio Calculation Method (In SRM Experiment)	
Use Scan at Peak Apex	Specifies that the application calculates the ion ratio based on the peak apex scan spectrum.
Use Average Scan	Specifies that the application calculates the ion ratio based on the average scan spectrum over the range of the peak's half height. The relative intensity in the configuration file must use the selected scan method.
Ion Ratio Window(%)	
Accurate Mass Experiment	
Exact Mass Window	Specifies a value in parts per million for the accurate mass experiment.
Exactive	
Adduct 1–*n*	Specifies the adducts listed in and applied throughout the configuration file. Adducts are polarity sensitive. For negative ionization, enter negative adduct values. Defaults: Adduct 1: H+, Adduct 2: NH4+, and Adduct 3: Na+
No Specified Retention Time	Specifies either First Peak or Highest Peak to use for processing when the search finds more than one *m/z* match in the raw data file.
Report All Compounds Listed in Configuration File	Specifies that in an Exactive experiment, the application reports all compounds in the configuration file whether or not matches are found for them. Default: Reports only those compounds where matches are found in the raw data file.

Figure 57. Example Target Screening Summary Report

Your Company Name
Summary Report

Raw File Name: C:\Xcalibur\examples\ToxID\Exact_Mass\Exact_Mass_Test.RAW
Config File Name: C:\Xcalibur\examples\ToxID\Exact_Mass\ConfigFile_Exact_mass.csv
Sample Name: Laboratory: Your Lab Name
Acquistion Start Time: 3/24/2008 4:46:43 PM
Screening Conditions: Based on accurate mass scans. Exact mass window (ppm): 30, RT window(min): 0.50.



Peak Number	Compound Name	Expected m/z	Detected m/z	Delta (mDa)	Delta (ppm)	Expected RT	Actual RT	Intensity
1	Albuterol	240.15940	240.15939	-0.0	-0.0	2.58	2.58	199505
2	Alprenolol	250.18040	250.18039	-0.0	-0.0	4.50	4.66	12604499
3	Amitriptyline	278.19060	278.19061	0.0	0.0	5.00	5.19	11769755
4	6-Acetylmorphine	328.15430	328.15433	0.0	0.1	3.30	3.57	2112090
5	6-Acetylcodeine	342.17020	342.17035	0.1	0.4	4.10	4.18	4593306
6	Acebutolol	337.21240	337.21246	0.1	0.2	3.80	3.98	9077282

Creating a Method Template

In the TraceFinder application, you can create a processing method using a method template that contains the basic settings.

Use the following procedures:

- To create a method template
- To specify peak criteria
- To identify the peaks
- 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. Click **Method Development** from the dashboard or the navigation pane.

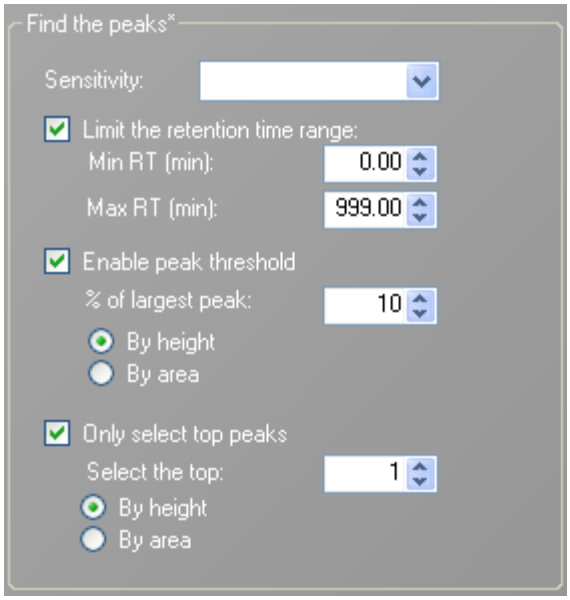
   The Method Development navigation pane opens.

2. Click **Method View** in the navigation pane.

3. From the main menu, choose **File > New > Method Template**.

   The Method Template Editor opens. For a complete description of the Method Template Editor, see "Method Template Editor dialog box" on page 195.

❖ To specify peak criteria



1. In the Find the Peaks area, select a sensitivity level.

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

   - The Genesis peak detection algorithm is provided for backward compatibility with Xcalibur 1.0 studies.
   - The ICIS peak detection algorithm is designed for MS data and has superior peak detection efficiency at low MS signal levels.
   - The Avalon peak detection algorithm is designed for integrating UV/Vis and analog chromatograms.

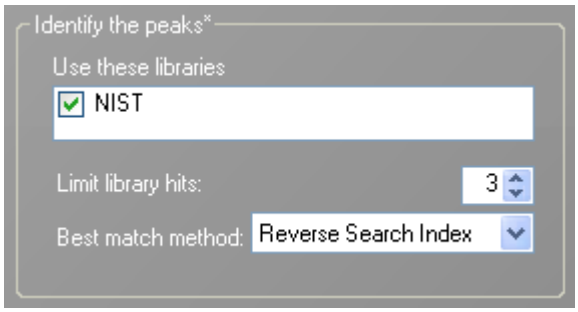
2. To look for peaks only in a certain range of the entire chromatogram, select the **Limit the Retention Time Range** check box and specify a retention time (RT) range.

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

   To consider a peak for a processing method, the TraceFinder 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 and enter the number of peaks to display.

❖ To identify the peaks



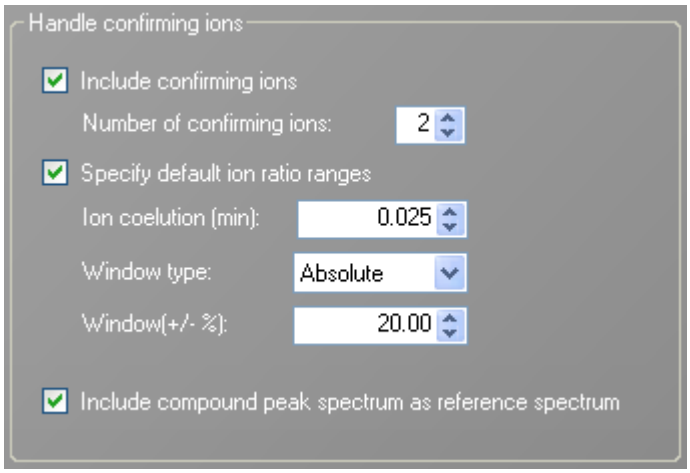
1. In the Use these Libraries box, select the libraries you want to search.

   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, select a value from the Best Match Method list.

❖ To specify confirming ions



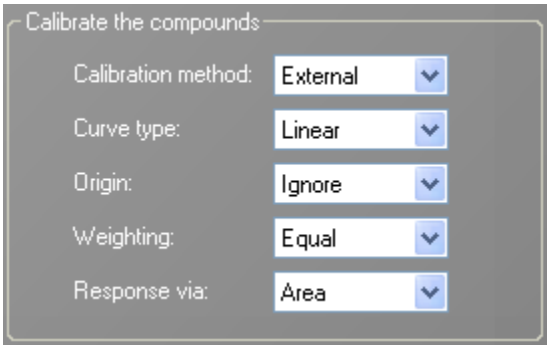
1. To set the number of confirming ions, select the **Include Confirming Ions** check box and enter a value in the Number of Confirming Ions box.

   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.

❖ 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 you select Include in the Origin list, all weighting values are unavailable except for Equal.
   - Quadratic: All other settings are available with this exception: When you select Include 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.

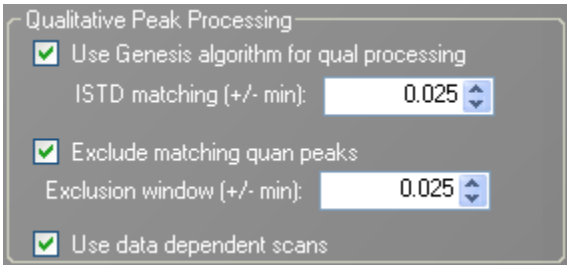
4. From the Weighting list, select one of the following:

    - 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, select **Area** or **Height**.

    - Area: Specifies that the TraceFinder application use this area value in response calculations.
    - Height: Specifies that the application use this height value in response calculations.

❖ To specify qualitative peak processing



1. Select the **Use Genesis Algorithm for Qual Processing** check box and specify a value for internal standard matching.

   The application uses the Genesis algorithm to match internal standards in a range plus/minus the value you specify. For additional information about the Genesis algorithm, see "Genesis Detection Method" on page 73.

2. Select or clear the **Exclude Matching Quan Peaks** check box and specify a value for the exclusion window.

   The application excludes quan peaks in a range plus/minus the value you specify.

3. To process samples that include data-dependent scans, select the **Use Data Dependent Scans** check box.

   When you process a sample using this feature, the application uses the TIC trace to find all data-dependent full scans, lists them, and performs a library search against the data-dependent MS/MS or MS^n scan.

   In addition to the peak information, the TIC Report and TIC Summary Report display information about the data-dependent filtered data. See Appendix A, "Reports."

❖ 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 to explain 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\1.1\Templates\Methods

Figure 58. Method Template Editor dialog box

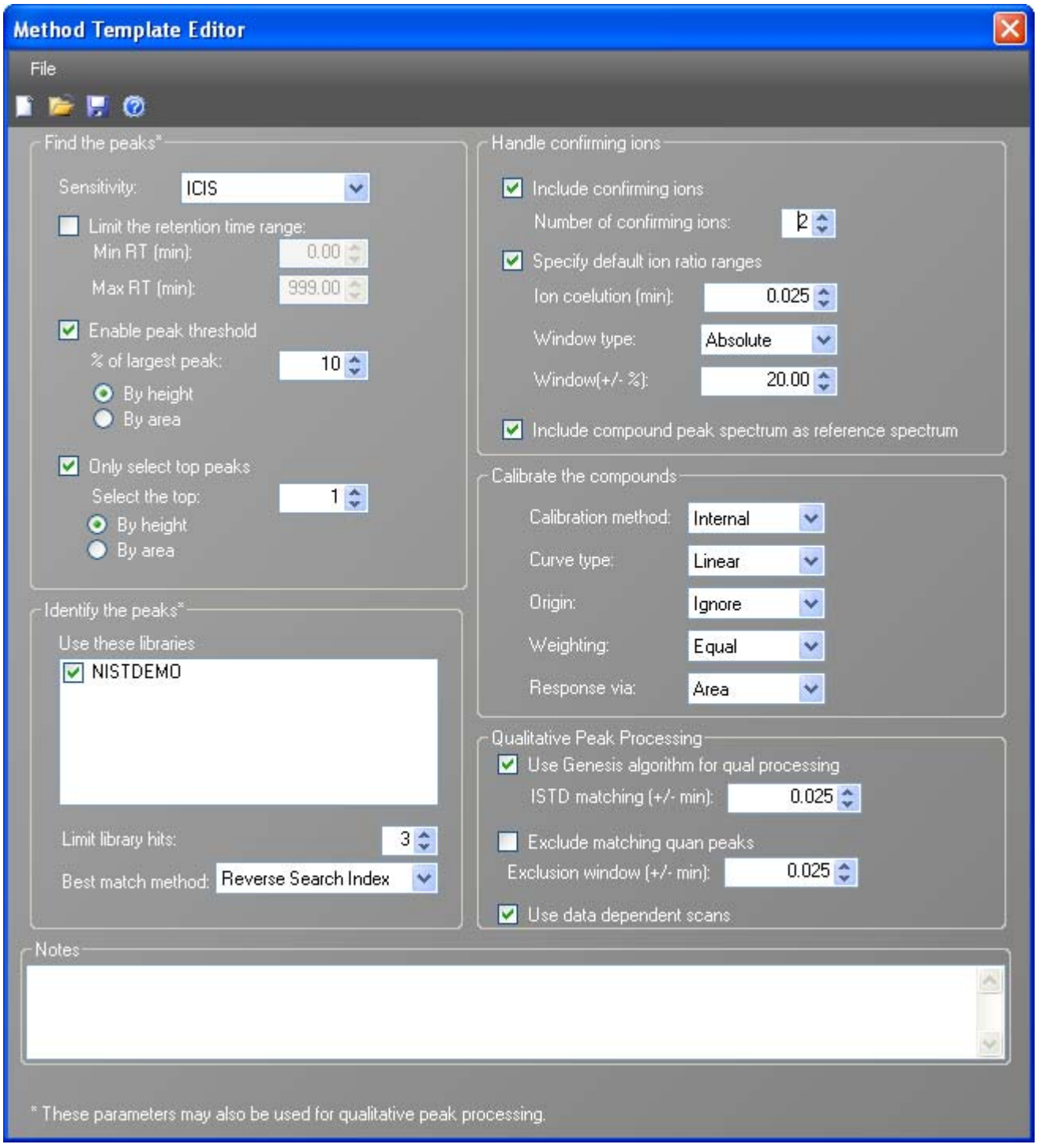


Table 52. Method Template Editor dialog box parameters (Sheet 1 of 3)

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. 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 results 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. Valid values: Search Index, Reverse Search Index, Match Probability
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. Ion Coelution specifies the maximum difference in retention time between a confirming ion peak and the quantification ion peak. Window Type specifies an Absolute or Relative calculation approach for determining the acceptable ion ratio range. Window (+/-%) specifies the acceptable ion ratio range.
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 52. Method Template Editor dialog box parameters (Sheet 2 of 3)

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 TraceFinder 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.
Qualitative Peak Processing	
Use Genesis algorithm for qual processing	The application uses the Genesis algorithm to match internal standards.
ISTD matching	Excludes all the target compounds found in the method and does not list these compounds in the TIC Report or in the Qual Mode view in the Data Review.

Table 52. Method Template Editor dialog box parameters (Sheet 3 of 3)

Parameter	Description
Exclude matching quan peaks	Compares the retention time of the internal standard in the method to the found retention time of the internal standard in the library search and excludes peaks outside the Exclusion Window range.
Exclusion window	Defines a range plus/minus the Exclusion Window value you specify.
Use data dependent scans	Constrains the Qual Mode view in the Data Review to only data-dependent scan spectra. See "Qual Mode" on page 312. In addition to the peak information, the TIC Report and TIC Summary report display information about the data-dependent filtered data.

Importing Published Master Methods

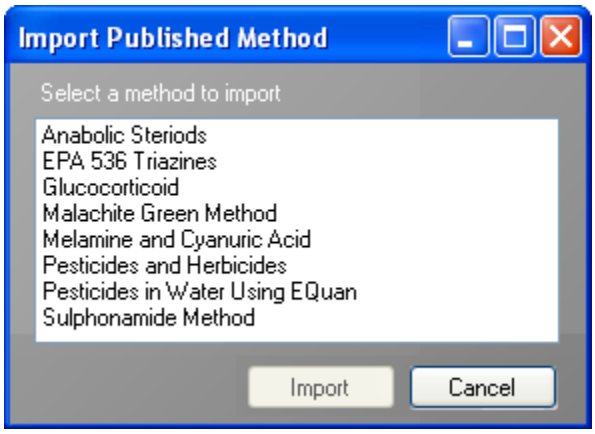
In the TraceFinder application, you can import published methods to use for detecting, processing, and reporting. The Tracefinder installation provides the following folder of published methods:

…\Thermo\TraceFinder\1.1\Published Master Methods

❖ To import a published master method

1. From the Method View task pane, click **Import Published Method**.

   The Import Published Method dialog box opens.



2. Select a method to import.
3. Click **Import**.

   The application reports that the method successfully imported and saves the method in the following folder:

   …\Thermo\TraceFinder\1.1\Methods

   You can use any of the Open Method commands to open this method just as you would a method you created.

Exporting SRM Data

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

❖ To export SRM data to an XML file

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

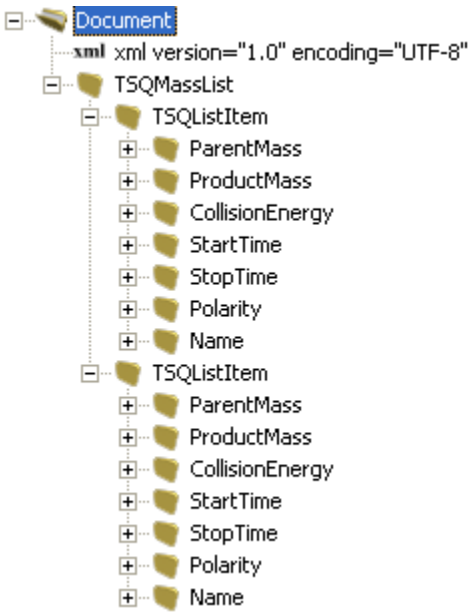
   The TraceFinder application writes the data in the SRM table to the following file:

   …\Thermo\TraceFinder\1.1\Methods*methodname*.xml

   The data in this file matches the TSQ .xml data, which you can use in the instrument method editor of the TSQ application.

> **Note** This command is available only when you select the Enable Compound Datastore option on the General page in the Application Configuration view. See "Application Configuration" on page 56.

Figure 59. SRM TSQ Quantum™ example



Working with Instrument Methods

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

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

Use the following procedures:

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

❖ To open the Instrument View

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

   The Method Development navigation pane opens.

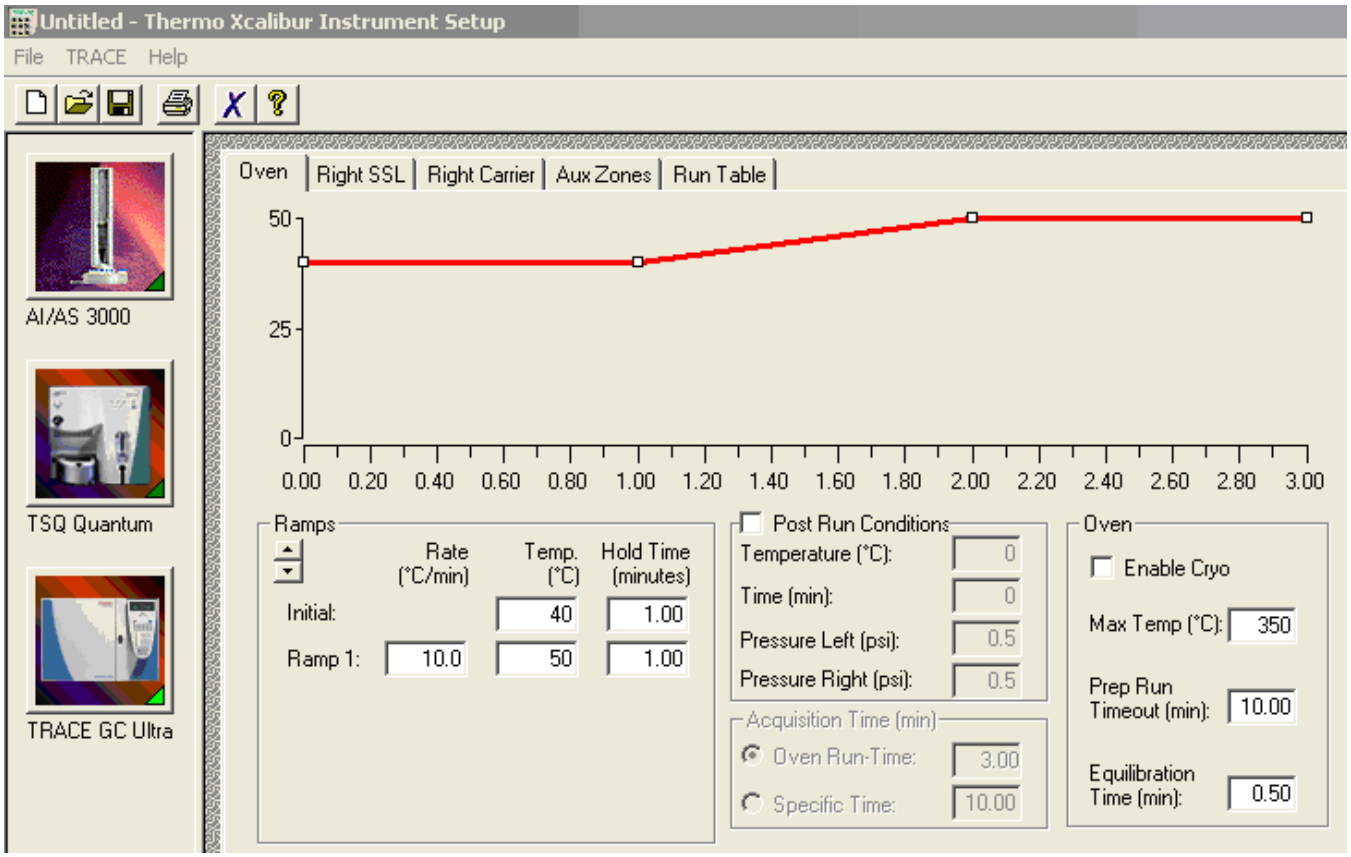
2. Click the **Instrument View** task pane.

❖ To create a new instrument method

1. Click **New Instrument Method** in the Instrument View task pane.

   The Thermo Xcalibur Instrument Setup window opens.

   This example instrument setup shows multiple configured instruments.

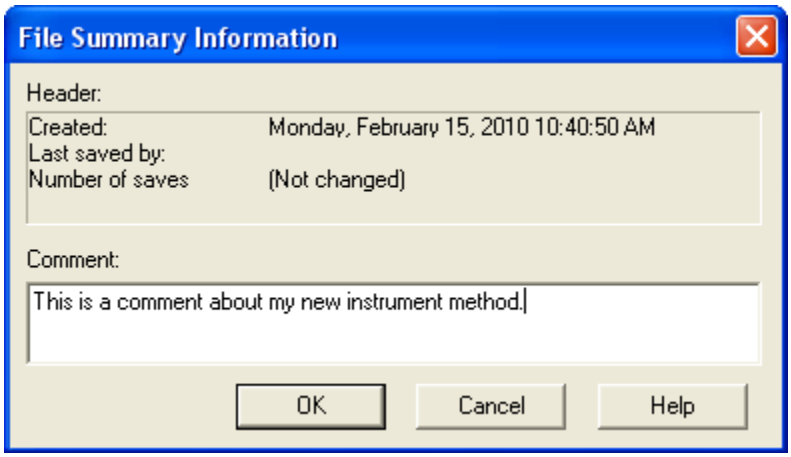


2. Click the icon for the instrument you want to use for the method.
3. Edit the values on the instrument page.
4. From the main menu in Thermo Xcalibur Instrument Setup window, choose **File > Save As**.

   The Save As dialog box opens.

5. Select an instrument method name to overwrite or type a new name for the instrument method, and click **Save**.

   The File Summary Information dialog box opens.



6. (Optional) Type a comment about the new instrument method.
7. Click **OK**.

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

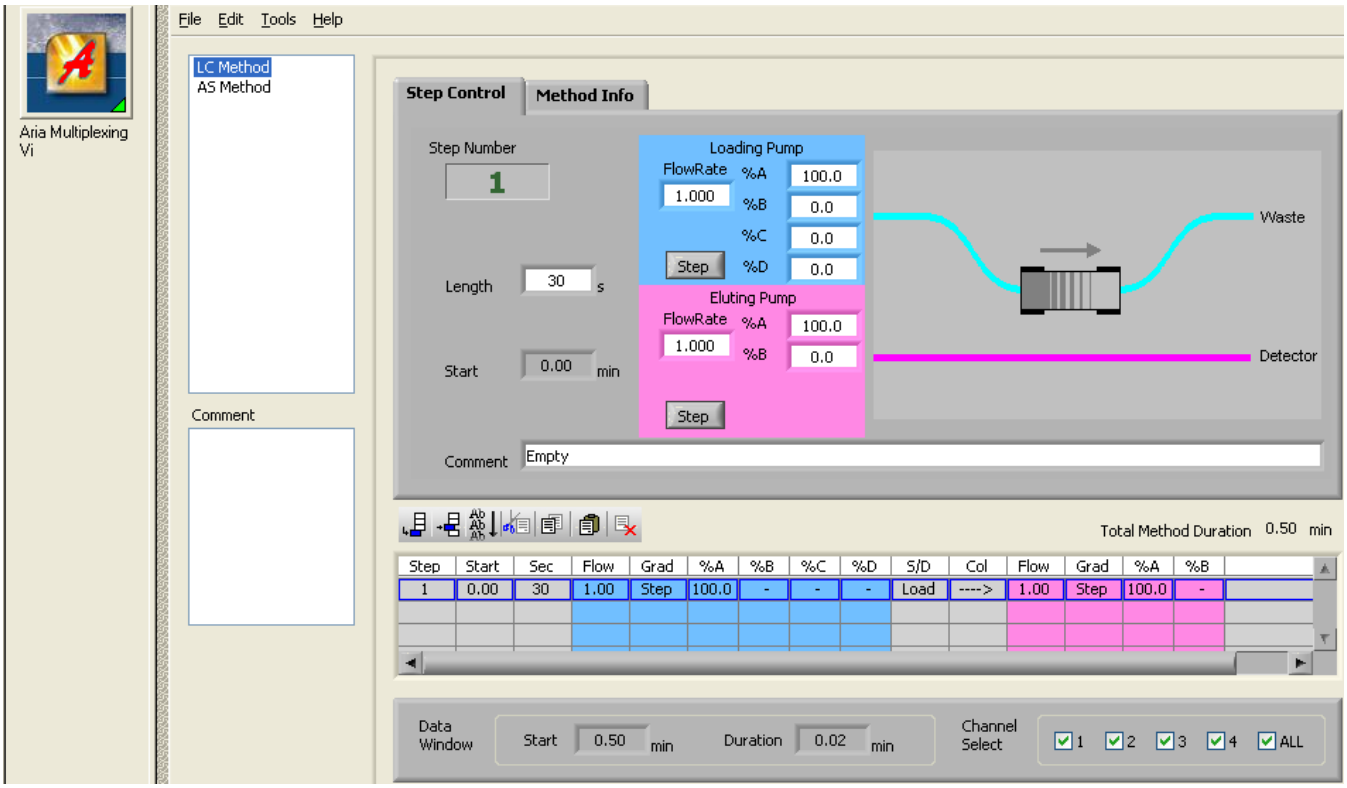
   …\Xcalibur\methods

❖ To create a new multiplexing instrument method

1. Click **New Instrument Method** in the Instrument View task pane.

   The Thermo Xcalibur Instrument Setup window opens.

Figure 60. Example instrument setup showing a configured multiplexed instrument



2. Click the icon for the instrument you want to use for the method.
3. Edit the values for the instrument method.

   For information about specifying multiplexing values, refer to the documentation for your multiplexed instrument.

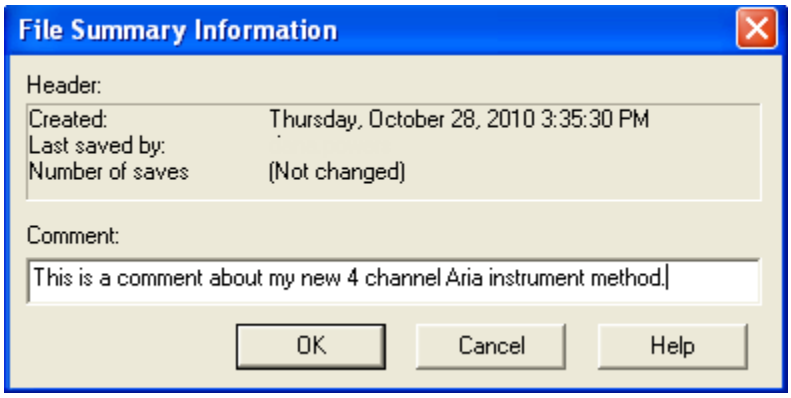
4. Specify the channels you want to use for acquisition. For example:

5. From the main menu in Thermo Xcalibur Instrument Setup window, choose **File > Save As**.

   The Save As dialog box opens.

6. Select an instrument method name to overwrite or type a new name for the instrument method, and click **Save**.

   The File Summary Information dialog box opens.



7. (Optional) Type a comment about the new instrument method.
8. Click **OK**.

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

   …\Xcalibur\methods

❖ To open an instrument method

1. Click **Open Instrument Method** on the Instrument View task pane.

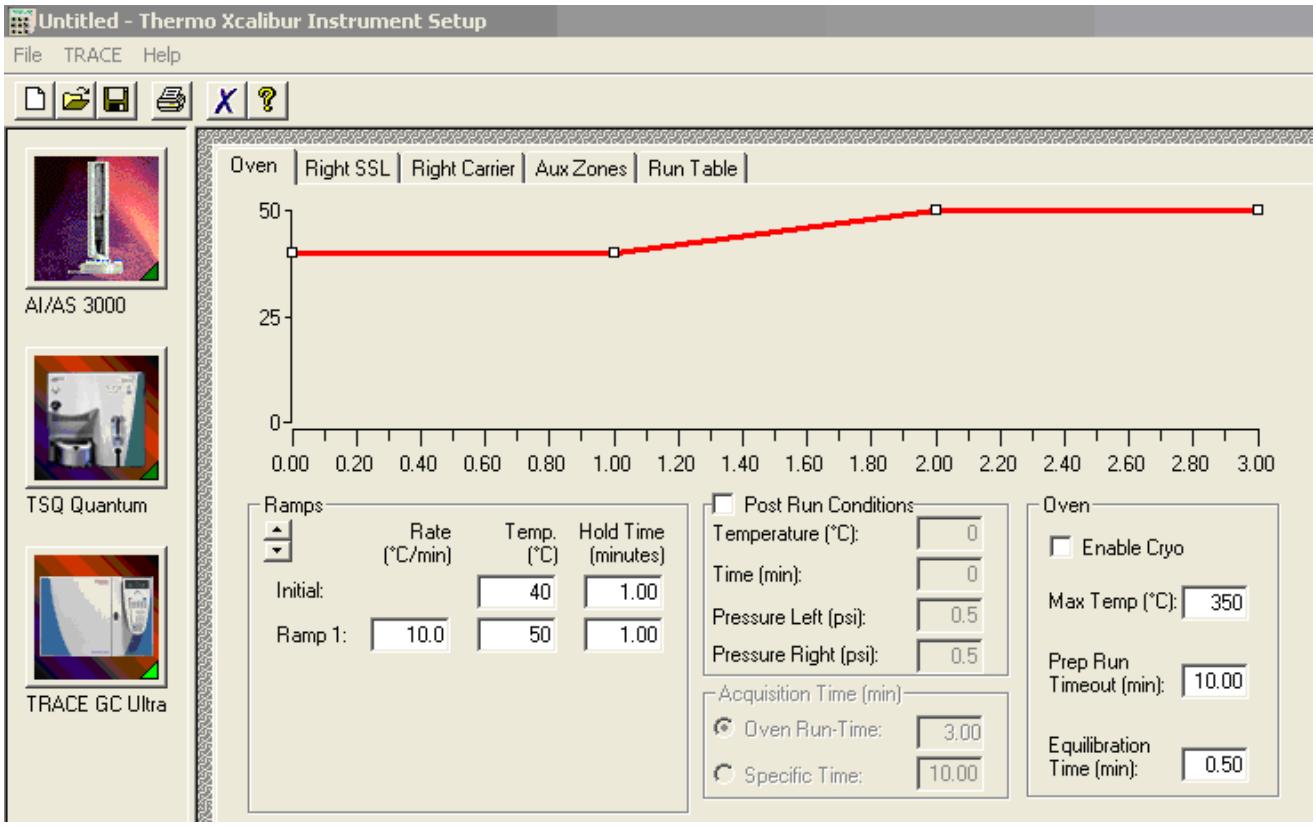
   An instrument method browser opens.

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

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

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

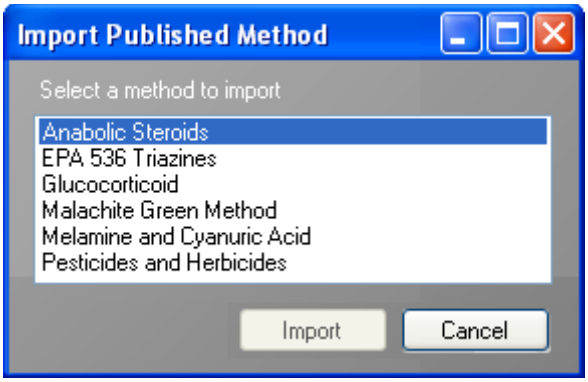
Figure 61. Example instrument setup showing multiple configured instruments



❖ To import an instrument method

1. From the Instrument View task pane, click **Import Published Method**.

   The Import Published Method dialog box opens. This dialog box lists the master methods in the Published Master Methods folder. You can import instrument methods that are associated with these published master methods.

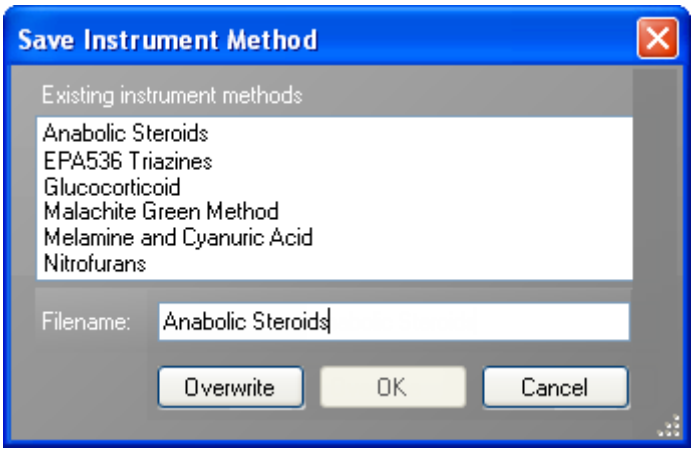


2. Select a method that includes the instrument method you want to import.

   For instructions for importing the master methods, see "Importing Published Master Methods" on page 198.

3. Click **Import**.

   The Save Instrument Method dialog box opens.



4. 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 application reports that the method successfully imported.

You can use any of the Open Instrument Method commands to open this method just as you would an instrument method that you created.

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 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; you can save only the raw data files created when you acquire the samples in the batch.

Use the following procedures:

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

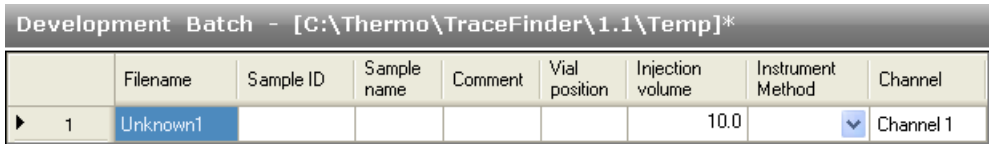
❖ To open the Development Batch view

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

The Method Development navigation pane opens.

2. In the Method Development navigation pane, click **Development Batch**.

The Development Batch view opens a new, empty batch.



Note The Channel column is available only when your configuration supports multiplexing.

❖ 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\1.1\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–

   Do the following:

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

   b. Click **Make New Folder**.

      The TraceFinder 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–

To add multiple sample rows, enter the number of rows and click the **Add Sample** icon.

The application adds the specified number of new, empty samples to 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–

   To insert multiple sample rows, enter the number of rows and click the **Insert Sample** icon.

   The TraceFinder application inserts new, empty samples above the selected sample.

   Note You cannot insert samples into an empty batch. You must have at least one sample to select before you can use this icon.

❖ 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 TraceFinder application adds a copy of the sample 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 the Copy Down or Fill Down commands 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.

   The minimum injection volume value allowed is 0.1µL; the maximum injection volume value allowed is 5000µL.
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.
6. To enter a channel for each sample, click the down arrow in the Channel column and select a channel from the list.

You cannot specify auto channel selection in a development batch.

Note The Channel column is available only when your configuration supports multiplexing.

Figure 62. Completed Development Batch

Development Batch - [C:\Thermo\TraceFinder\1.1\Temp]*

	Filename	Sample ID	Sample name	Vial position	Injection volume	Instrument Method	Channel
1	File1	1		1	10.0	Anabolic Steroids	Channel 1
2	File2	2		2	10.0	Anabolic Steroids	Channel 2
3	File3	3		3	10.0	Anabolic Steroids	Channel 1
4	File4	4		4	10.0	Anabolic Steroids	Channel 2

❖ 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.

   Use the first column to ensure that the samples are selected.

Selected samples

	Filename	Sample ID	Sample name	Comment	Vial p
1	file1	1	sample1		1
2	file2	2	sample2		2
3	file3	3	sample3		3
4	file4	4	sample4		4
5	file5	5	sample5		5

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.

   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.

2. 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 TraceFinder application saves only the generated raw data 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 acquire selected samples

1. Select the samples you want to acquire.
2. 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 data files and all temporary working files to the following folder:

   …\Thermo\TraceFinder\1.1\Temp

   When the acquisition is complete, the application deletes all the temporary working files. Only the raw data 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 acquire the batch

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 an .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 data 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.

Viewing Raw Data Files in the Qual Browser

You can view the chromatogram and spectra for completed samples in a development batch.

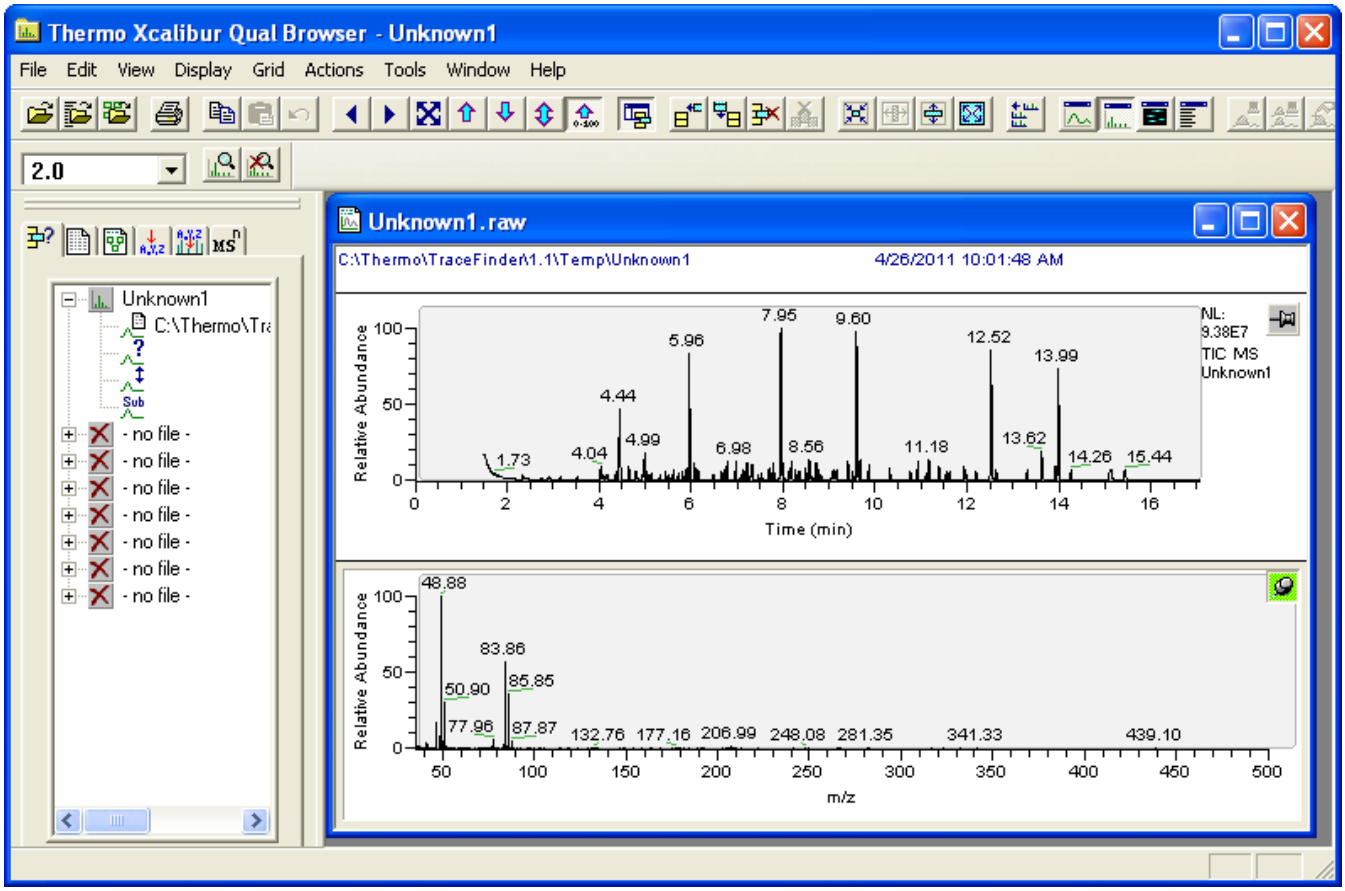
Use the following procedures:

- To open the Qual Browser
- To display the last completed raw data file in the Qual Browser

❖ To open the Qual Browser

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

The Thermo Xcalibur Qual Browser window opens.



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

❖ To display the last completed raw data file in the Qual Browser

In Acquisition page of the real-time viewer, right-click and choose **View Last File in Qual Browser** from the shortcut menu.

The last completed file opens in the Qual Browser.

When all samples are completed, you can view the last raw data file for the batch.

Using the Acquisition Mode

This chapter describes the tasks associated with the Acquisition mode.

Contents

- Working with Batches
- Real-time Display
- Sample Types

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 LabDirector or Supervisor role 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:

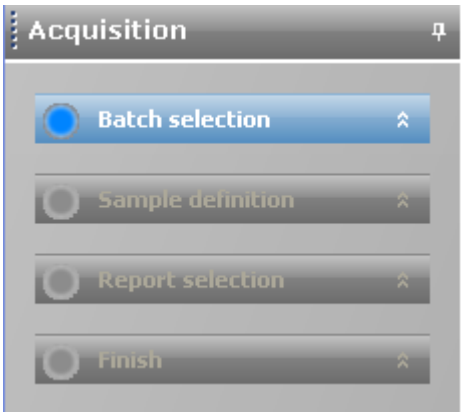
- Opening and Navigating the Acquisition Mode
- Creating Batches

Opening and Navigating the Acquisition Mode

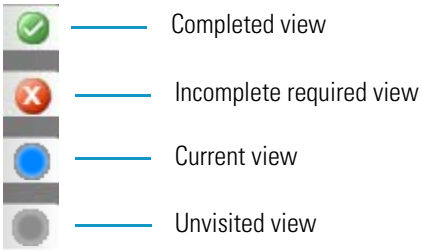
To open the Acquisition mode, click **Acquisition** in the navigation pane or from the dashboard.

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 63. Task pane when you enter the Acquisition mode

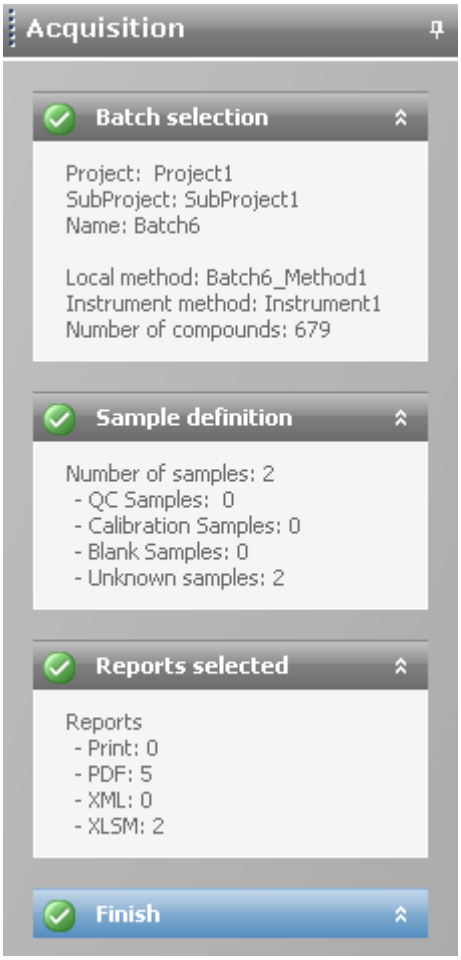


The status of each view in the Acquisition mode shows you which tasks are completed and which tasks are not.



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

Figure 64. Example task pane when you have completed the Acquisition mode



Creating Batches

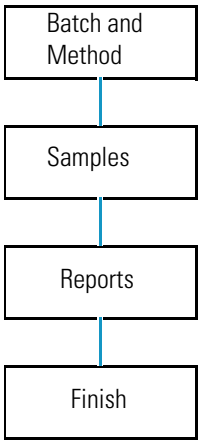
These are the major steps you use in Acquisition mode to create a batch:

1. Selecting a Batch
2. Defining the Sample List
3. Selecting and Reviewing Reports
4. Submitting the Batch

Workflows

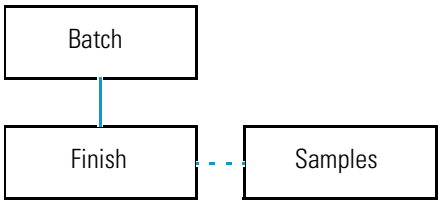
Depending on how you create your batch, you use different views in the Acquisition mode. The following workflows show the Acquisition views required for each batch creation approach. Depending on your approach to creating a batch, use one of these specific workflows.

❖ **Creating an original batch**



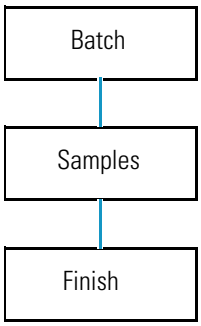
To create an original batch, start with the instructions "To start a new batch" on page 220.

❖ **Acquiring a previously saved (.tbr) batch**



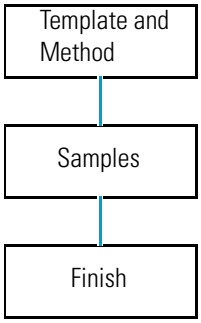
To acquire a previously saved batch, start with the instructions "To select a ready-to-acquire batch" on page 221.

❖ 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 222.

❖ Creating a batch template



When user security is enabled, this workflow is available only to users in the LabDirector or Supervisor role.

To create a batch template, start with the instructions "To create a batch template" on page 223 and then click **Save** on the Finish page

Selecting a Batch

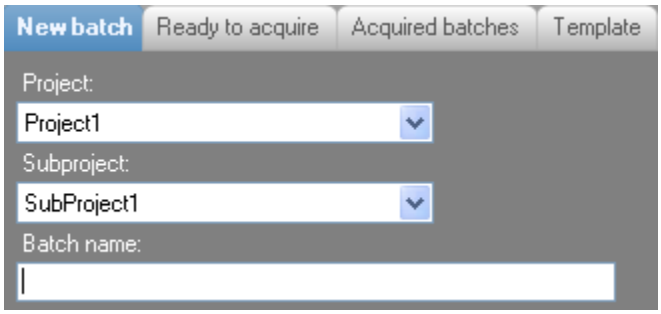
In a Template Selection view of the Acquisition mode, you can choose to create a new batch in any of your current projects/subprojects.

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

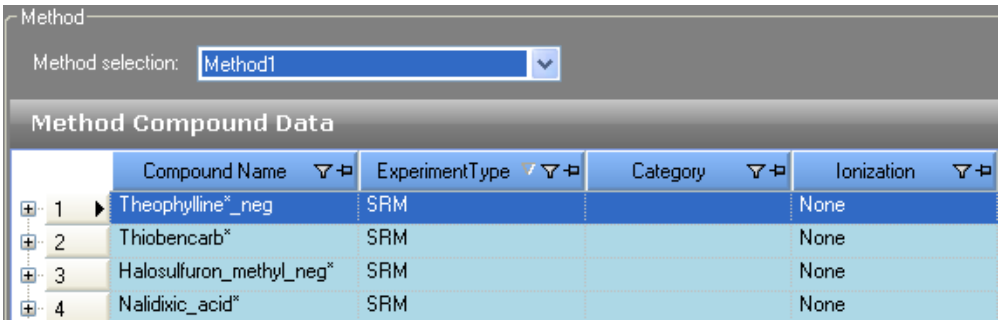
❖ To start a new batch

1. Click the **New Batch** tab.
2. Select the project and subproject where you want to create the new batch.
3. Type a name for the new batch in the Batch Name box.



4. Select a method from the Method Selection list.

   The Method Compound Data pane displays the compounds in the method. You cannot edit the compounds list from the Acquisition mode.



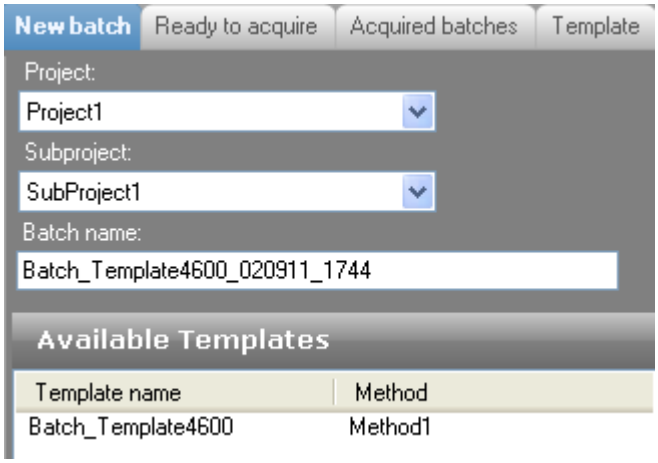
5. To continue to the next view, click **Next**.

   The Sample Definition view opens. See "Defining the Sample List" on page 224.

❖ To select a template for the new batch

1. Click the **New Batch** tab.
2. In the Available Templates pane, 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. You can change the default project, subproject, and method associated with this template.
3. (Optional) Select a different project and subproject where you want to create the new batch.



4. (Optional) Select a different method to use for the new batch.
5. To continue to the next view, click **Next**.

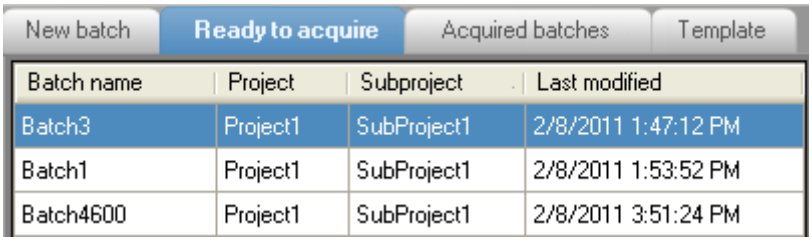
   The Sample Definition view of the Acquisition mode opens. See "Defining the Sample List" on page 224.

❖ 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 located in the following folder:

   …\Thermo\Tracefinder\1.1\Projects*projectname**subprojectname*
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 **Submit**.

     For detailed instructions, see "Submitting the Batch" on page 237.

   –Or–

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

     For detailed instructions on editing a samples list, see "Defining the Sample List" on page 224.

   –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.

     The application saves the .tbr batches in the following folder:

     …\Thermo\TraceFinder\1.1\Projects*projectname**subprojectname*

❖ 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**.

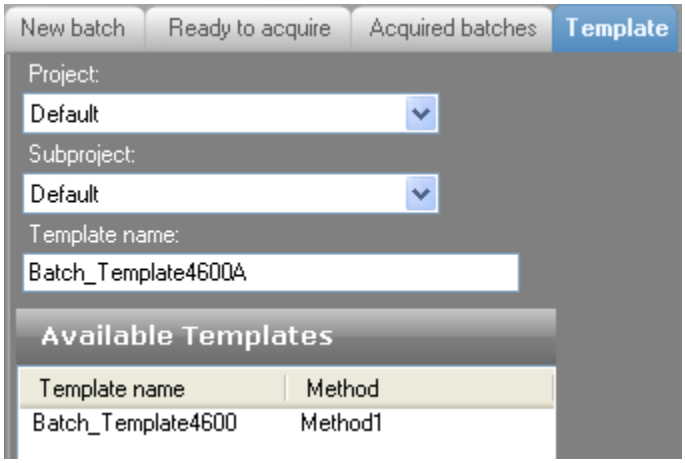
   The Sample Definition view of the Acquisition mode opens. See "Defining the Sample List" on page 224.

❖ To create a batch template

1. Click the **Template** tab.

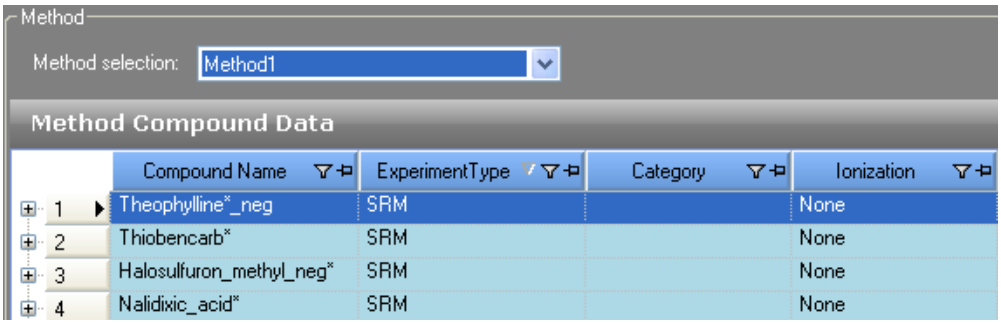
   Note When user security is enabled, this page is available only to users in the LabDirector or Supervisor role.

2. Select the project and subproject where you want to create the new batch template.
3. Type a name for the new batch template in the Template Name box.



4. Select a method from the Method Selection list.

   The Method Compound Data pane displays the compounds in the method. You cannot edit the compounds list from the Acquisition mode.



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 224.

Defining the Sample List

In 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. See "Sample Definition view" on page 230.

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
- To reinject a sample from a previously acquired batch
- To select channels for the batch
- To assign a specific channel to a sample

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

- When 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 233.
- When you are editing a previously acquired batch or a .tbr batch, the Finish Selection view opens. See "Submitting the Batch" on page 237.

❖ To add samples to the list

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

.

   Tip To quickly add a single row, right-click and choose **Add Sample** from the shortcut menu.

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

   Each file name must be unique.

3. Select a sample type from the Sample Type list for each sample.

Available Environmental and Food Safety sample types		
Matrix Blank	Solvent	Unknown/TIC
Cal Std	Chk Std	Unknown
LCS	MDL	MS
LCSD	Method Val	MSD

Available General Quantitation sample types		
Matrix Blank	Unknown/TIC	Unknown
Cal Std	Chk Std	Solvent

For a detailed description of sample types, see "Sample Types" on page 259.

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 LabDirector 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.

   The minimum injection volume value allowed is 0.1µL; the maximum injection volume value allowed is 5000µL.

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 the **Insert** button,

.

   The application inserts the unknown samples above the selected sample.

Inserted samples

	Status	Filename	Sample type	Sample level	Sample ID
1		cal_std_5	Cal Std	10	cal std = 5 ng/uL
2		Unknown2	Unknown		
3		Unknown1	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.

   Each file name must be unique.

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

   For a detailed description of each sample type, see "Sample Types" on page 259.

Available Environmental and Food Safety sample types		
Matrix Blank	Solvent	Unknown/TIC
Cal Std	Chk Std	Unknown
LCS	MDL	MS
LCSD	Method Val	MSD

Available General Quantitation sample types		
Matrix Blank	Unknown/TIC	Unknown
Cal Std	Chk Std	Solvent

5. For each Cal Std or Chk Std sample, click the Sample Level cell and select a level from the 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 LabDirector 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.

   The minimum injection volume value allowed is 0.1µL; the maximum injection volume value allowed is 5000µL.

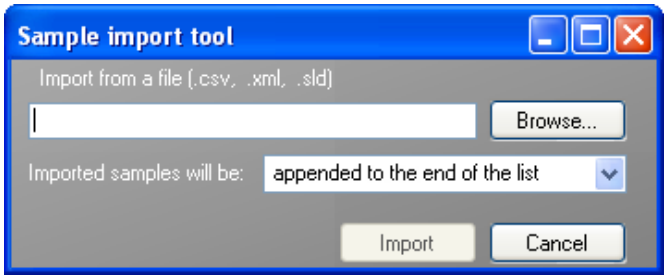
8. (Optional) Type or edit the values for the remaining columns.

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

❖ To import samples into the list

1. Click the **Import** button, Import.

   The Sample Import Tool dialog box opens.



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

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

   Note The .csv, .xml, or .sld 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.

   When you import samples from an Xcalibur sequence file (.sld), the TraceFinder application makes the following column name substitutions:

Xcalibur column	TraceFinder column
Level	Sample Level
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conv Factor

   When you import samples from an Xcalibur sequence file (.sld), the TraceFinder application makes the following sample type substitutions:

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	Chk Std
Std Bracket	Cal Std

5. For each Cal Std or Chk Std sample, click in the Sample Level cell and select a level from the 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 LabDirector 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.

   The minimum injection volume value allowed is 0.1µL; the maximum injection volume value allowed is 5000µL.

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, Filename, Sample Type, and Sample Level columns stay fixed while the other columns scroll right and left.

9. (Optional) When using multiplexing, select a channel for each imported sample.

   Imported samples default to Auto.

❖ 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.

❖ To reinject a sample from a previously acquired batch

1. In the sample list, select the sample you want to reinject.
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 reinjections of the same sample are numbered INJ002, INJ003, and so forth.

   The TraceFinder application copies all parameter values from the original sample.

A green status icon indicates previously acquired samples (acquired and processed), and the sample name is grayed out. A blue status icon indicates samples created for reinjection (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

When you submit this batch, the application acquires only the reinjection samples.

❖ To select channels for the batch

To disable a configured channel, clear the check box for the channel in the Multiplexing Channels area at the bottom of the page.

By default, all configured channels are selected. The configured channels are determined by the multiplexing settings in the Configuration mode. See "Specifying Multiplexing Parameters" on page 70.

Note Disabling a channel in the Multiplexing Channels area does not remove this channel selection from the Channels list for each sample. When you assign a channel to a sample, be careful not to assign a channel that you disabled.

❖ To assign a specific channel to a sample

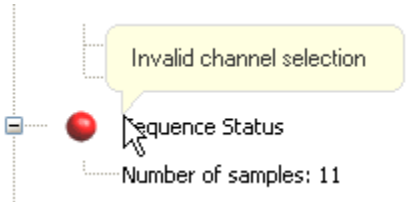
1. Scroll to the Channel column (the rightmost column in the sample list).

   All samples default to Auto.

2. Select a channel from the Channel list.

When you submit the batch, samples that are set to Auto run on any of the available channels and samples that are set to a specific channel run only on that channel.

If you select a channel that is not available for this batch, the sample sequence is flagged on the Finish page of the Acquisition mode. See the previous procedure, To select channels for the batch.



3. If you see this error, do the following:
   a. Click **Previous** to return to the Sample Definition page.

      The incorrect sample is marked with an error flag.

   b. Correct the channel selection.

Figure 65. Sample Definition view

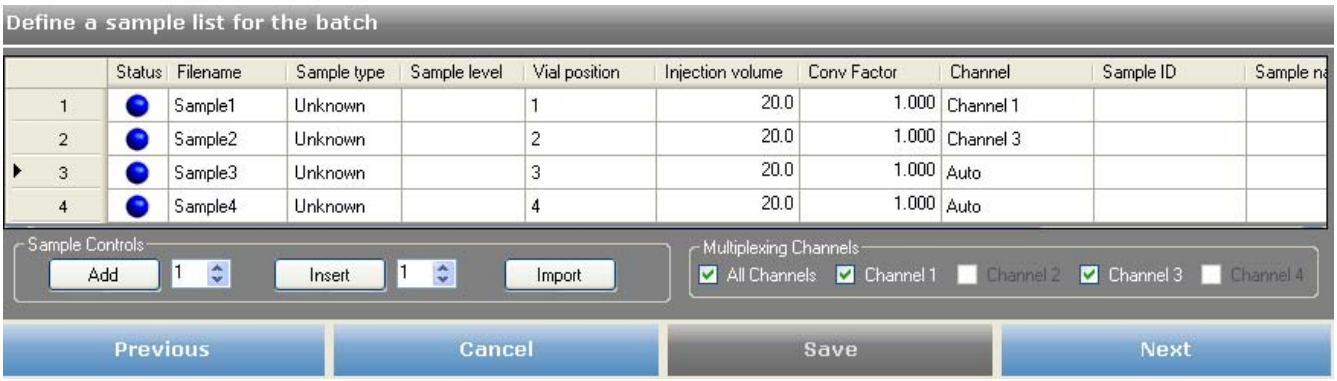


Table 53. Sample Definition parameters (Sheet 1 of 3)

Parameter	Definition
Sample Controls	
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.
Multiplexing Channels	
All Channels	Uses all configured channels to acquire this batch.
Channel 1-*n*	Uses only the selected channels to acquire this batch.
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.
Save	Saves this batch as a to-be-run (.tbr) batch.

Table 53. Sample Definition parameters (Sheet 2 of 3)

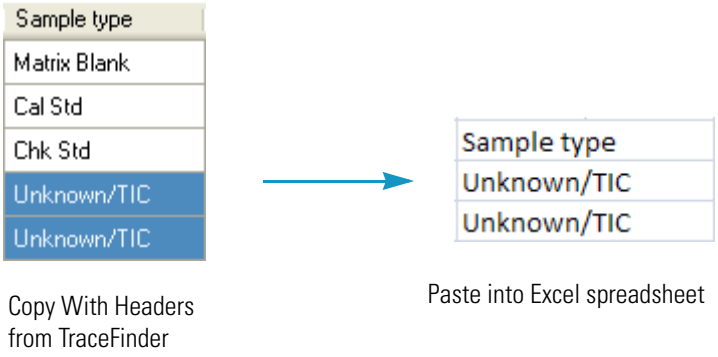
Parameter	Definition
Next	Takes you to the next Acquisition mode view.
Shortcut menu	
Add Sample	Adds a single empty row to the sample grid.
Insert Sample	Inserts a single empty row to the sample grid above the selected row.
Insert Copy Sample	Copies the currently selected row and inserts a copy above the row.
Reinject selected samples	Creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections 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 227.
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."
Modify columns	Opens the Modify Columns dialog box. See "Column Display" on page 284.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information to another application, such as an Excel spreadsheet. You cannot paste this data back into the Acquisition mode sample list.
Copy With Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information to another application, such as an Excel spreadsheet. You cannot paste this data back into the Acquisition mode sample list. For example:  Copy With Headers from TraceFinder Paste into Excel spreadsheet
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column.
Undo Last Paste	Removes the last pasted item in the Acquisition mode sample list.

Table 53. Sample Definition parameters (Sheet 3 of 3)

Parameter	Definition
Export to CSV file	Opens the Save As dialog box where you can save the current sample list to a .csv file.
Status color codes	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed.

Selecting and Reviewing Reports

On the Report Selection view, you can specify the types of reports you want to create. See "Report Selection view" on page 235. For a complete list of report types and examples of output files, see Appendix A, "Reports." In addition to the report type, you can specify a report description for each of your reports.

For each standard report you generate, you can create a hardcopy printout, a PDF file, or an XML file.

For each custom report you generate, you can create a hardcopy printout or an XLSM file.

When you have finished specifying your report options, click **Next** to go to the Finish view. See "Submitting the Batch" on page 237.

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

…\Projects*projectname**subprojectname**batchname*\Reports

Use the following procedures:

- To edit a report description
- To preview a standard report
- To specify a standard report in print format or as a PDF, XML, or XLSM file
- To export reports to a specific folder

❖ To edit a report description

Select the Report Description column and edit the default description.

The default report description is the same as the report name.

❖ To preview a standard report

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

Note Only Standard report types have preview documents.

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

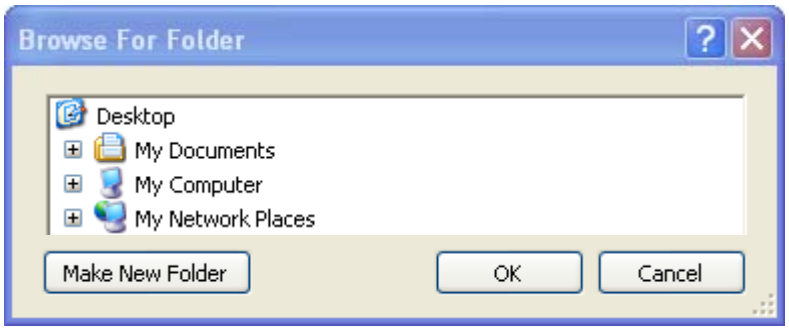
1. For each type of report you want to create, select the check box in the Print, Create PDF, Create XML, or Create XLSM columns.
2. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell. You can duplicate the output type only for reports that have this output format available.

❖ To export 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**.

   The application writes all reports to the specified folder in addition to the batch Reports folder.

Figure 66. Report Selection view

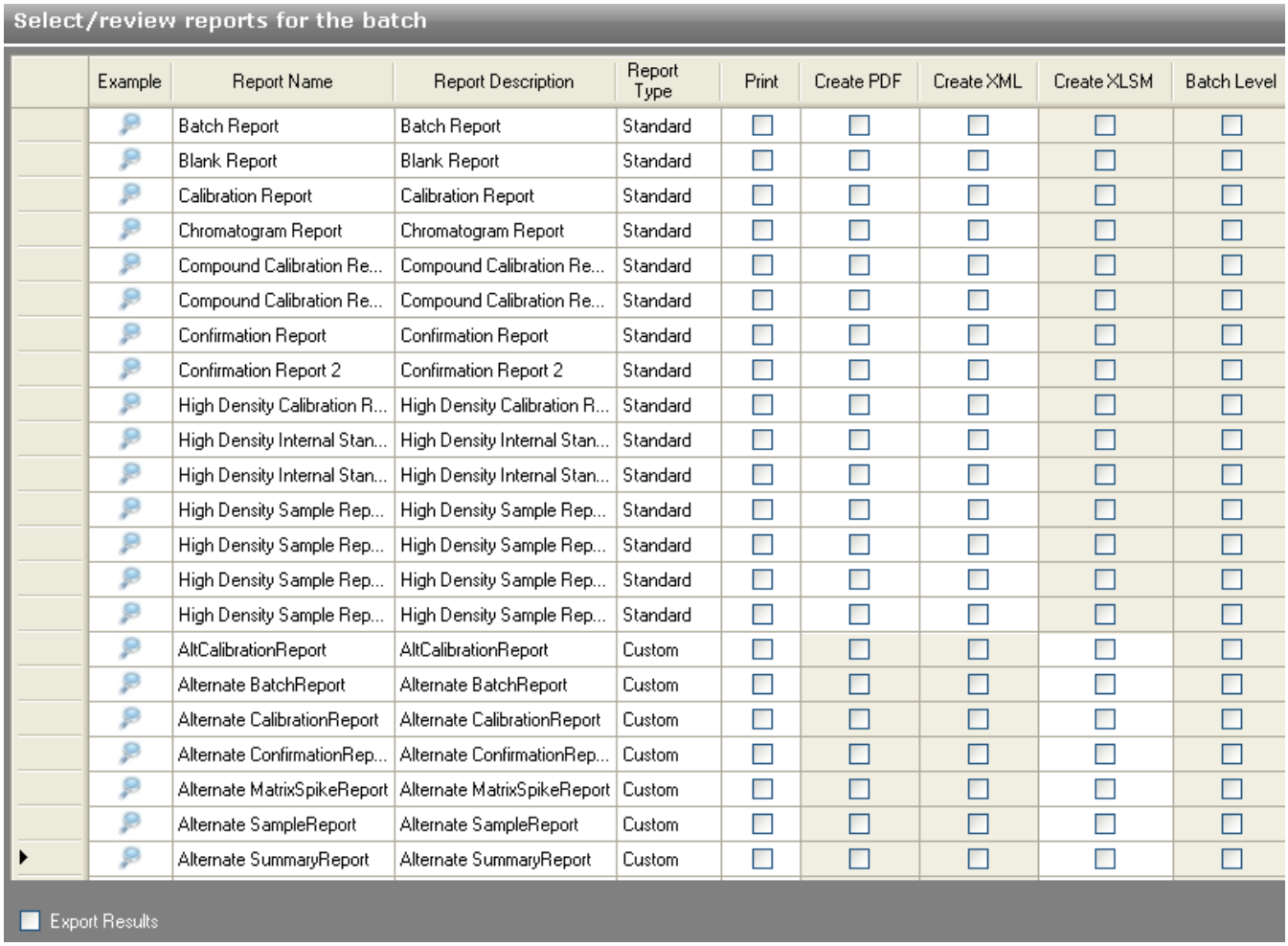


Table 54. Report Selection parameters (Sheet 1 of 2)

Parameter	Description
	Displays an example PDF for the report type. This example provides a model of the report type only; it does not reflect your specific data. This is available for standard reports only.
Report Name	The name of a report.
Report Description	User-editable title to be used on a report.
Report Type	The type of report: Standard, Custom, or Target Screening.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files. Available only for standard reports.
Create XML	Reports to be exported in XML format. Available only for standard reports.

Table 54. Report Selection parameters (Sheet 2 of 2)

Parameter	Description
Create XLSM	Reports to be exported in Excel Macro-Enabled Workbook (.xlsm) format. Available only for custom reports.
Batch Level	Rather than creating separate reports for each sample, the application uses a composite of the data from all the samples to create a single report for the entire batch. Batch-level reports are prepended with a **B** to differentiate them. You cannot select this option from the Report Selection page. You must select the Batch Level option for the report in the report configuration. See "Specifying the Reports Configuration" on page 58.
Shortcut menu: Copy Down	Copies the selected or cleared state to all subsequent reports in the column.

Submitting the Batch

In 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 acquire and process data and optionally create reports. See "Finish view" on page 244.

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.

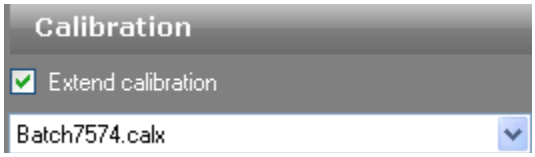
   The TraceFinder application runs this method before running the batch. No autosampler injection takes place. This feature is not available for all instruments.

2. (Optional) Select a method from the System Shutdown Method list.

   The TraceFinder application runs this method after running the batch. 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.



Note You must acquire at least one batch with the current method to create a .calx calibration file.

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 55. Instrument states

Instrument state	Description
Turn Device On	Keeps the system in the On state when the current run finishes, 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 finishes, 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 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 finishes. The Off state indicates that all power to the instrument, which the TraceFinder application can control, 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.
Instrument status indicators	
	Green indicates that the device is turned on or is running.
	Yellow indicates that the device is in standby mode or is waiting for contact closure.
	Red indicates that the device is turned off or that there is an error with the device.

❖ 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 **Submit**.

   The Submit Options dialog box opens. For a detailed description of the parameters, see "Submit Options dialog box" on page 241.

2. (Optional) Select the **Create Reports** check box.

   Note By default, the application acquires and processes data when you submit the batch.

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 will initiate communication with the other instruments.

   This is usually the autosampler.

5. (Optional) Select the **Start When Ready** check box, which starts 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 with multiplexing enabled) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.

7. (Optional without multiplexing enabled) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   - **Next Available Batch** places the batch immediately after the currently acquiring batch.
   - **Next Available Sample** places the batch immediately after the currently acquiring sample.

8. (Optional) Click **Cancel** to exit the Acquisition mode without performing any tasks.

9. 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 67. Submit Options dialog box

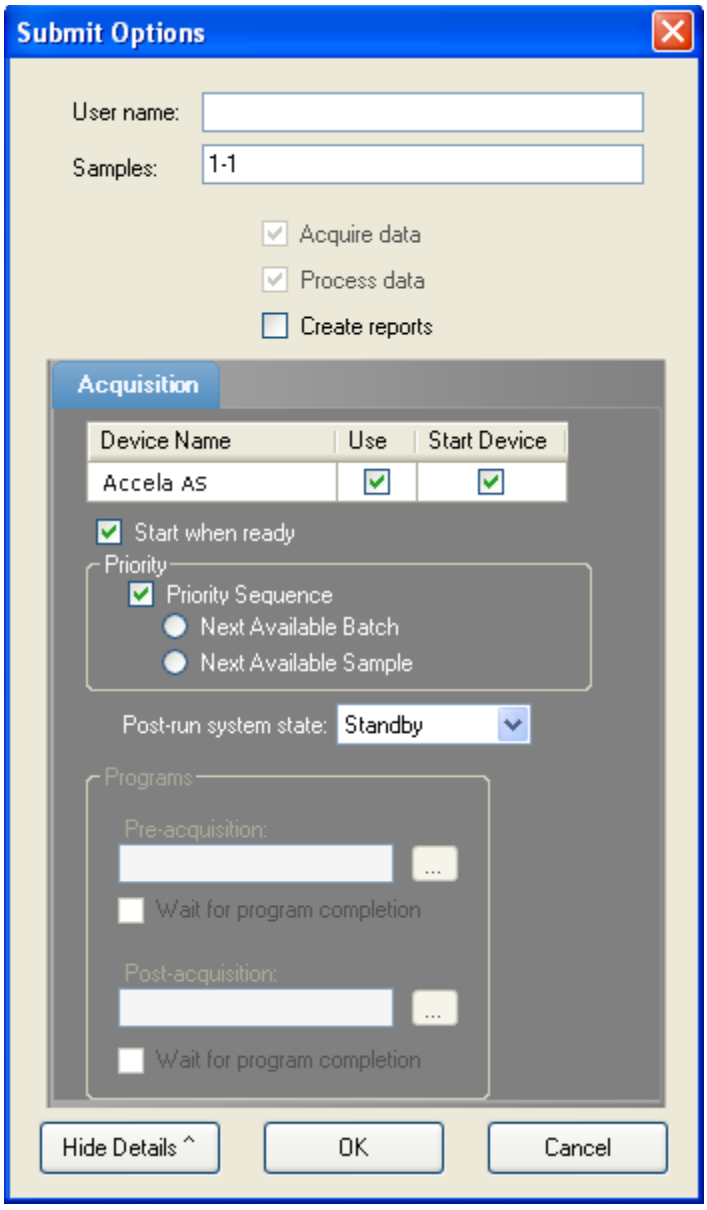


Table 56. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Acquire Data	(Default) Submits the current batch to acquisition.
Process Data	(Default) Processes the data for the current batch.
Create Reports	Creates reports for the current batch.

Table 56. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
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.
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 Sequence	With multiplexing enabled, places the batch immediately after the currently acquiring batch. Without multiplexing enabled, specifies one of the following priority options to place the batch in the queue: • **Next Available Batch** places the batch immediately after the currently acquiring batch. • **Next Available Sample** places the batch immediately after the currently acquiring sample.
Post-run system state	Specifies the system state after it acquires the last batch. On (default), Standby, or Off.
Programs	
Pre-acquisition	
Post-acquisition	
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 subproject folder with the file extension .tbr (to be run):

  …\TraceFinder\1.1\Projects*projectname**subprojectname*

- For each acquired sample, the application writes an RSX file to the batch Data folder:

  …*projectname**subprojectname**batchname*\Data

- The application saves method information to the batch Methods folder:

  …*projectname**subprojectname**batchname*\Methods*methodname*

- The application writes the reports to the batch Reports folder:

  …*projectname**subprojectname**batchname*\Reports

Figure 68. Finish view

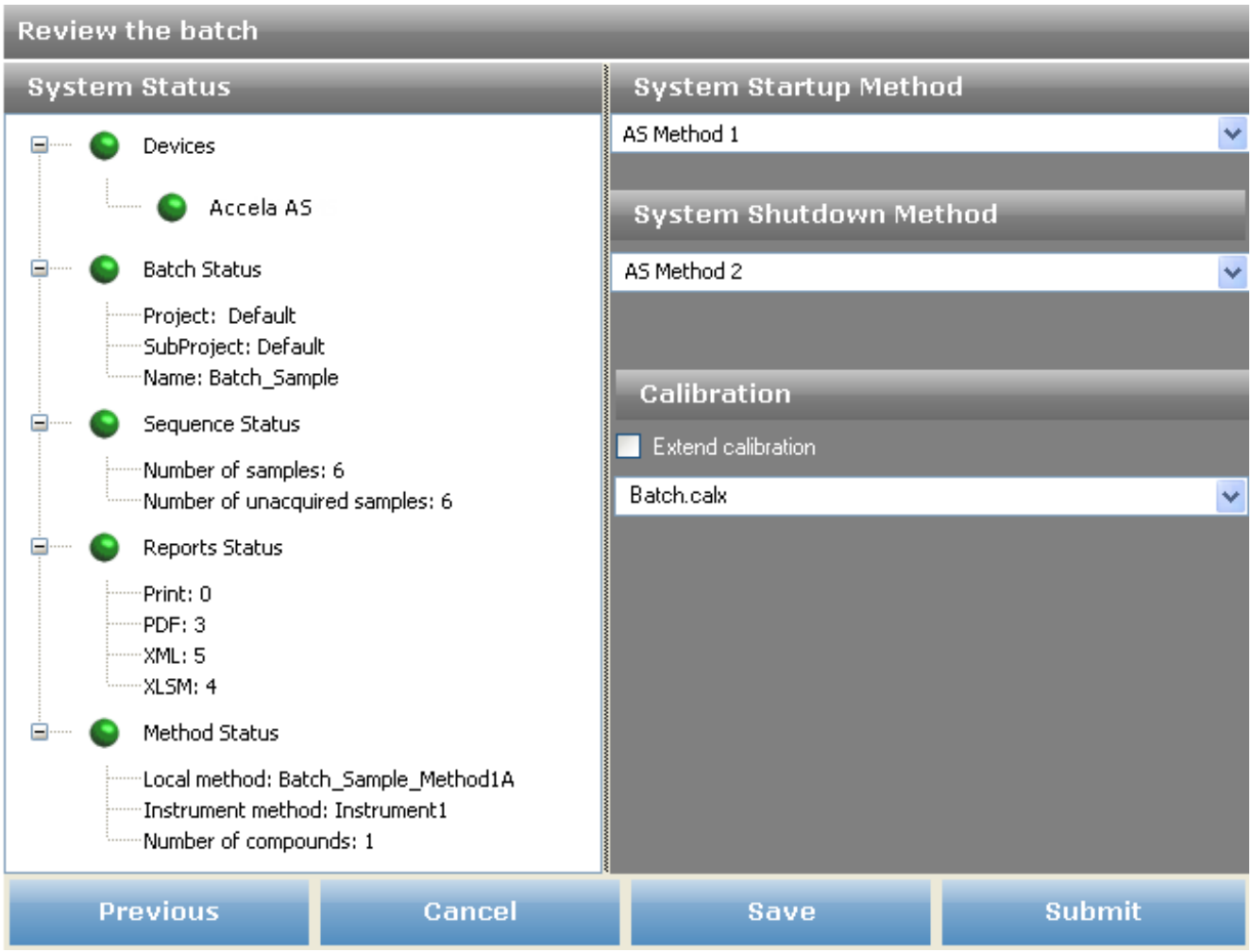


Table 57. Finish view parameters (Sheet 1 of 2)

Parameter	Description
System Status	The System Status pane displays the following: • Devices used for the acquisition • Project, subproject, and name of the batch • Number of samples in the batch • Number of standard and custom reports to be printed and saved as PDF, XML, or XLSM files • Local method and instrument method used for the batch • 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 57. 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.
Submit	Opens the Submit Options dialog box where you can optionally choose to generate 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**.

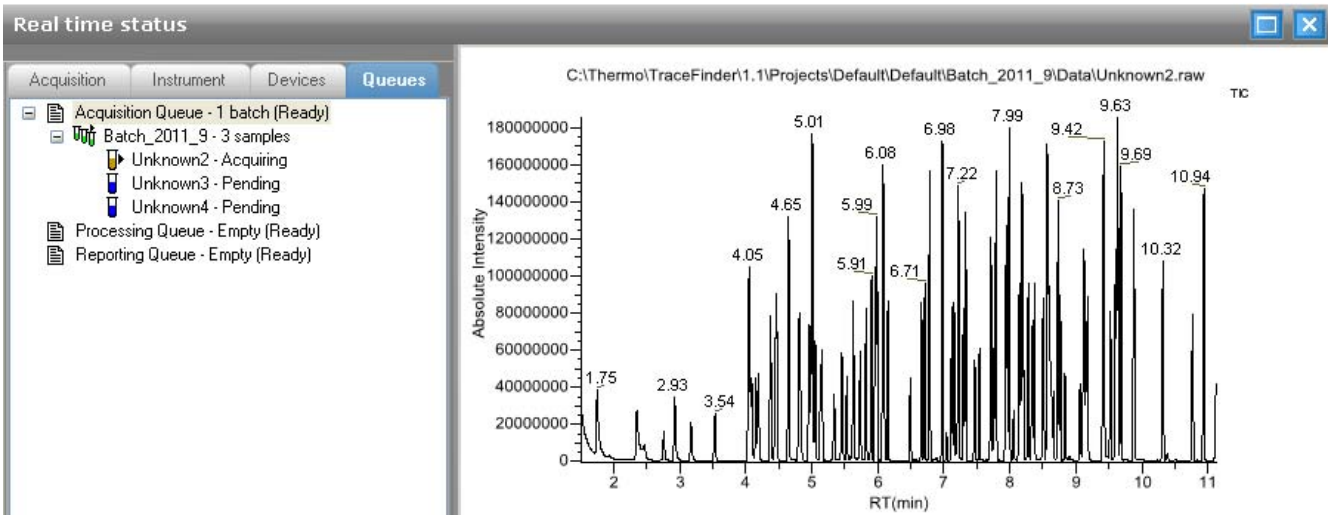
The real-time status displays at the bottom of the dashboard.

❖ **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.

Figure 69. Real Time Status display

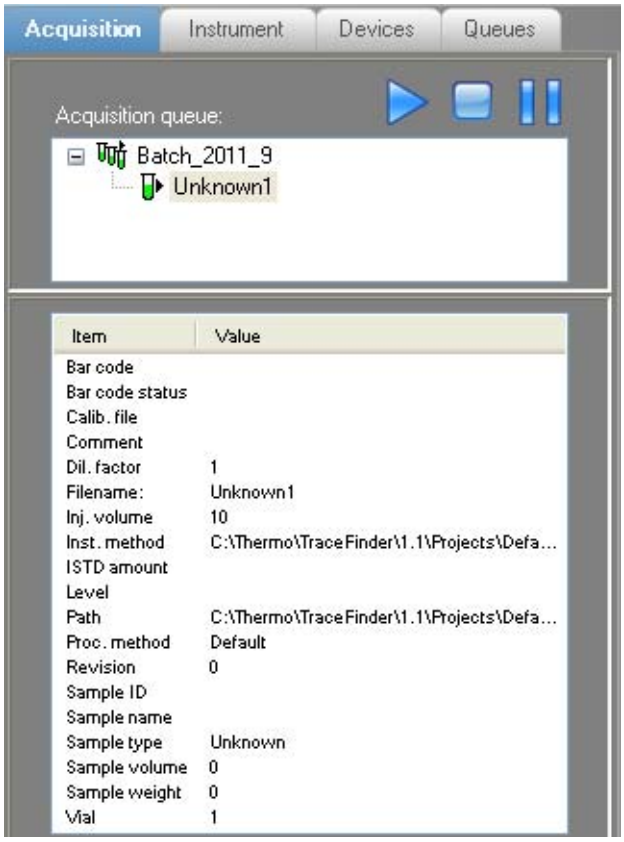


The real-time status display has four pages of information and a real-time trace pane:

- Acquisition Page
- Instrument Page
- Devices Page
- Queues Page
- Real-time Trace Display

Acquisition Page

Use the Acquisition page to monitor the progress as the application acquires the samples.

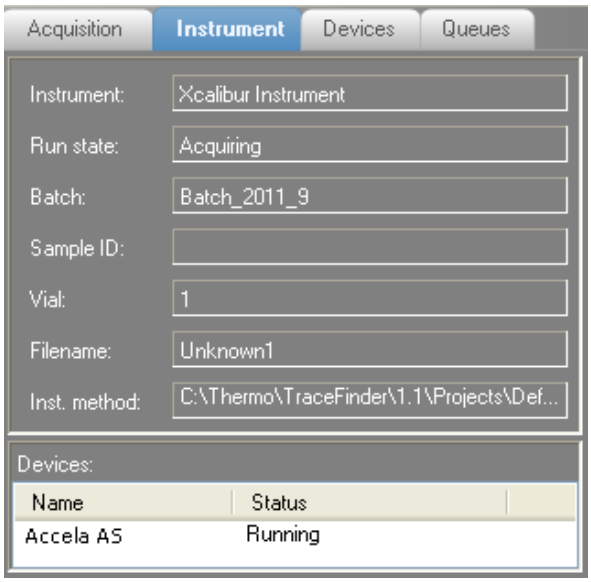


❖ **To pause or stop the batches in the queue**

Use the **Start**, , **Stop**, , or **Pause**, , buttons to control batches in the Acquisition queue.

Instrument Page

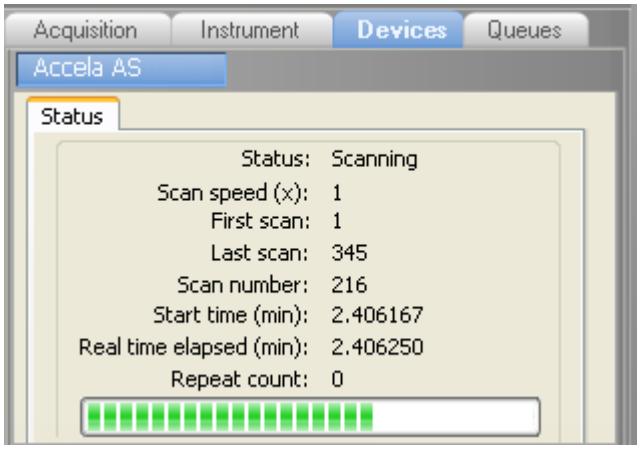
Use the Instrument page to monitor the currently acquiring sample.



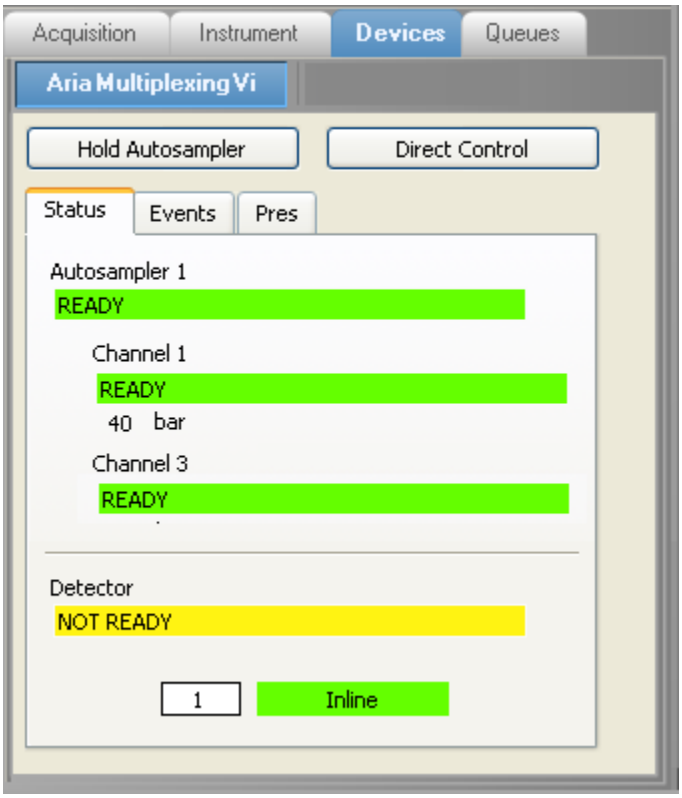
Devices Page

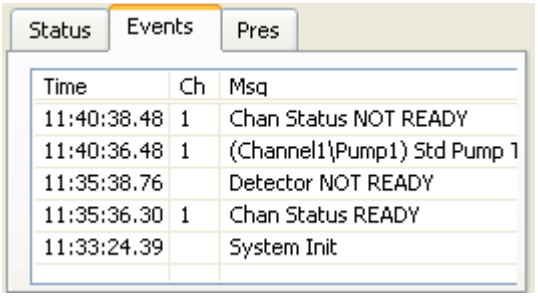
Use the Devices page to monitor the status of the instrument. The feedback you see on the Devices page depends on the instrument you are using. The following examples show an Accela autosampler and an Aria multiplexing device.

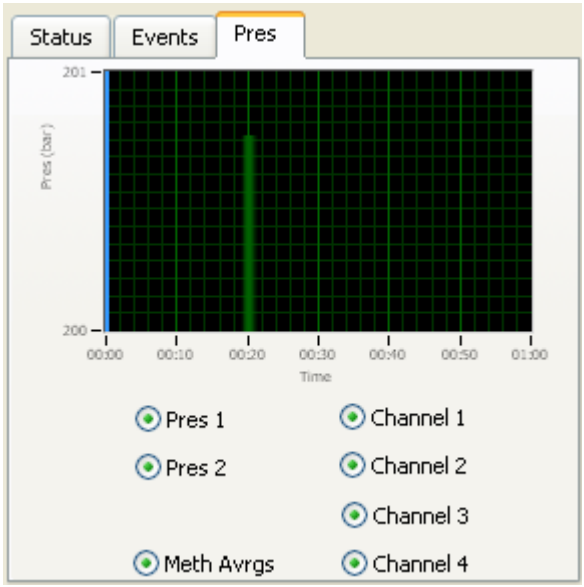
Accela Autosampler Feedback



Aria Multiplexing Feedback







Use the following procedures:

- To pause the autosampler
- To access the Aria multiplexing controls
- To control the channels
- To view the pressure trace

❖ To pause the autosampler

1. Click **Hold Autosampler**.

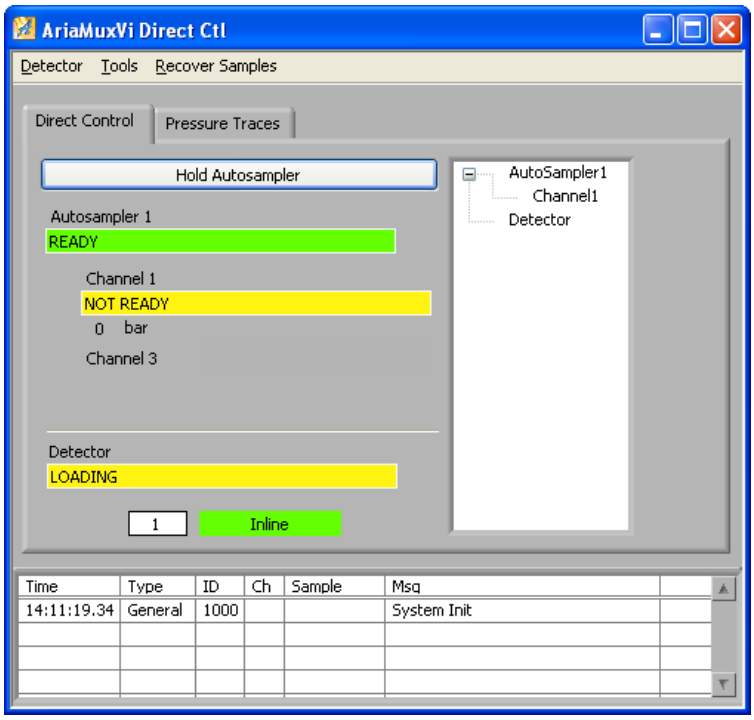
   The autosampler finishes the current autosampler step and then pauses. The LC pumps and autosampler continue.

2. To restart the autosampler, click **Hold Autosampler** again.

❖ To access the Aria multiplexing controls

Click **Direct Control**.

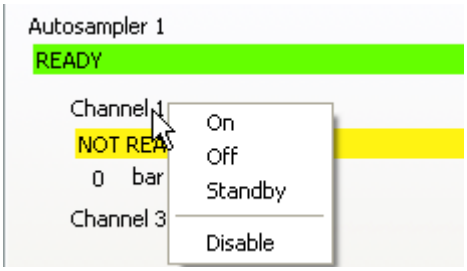
The AriaMuxVi Direct Ctl dialog box opens.



For a detailed description of the features in this dialog box, refer to the *Transcend Systems with Xcalibur Software User Guide*.

❖ To control the channels

Right-click the channel name and choose a command from the shortcut menu.

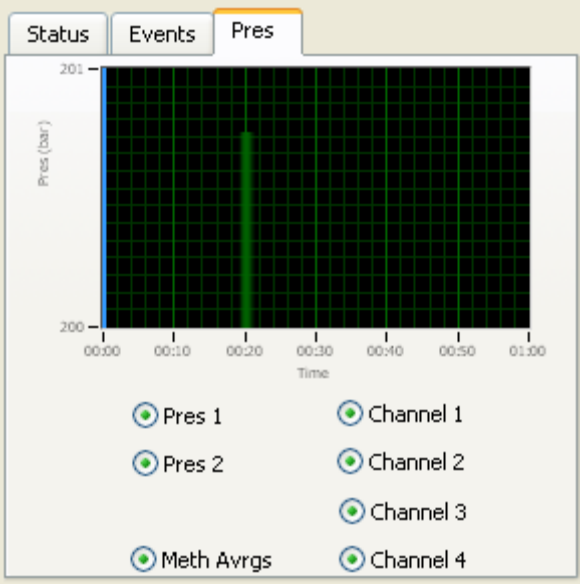


Parameter	Description
On	Turns on a stopped pump and continues acquiring the sample list assigned to that channel.
Off	After the current sample completes, the application stops acquiring and the pump shuts down.
Standby	After the current sample completes, the application stops acquiring. The pump continues to run.
Disable / Enable	• **Disable** prevents the channel from receiving samples. When you choose **Disable** during a run, the application finishes the current sample on the channel and then stops. • **Enable** allows the channel to receive samples. When you disable a channel that is set to **On**, the channel is highlighted in green and the status is READY. You can turn the channel to **Off** or **Standby**.

❖ To view the pressure trace

1. Click the **Pres** tab.

   The Pressure page displays a pump pressure graph for each sample in the batch. A fluctuation or change in the pump pressure could indicate a change in the chromatography conditions.



2. To view the pressure for a specific pump, select the **Pres 1** or **Pres 2** option.

   By default, the pressure for all pumps are displayed.

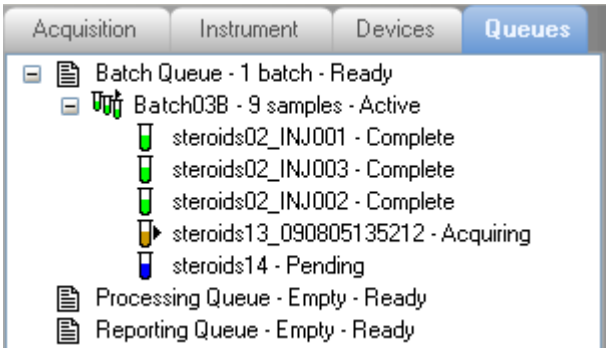
3. To view the pressure for a specific channel, select the corresponding channel number.

   By default, the pressure for all channels is displayed.

Queues Page

Use the Queues page to monitor and control the Acquisition, Processing, and Reporting queues:

- Use the Queue-level Commands to pause or remove batches in any of the queues.
- Use the Batch-level Commands to pause or remove entire batches or samples within batches from any of the queues.



Queue-level Commands

Use the queue-level commands to pause or remove batches in any of the queues on the Queues page.

Use the following procedures:

- To pause all batches in a queue
- To remove a single batch from a queue
- To remove all batches in a queue
- To remove all pending batches

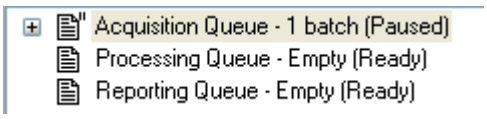
❖ To pause all batches in a queue

1. Select a queue (Acquisition, Processing, or Reporting).

   Note When multiplexing is enabled, as many as four samples can acquiring at once. Pausing the Acquisition queue does not affect any acquiring samples.

2. Right-click and choose **Pause Queue** from the shortcut menu.

   After the current sample completes, the application pauses all batches and samples in the specified queue. Only the selected queue is affected.

3. To restart a paused queue, select the queue, right-click, and choose **Resume Queue** from the shortcut menu.

❖ To remove a single batch from a queue

1. Select a queue (Acquisition, Processing, or Reporting).
2. Right-click and choose **Stop Active Batch** from the shortcut menu.

> **Note** This command is available only when there are active batches in the queue. Paused batches and batches that contain only pending samples are not "active".

The application confirms that you want to remove the active batch from the selected queue. After the current sample completes, the application removes the batch and all pending samples from the queue. Only the selected queue is affected.

❖ To remove all batches in a queue

1. Select a queue (Acquisition, Processing, or Reporting).
2. Right-click and choose **Stop All Batches** from the shortcut menu.

The application removes all batches with pending samples from the selected queue. The current sample continues to acquire. Only the selected queue is affected.

❖ To remove all pending batches

1. Select a queue (Acquisition, Processing, or Reporting).
2. Right-click and choose **Remove Pending Batches** from the shortcut menu.

> **Note** A pending batch is a batch in which all samples are pending. If any sample in the batch is active, the batch is not affected by this command.

The application removes all batches that contain only pending samples. Only the selected queue is affected.

Figure 70. Queue-level shortcut menu

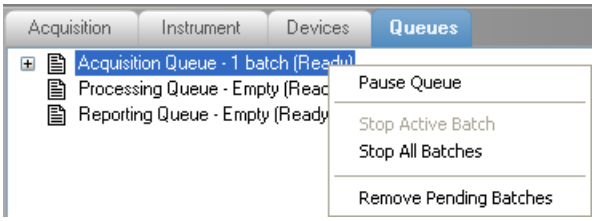


Table 58. Queue-level shortcut menu commands (Sheet 1 of 2)

Parameter	Description
Pause Queue	After the current sample completes, the application pauses the specified queue. Only the selected queue is affected.
Stop Active Batch	Removes all pending samples from the specified queue. The active sample is not affected.

Table 58. Queue-level shortcut menu commands (Sheet 2 of 2)

Parameter	Description
Stop All Batches	Removes all pending samples and batches from the specified queue. The active sample is not affected.
Remove Pending Batches	Removes all pending batches from the specified queue. The active batch is not affected.

Batch-level Commands

Use the batch-level commands to pause or remove entire batches or samples within batches from any of the queues on the Queues page.

Use the following procedures:

- To stop a batch
- To remove a pending batch
- To remove pending samples from a batch
- To remove a single pending sample from a batch

❖ To stop a batch

1. Select an active batch in any of the queues (Acquisition, Processing, or Reporting).

   Note The batch must have at least one active sample and one pending sample.

2. Right-click and choose **Stop Batch** from the shortcut menu.

   The application confirms that you want to remove the selected batch from the queue. After the current sample completes, the application removes the batch and all pending samples from the queue.

❖ To remove a pending batch

1. Select a pending batch in any of the queues (Acquisition, Processing, or Reporting).

   Note A pending batch is a batch in which all samples are pending. If any sample in the batch is active, this command is not available.

2. Right-click and choose **Remove Pending Batch** from the shortcut menu.

   The application confirms that you want to remove the selected batch from the queue and then removes the batch from the queue.

❖ To remove pending samples from a batch

1. Select a batch in any of the queues (Acquisition, Processing, or Reporting).

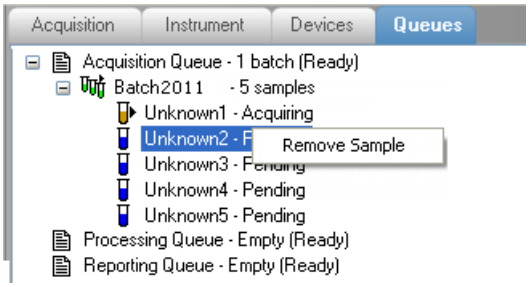
   Note The batch must have at least one pending sample.

2. Right-click and choose **Remove Pending Samples** from the shortcut menu.

   The application confirms that you want to remove all pending samples from the batch and then removes the samples. If the batch includes only pending samples, the application removes the batch from the queue.

❖ To remove a single pending sample from a batch

1. Select a pending sample.
2. Right-click and choose **Remove Sample** from the shortcut menu.



The application confirms that you want to remove the selected sample from the batch and then removes the sample.

Figure 71. Batch-level shortcut menu

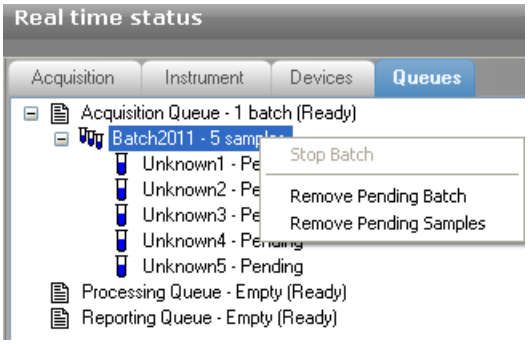
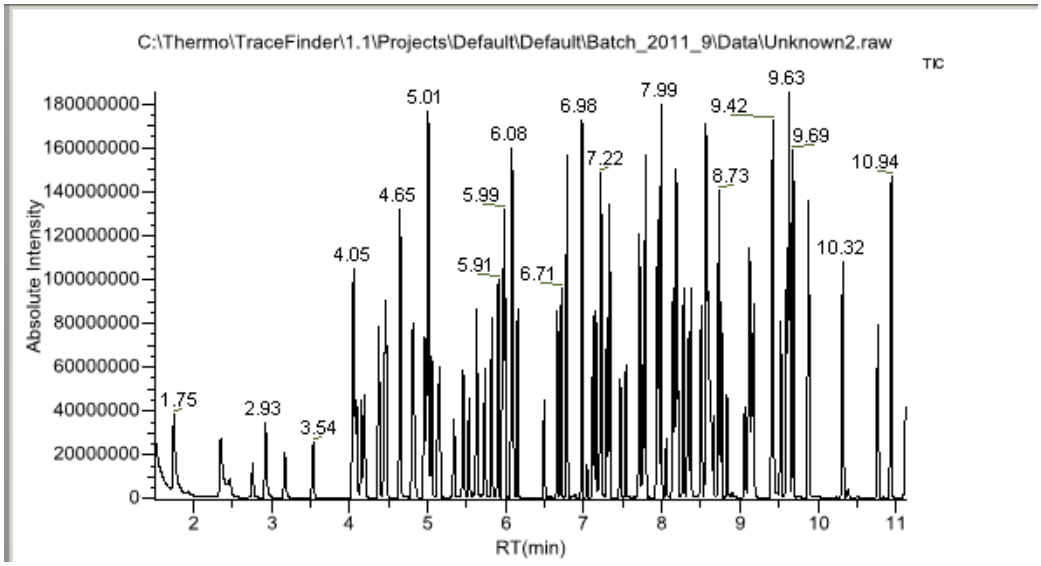


Table 59. Batch-level shortcut parameters

Parameter	Description
Stop Batch	After the current sample completes, the application removes all samples in the selected batch.
Remove Pending Batch	Removes all samples from the selected pending batch.
Remove Pending Samples	Removes all pending samples from the selected batch.

Real-time Trace Display

As each sample acquires, the real-time chromatogram pane shows the retention time and intensity of the TIC trace.

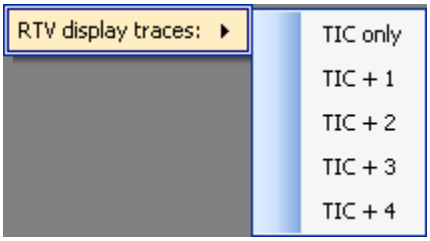


By default, the real-time display shows only the TIC trace as each sample acquires. To observe specific traces, such as the internal standard, use the RTV Display Traces function to display multiple traces.

When you create your method, you can specify additional traces to display in the real-time viewer and in which order the traces are displayed. The application always displays the TIC trace in the top pane. See "Real Time Viewer" on page 156.

❖ To display multiple traces

Right-click in the chromatogram pane and choose the number of traces you want to display.

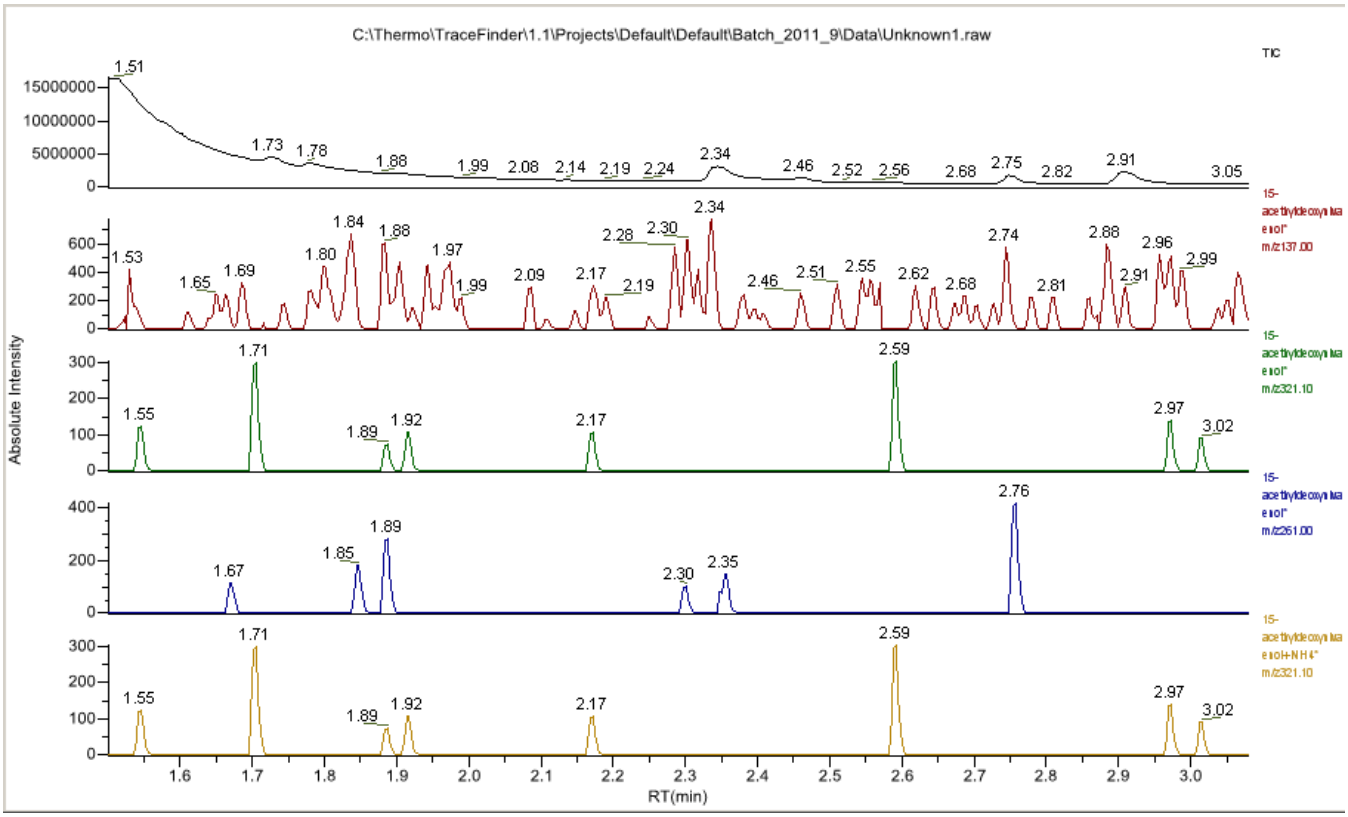


The chromatogram pane displays real-time chromatograms for the selected number of traces.

The TIC is always displayed at the top. When there are more traces than can fit in the pane, you can scroll through the traces.

For each trace, the application displays the mass or precursor mass.

Figure 72. Real-time display with multiple traces



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 60. 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 Chk Std sample, it compares the measured quantity with the expected value and an acceptability range. The quantitative analysis of a Chk Std sample is classified as *passed* if the difference between the observed and expected quantities is within the user-defined tolerance. A Chk Std sample is classified as *failed* if the difference between the observed and expected quantities is outside the user-defined tolerance.
Solvent	Contains only solvent.
Unknown	Used for quantitative analysis of samples.
Unknown/TIC	Used for quantitative and qualitative analysis of samples.
LCS	Lab control sample. (Environmental and Food Safety only)
LCSD	Lab control sample duplicate. (Environmental and Food Safety only)
MDL	Method detection limits sample. (Environmental and Food Safety only)
Method Val	Method validation sample. (Environmental and Food Safety only)
MS	Matrix spike sample. (Environmental and Food Safety only)
MSD	Matrix spike duplicate sample. (Environmental and Food Safety only)

Using the Data Review Mode

This chapter includes instructions for using the features of the Data Review mode.

Contents

- Working in Batch View
- Working in Data Review View
- Working in Report View
- Working in the Local Method View

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 and process data and optionally create reports for the submitted samples.

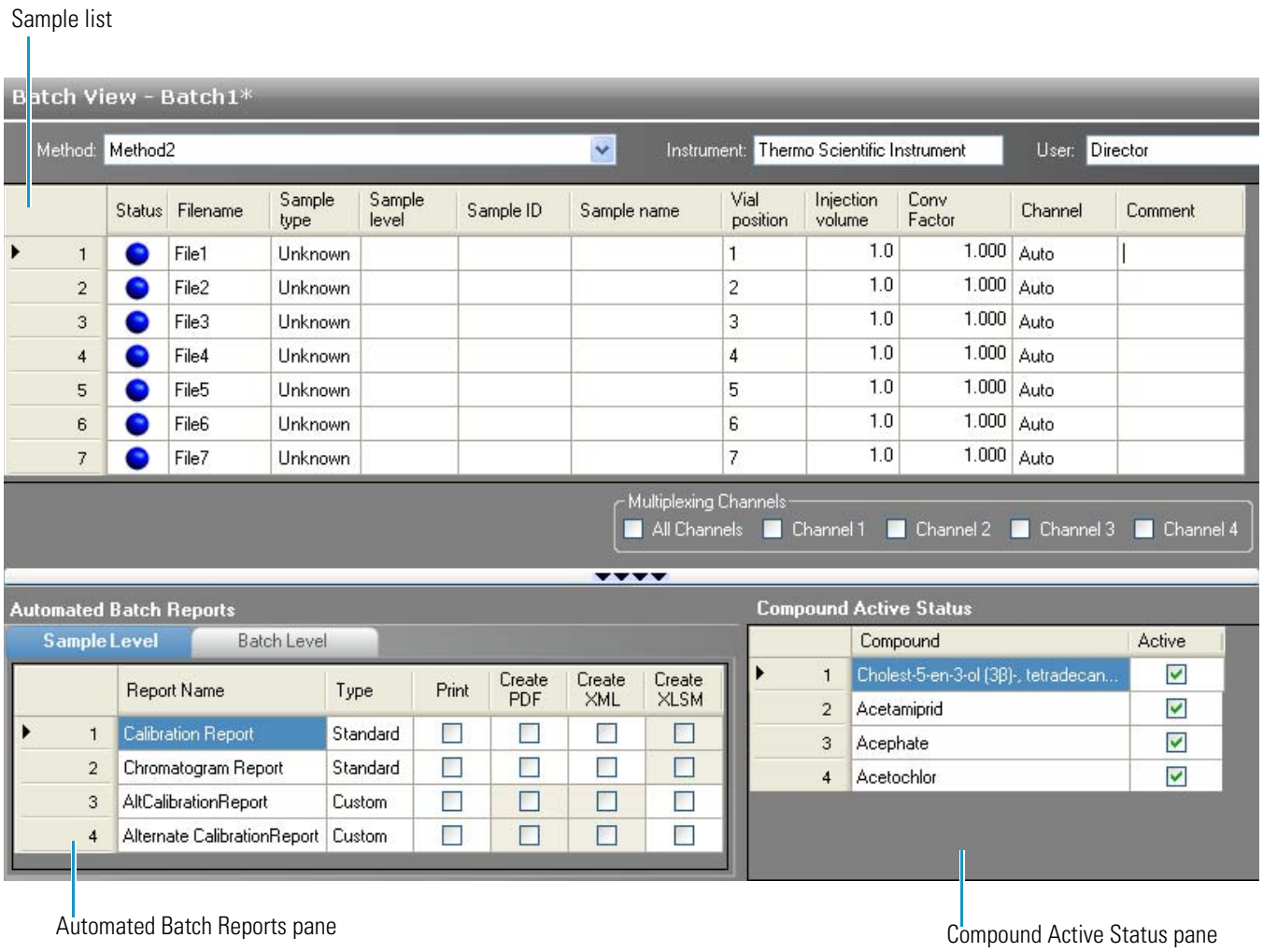
This section contains information about the following topics:

- Batch View Panes
- Creating a New Batch
- Editing a Batch
- Editing Report Output Formats
- Submitting a Batch

Batch View Panes

The Batch View is divided into three panes:

- Use the sample list to create a batch. See "Creating a New Batch" on page 264.
- Use the Automated Batch Reports pane to select the type of output formats you want to generate for the reports. See "Editing Report Output Formats" on page 274.
- Use the Compound Active Status pane to make specific compounds active or inactive. See "Setting Compound Active Status" on page 276.



Tip To resize the panes, drag the separators that divide the panes.

Creating a New Batch

In the Batch View, you can create a new batch.

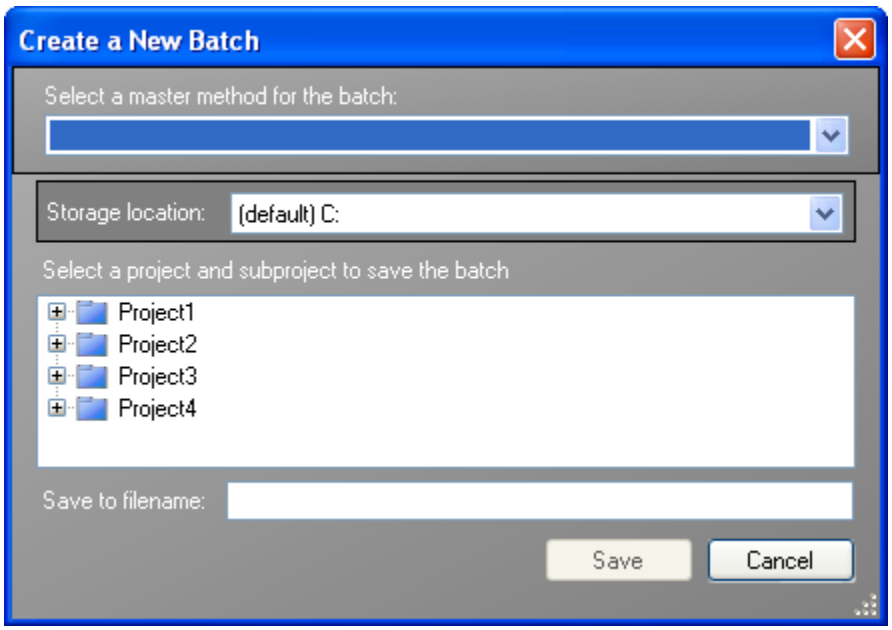
Use the following procedures:

- To create a new batch
- To add samples to the list
- To insert samples into the list
- To import samples into the list
- To remove samples from the list
- To copy a sample
- To reinject a sample
- To edit sample values
- To customize the column display
- To temporarily customize the column display

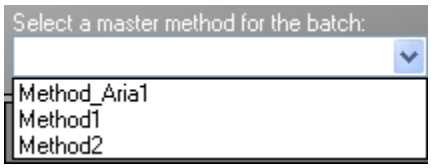
❖ To create a new batch

1. Click **New Batch** in the Batch View task pane or choose **File > New > Batch**.

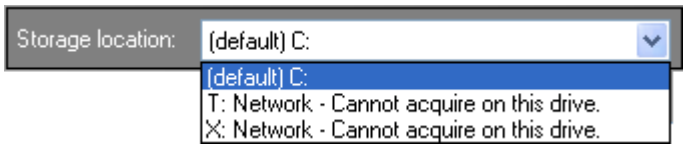
   The Create a New Batch dialog box opens.



2. Select a master method from the Method list.



3. Select a drive from the Storage Location list.



The project list displays all projects, subprojects, and batches on the selected drive.

Tip The application does not display drives that do not have a project and subproject.

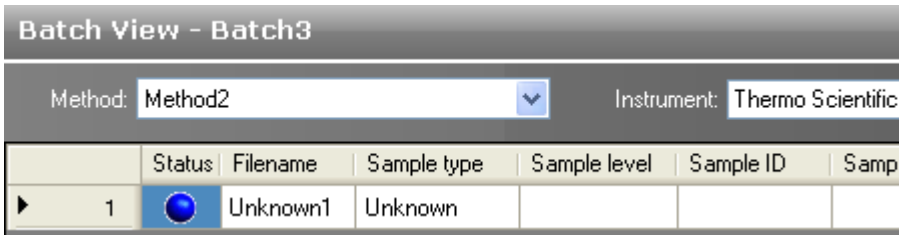
You cannot use network drives to acquire data. For more information about network drives, see "Working with Drives" on page 40.

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**.

A new, unnamed batch opens with one Unknown sample.



❖ To add samples to the list

1. To add a single sample row, right-click the sample list and choose **Add Sample** from the shortcut menu.

2. To add multiple sample rows, select the number of rows and then click the **Add Sample** button,

The application adds the specified number of new, empty samples to the end of the sample list.

❖ To insert samples into the list

Select the sample above which you want to insert unknown samples, and do one of the following:

- To insert a single sample row, right-click and choose **Insert Sample** from the shortcut menu.
- To insert multiple sample rows, select the number of rows and then click the **Insert Sample** button

.

The TraceFinder application inserts a new, empty sample or samples above the selected sample.

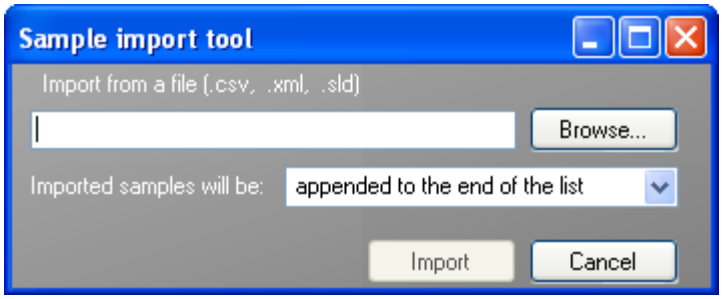
Inserted samples

	Status	Filename	Sample type	Sample level	Sample ID
1		cal_std_5	Cal Std	10	cal std = 5 ng/uL
2		Unknown2	Unknown		
3		Unknown1	Unknown		
4		cal_std_10	Cal Std	10	cal std = 10 ng/uL

❖ To import samples into the list

1. Choose **Batch > Import Samples** from the main menu, or click the **Import Samples** button,
.

   The Sample Import Tool dialog box opens.



   From this dialog box, you can import samples from a .csv, .xml, or .sld file.

2. Click **Browse** and select a .csv, .xml, or .sld 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.

When you import samples from an Xcalibur sequence file (.sld), the TraceFinder application makes the following column name substitutions:

Xcalibur column	TraceFinder column
Level	Sample Level
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conv Factor

When you import samples from an Xcalibur sequence file (.sld), the TraceFinder application makes the following sample type substitutions:

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	Chk Std
Std Bracket	Cal Std

5. (Optional) When using multiplexing, select a channel for each imported sample.

   Imported samples default to Auto.

❖ 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.

❖ 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 TraceFinder application inserts the copy above the selected sample.

❖ To reinject a sample

1. In the sample list, select the sample you want to reinject.
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 reinjections 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, do one of the following:

   Double-click the Filename column and type a file name.

   –Or–

   Right-click and choose **Browse in Raw File** from the shortcut menu and locate a raw data file to use for the sample.

2. For each sample, click the Sample Type column and select a sample type from the list.

Available Environmental and Food Safety sample types		
Matrix Blank	Solvent	Unknown/TIC
Cal Std	Chk Std	Unknown
LCS	MDL	MS
LCSD	Method Val	MSD

Available General Quantitation sample types		
Matrix Blank	Unknown/TIC	Unknown
Cal Std	Chk Std	Solvent

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 are 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 click **Update**.

   For detailed instructions, see Chapter 4, “Using the Method Development Mode.”

4. Enter or edit the values for the remaining columns.

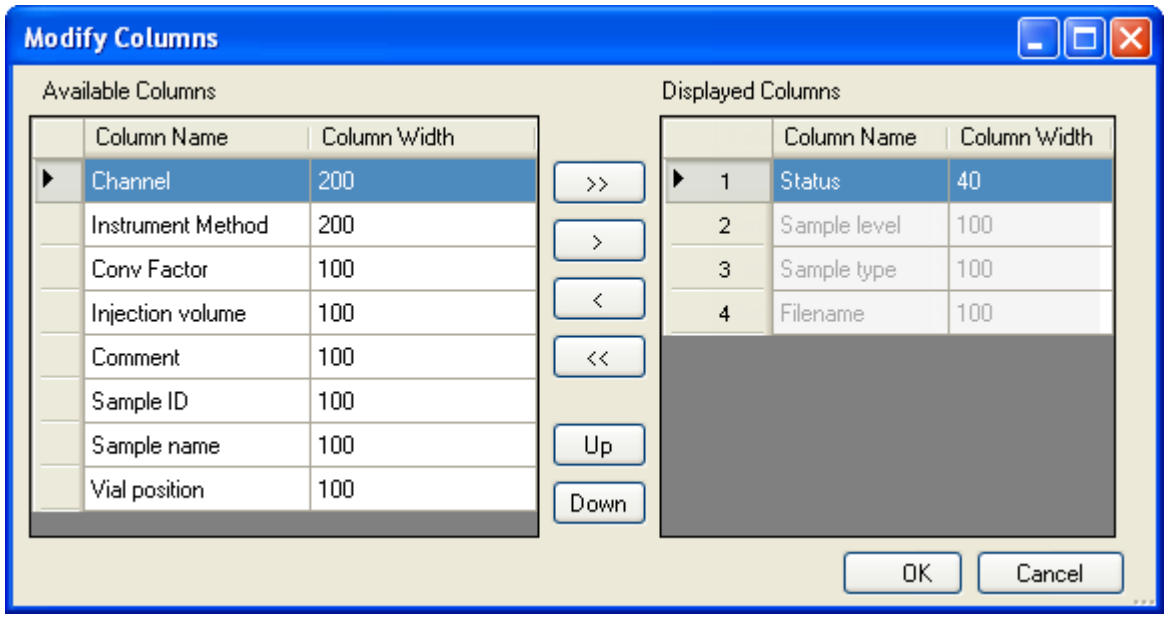
   When you use the scroll bar at the bottom of the samples list, the Status, Flags, Filename, and Sample Type columns remain fixed and only the other columns scroll right and left.

   For instructions to automatically copy or fill values in these columns, see Appendix B, "Using Copy Down and Fill Down."

❖ To customize the column display

1. Right-click the Batch View sample list and choose **Modify Columns** from the shortcut menu.

   The Modify Columns dialog box opens.



Parameter	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
<	Moves the selected column to the Available Columns pane. You cannot move the Status, Sample Level, Sample Type, or Filename columns.
<<	Moves all columns except Status, Sample Level, Sample Type, and Filename to the Available Columns pane.
Up	Moves the selected column name in the Displayed Columns pane one row up in the column order. You cannot move the Status, Sample Level, Sample Type, or Filename columns.
Down	Moves the selected column name in the Displayed Columns pane one row down in the column order. You cannot move the Status, Sample Level, Sample Type, or Filename columns.

2. Use the arrow buttons to move all the columns you want to display to the Displayed Columns pane.

   All the columns you select are displayed after the Status, Sample Level, Sample Type, and Filename columns.

3. To arrange the order of the columns, do the following:

   a. In the Displayed Columns pane, select a column name.

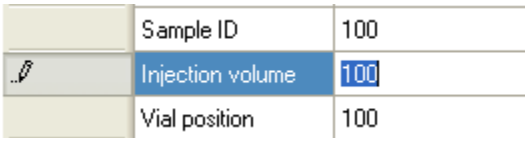
   b. Use the **Up** and **Down** buttons to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Batch View sample list; the last column in the list represents the rightmost column in the Batch View sample list.

      Note You cannot move the Status, Sample Level, Sample Type, or Filename columns.

4. To change the width of a column, do the following:

   a. In the Displayed Columns pane, select the column width.

   b. Type a new value for the width.

5. When you have completed your changes, click **OK**.

   The columns in the sample list immediately reflect your changes. The application uses these settings for all sample lists in the Batch View.

   You can use the drag-and-drop method to temporarily reorder the columns in your sample list, but you cannot save this order. When you restart the TraceFinder application, the Batch View displays your columns in the order specified in the Modify Columns dialog box.

❖ To temporarily customize the column display

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, Sample Level, Sample Type, and Filename columns can be swapped with each other, but they must always be the first four columns in the sample list.

   You cannot save these changes. When you restart the TraceFinder application, the Batch View displays your columns in the order specified in the Modify Columns dialog box.

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 reinjection. If the batch has unacquired samples when you complete your edits, you can save it as a to-be-run (.tbr) batch.

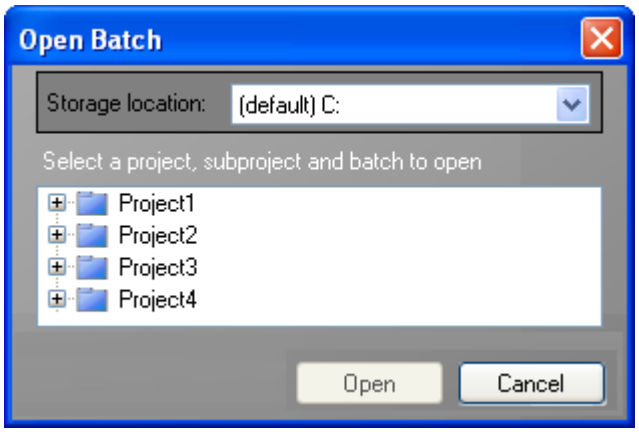
Use the following procedures:

- To open a saved batch
- To open a recent batch
- To edit samples in a batch
- To reinject a sample from a previously acquired batch
- To submit all samples in the batch
- To submit selected samples

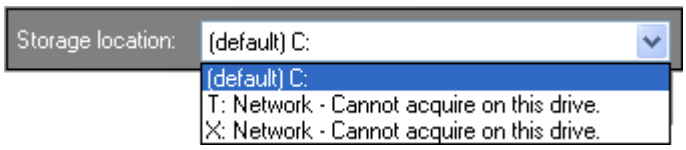
❖ To open a saved batch

1. From the Batch View task pane, click **Open Batch.**

   The Open Batch dialog box opens.



2. Select a drive from the Storage Location list.



   The project list displays all projects, subprojects, and batches on the selected drive.

3. Select a project, subproject, and batch.
4. Click **Open**.

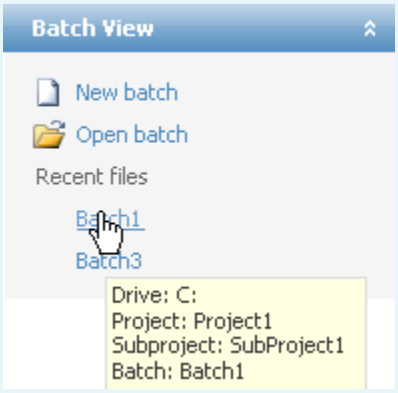
   The selected batch opens in the Batch View.

❖ To open a recent batch

Click a batch name in the Recent Files list.

The selected batch opens in the Batch View.

Tip To view the drive, project, and subproject for a recent batch, hold your cursor over the batch name.



❖ To edit samples in a batch

Use the commands described in "Working in Batch View" on page 262.

You can edit samples, add new samples, reinject acquired samples, or delete samples.

❖ To reinject a sample from a previously acquired batch

1. In the sample list, select the sample you want to reinject.
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 reinjections of the same sample are numbered INJ002, INJ003, and so forth.

The TraceFinder application copies all parameter values from the original sample.

A green status icon indicates previously acquired samples (acquired and processed), and the sample name is grayed out. A blue status icon indicates samples created for reinjection (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

When you submit all samples in this batch, all samples (including previously acquired samples) are acquired.

3. To save this batch with the new samples for reinjection, 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 submit the batch. All submitted samples—both the reinjection samples and the previously acquired samples—are acquired. The application appends a timestamp to the acquired raw data files to differentiate each acquisition.

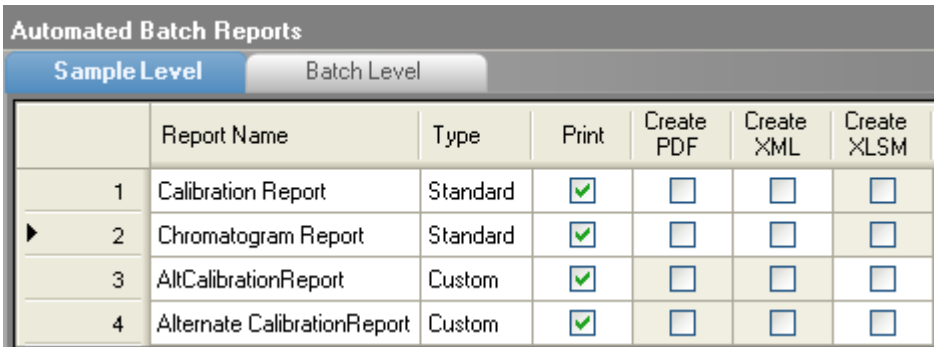
Editing Report Output Formats

In the Automated Batch Reports pane, you can view the reports that are selected for this batch and modify which output formats are generated for each report.

❖ To edit the sample-level output formats

1. Click the **Sample Level** tab.

   The application displays reports and the output formats as they were specified in the method.



	Report Name	Type	Print	Create PDF	Create XML	Create XLSM
1	Calibration Report	Standard	☑	☐	☐	☐
2	Chromatogram Report	Standard	☑	☐	☐	☐
3	AltCalibrationReport	Custom	☑	☐	☐	☐
4	Alternate CalibrationReport	Custom	☑	☐	☐	☐

   For detailed instructions for specifying which reports and output formats are generated, see "Specifying the Reports Configuration" on page 58.

2. Select or clear any of the check boxes for your reports.

3. To duplicate an output format for all reports for this sample, 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. This action applies only to report types for which this output format is available.

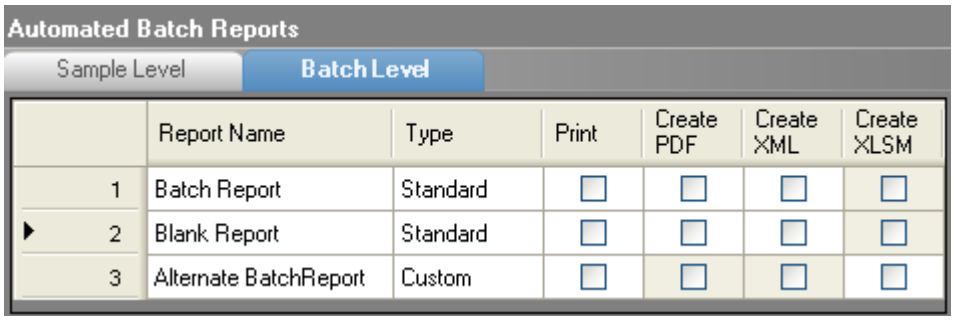
4. To duplicate the output format for all samples in the batch, right-click the cell and choose **Apply Selection to All Samples** from the shortcut menu.

   This action applies only to report types for which this output format is available.

❖ To edit the batch-level output formats

1. Click the **Batch Level** tab.

   The application displays the reports and the output formats as they were specified in the method.



   For detailed instructions for specifying which reports and output formats are generated and which reports are batch-level, see "Specifying the Reports Configuration" on page 58.

2. Select or clear any of the check boxes for your reports.

3. To duplicate the output format 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. This action applies only to reports for which this output format is available.

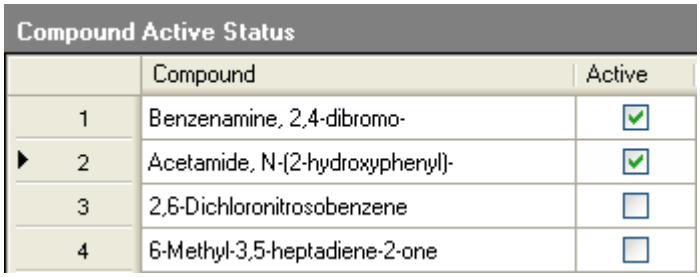
Setting Compound Active Status

In the Compound Active Status pane, you can choose specific compounds to be active or inactive.

❖ To set a compound as active or inactive

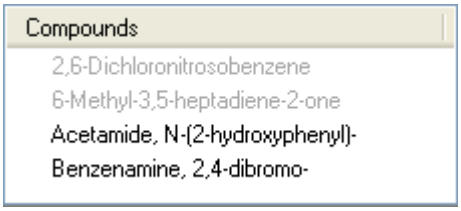
1. In the samples list, select a sample.

   All compounds in the selected sample are listed in the Compound Active Status pane. The default active/inactive status is determined by the settings in the local method. See "Identification" on page 119.



2. Select or clear the Active check box for the compound.

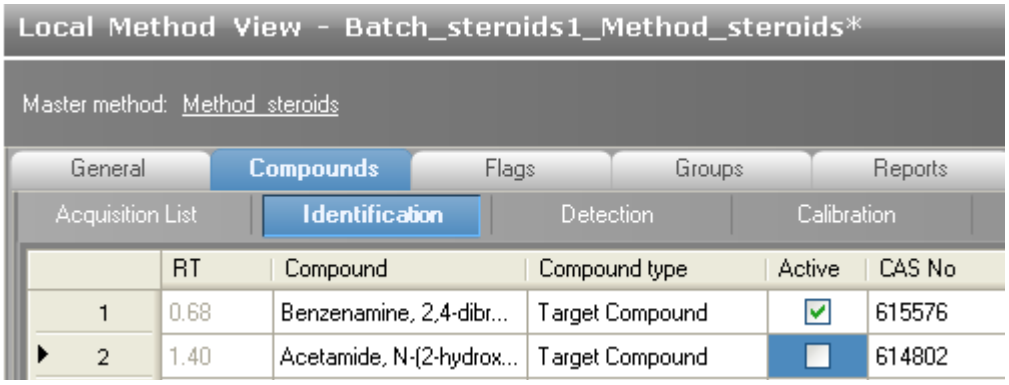
   When you specify a compound as inactive in this pane, it becomes inactive in the Compounds pane in the Data Review view. Inactive compounds are grayed out:



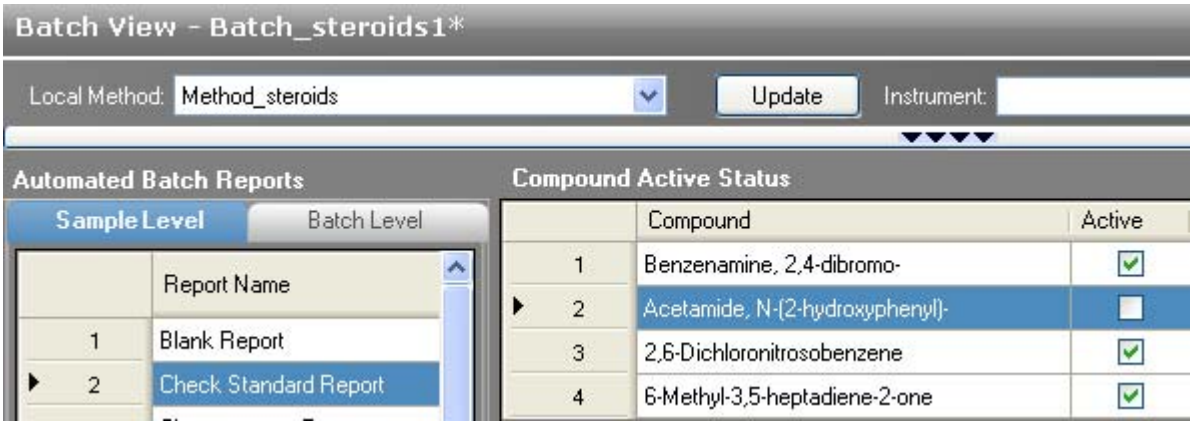
   For instructions for changing the active/inactive status in the Data Review view, see "Inactive and Excluded Compounds" on page 290.

Compound Active/Inactive Status

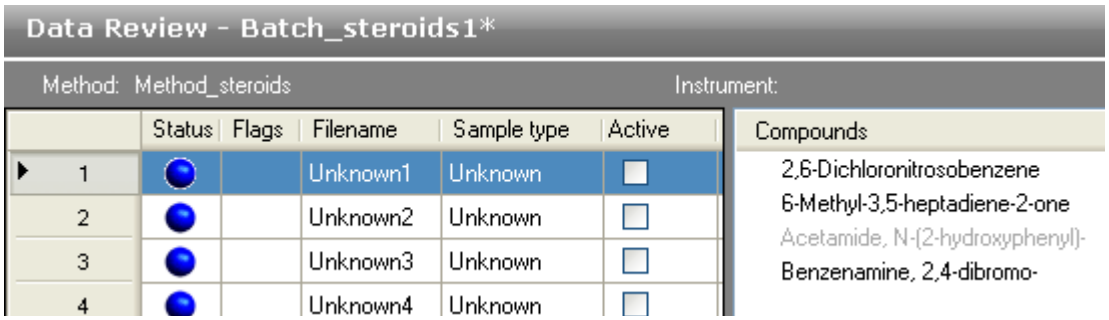
You can specify which compounds are active or inactive in the Local Method View, the Batch View, or the Data Review view.



For details about the setting the status on the Identification page, see "Identification" on page 119.



For details about setting the status in the Batch View, see "Setting Compound Active Status" on page 276.



For details about setting the status in the Data Review view, see "Inactive and Excluded Compounds" on page 290.

Submitting a Batch

In Batch View, you can submit an entire batch or only selected samples in the batch. When you submit a batch for acquisition and processing, you can choose to create reports for the submitted samples. See "Submit Options dialog box" on page 280.

Use the following procedures:

- To submit all samples in the batch
- To submit selected samples

For a description of commands on the shortcut menu, see "Batch View shortcut menu commands" on page 282.

❖ To submit all samples in the batch

1. Click the **Submit Batch** button, .

   The Submit Options dialog box opens. See "Submit Options dialog box" on page 280.
2. Select the tasks you want to perform: acquire data, process data, or create reports.
3. (Optional) Click **Show Details** to display additional Acquisition parameters.
4. Select the **Use** check box for the device that you want to use for this acquisition.
5. (Optional) Select the **Start Device** check box to indicate the device that will initiate the communication with the other instruments.

   This is usually the autosampler.
6. (Optional) Select the **Start When Ready** check box to have all instruments start together when they are all ready.

   When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
7. (Optional with multiplexing enabled) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.
8. (Optional without multiplexing enabled) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:
   - **Next Available Batch** places the batch immediately after the currently acquiring batch.
   - **Next Available Sample** places the batch immediately after the currently acquiring sample.
9. To start the selected processes, click **OK**.

❖ To submit selected samples

1. Select the samples you want to submit.
2. Click the **Submit Selected Samples** button, .

   The Submit Options dialog box opens. See "Submit Options dialog box" on page 280.
3. Select the tasks you want to perform: acquire data, process data, or create reports.
4. Select the **Use** check box for the device that you want to use for this acquisition.
5. (Optional) Click **Show Details** to display additional Acquisition parameters.
6. (Optional) Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

   This is usually the autosampler.
7. (Optional) Select the **Start When Ready** check box to have all instruments start together when they are all ready.

   When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
8. (Optional with multiplexing enabled) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.
9. (Optional without multiplexing enabled) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:
   - **Next Available Batch** places the batch immediately after the currently acquiring batch.
   - **Next Available Sample** places the batch immediately after the currently acquiring sample.
10. To start the selected processes, click **OK**.

Figure 73. Submit Options dialog box

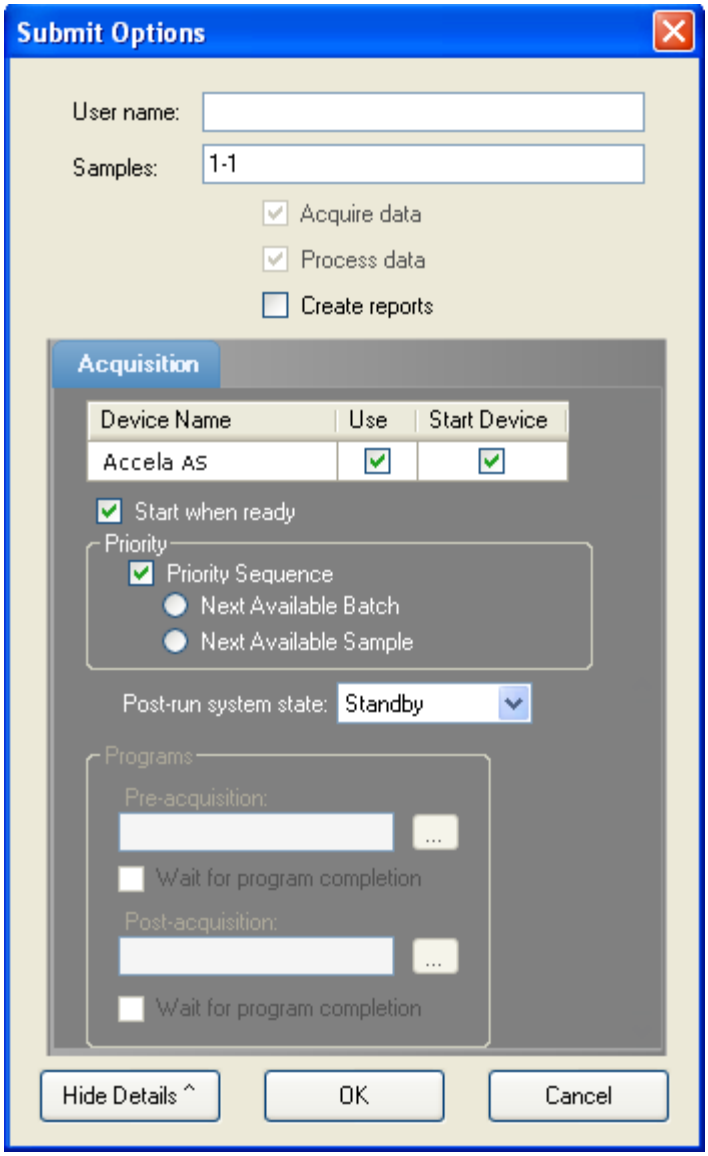


Table 61. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Samples	Reports the batch number and number of samples.
Acquire Data	(Default) Submits the current batch to acquisition.
Process Data	(Default) Processes the data for the current batch.
Create Reports	Creates reports for the current batch.

Table 61. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
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 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 will initiate communication with the other instruments. This is usually the autosampler.
Start When Ready	Starts 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 must wait for the last instrument to be ready.
Priority Sequence	With multiplexing enabled, places the batch immediately after the currently acquiring batch. Without multiplexing enabled, specifies one of the following priority options to place the batch in the queue: • **Next Available Batch** places the batch immediately after the currently acquiring batch. • **Next Available Sample** places the batch immediately after the currently acquiring sample.
Post-run system state	TBD
Programs	TBD
Pre-acquisition	TBD
Post-acquisition	TBD
Buttons	
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.

Figure 74. Batch View

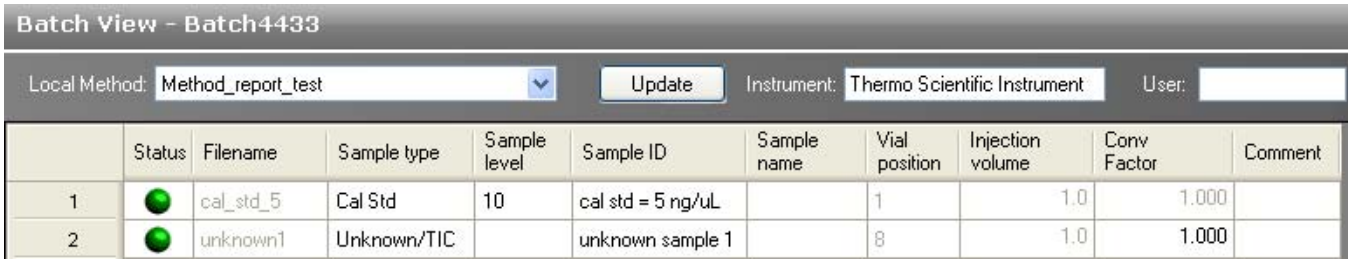
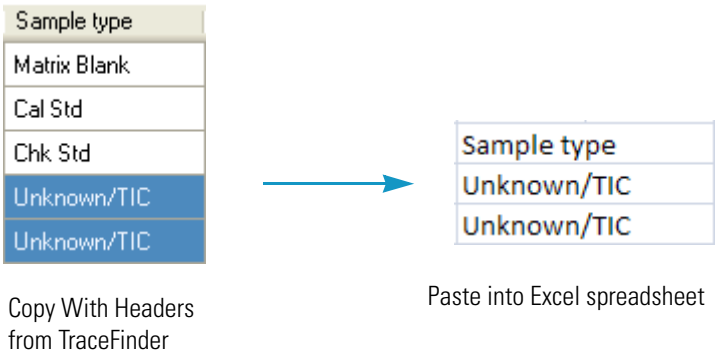


Table 62. Batch View shortcut menu commands (Sheet 1 of 2)

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 selected samples	Creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections 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 266.
Browse in raw file	Opens a dialog box where you can select a raw data file to use for the sample row.
Map raw files to samples	Opens a dialog box where you can select raw data files to use for the sample rows.
Copy down	Copies the value in the selected row to all rows below it. This command is available only when you have selected a value that can be copied 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. This command is available only when you have selected a value that can be filled down.
Modify columns	Opens the Modify Columns dialog box. See "Column Display" on page 286.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information to another application, such as an Excel spreadsheet. You cannot paste this data back into the Batch View sample list.

Table 62. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
Copy With Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information to another application, such as an Excel spreadsheet. You cannot paste this data back into the Batch View sample list. For example:  Copy With Headers from TraceFinder Paste into Excel spreadsheet
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column.
Undo Last Paste	Removes the last pasted item in the Batch View.
Export to CSV file	Opens the Save As dialog box where you can save the current sample list to a .csv file.

Working in Data Review View

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.

The Data Review view uses a samples list and one of two modes: Quan Mode or Qual Mode. The Qual Mode is available only for Unknown/TIC sample types. When you view the data for an Unknown/TIC sample type, you can switch between Qual Mode and Quan Mode.

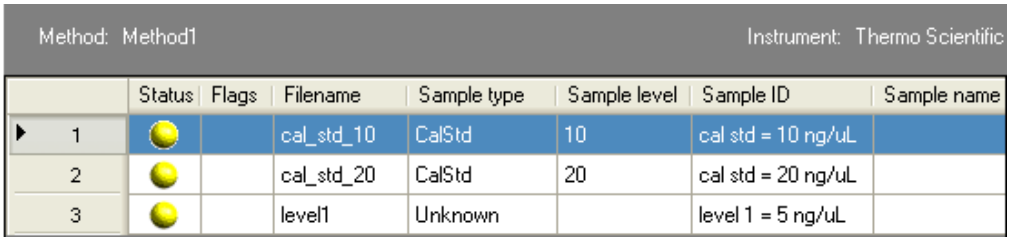
This section includes the following topics:

- Samples List
- Quan Mode
- Qual Mode

Samples List

Use the samples list to select a particular sample. For detailed descriptions of the columns in a samples list, see "Samples list" on page 291.

Status indicators for each sample indicate if the sample is unacquired, acquired, currently acquiring, or processed.



The samples list includes the following features:

- Column Display
- Status Indicators
- Sample Flags
- Compound Flags
- Inactive and Excluded Compounds

The samples list is the same in both Quan Mode and Qual Mode and displays all the quantitative data for the samples of a batch.

- In Quan Mode, the samples list works with the Compounds pane to select a unique sample and compound combination, which then has its textual and graphical values displayed in the Quan Mode pane. The list of compounds that are available for a specific method is displayed in the Compounds pane.

  From the samples list, 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 the appearance of that compound for that particular sample and grays the compound 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.

- In Qual Mode, the samples list works with the peaks pane to select a unique sample and peak combination, which then has its textual and graphical values displayed in the Qual Mode pane.

Column Display

The samples list can contain many columns of information. You can scroll to see all the columns of information, and you can customize which columns you want to display and their display order.

Use the following procedures:

- To scroll the samples list
- Status Indicators
- To customize the column display

❖ To scroll the samples list

Use the scroll bar at the bottom of the samples list to view all the information.

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 temporarily customize the column display

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.

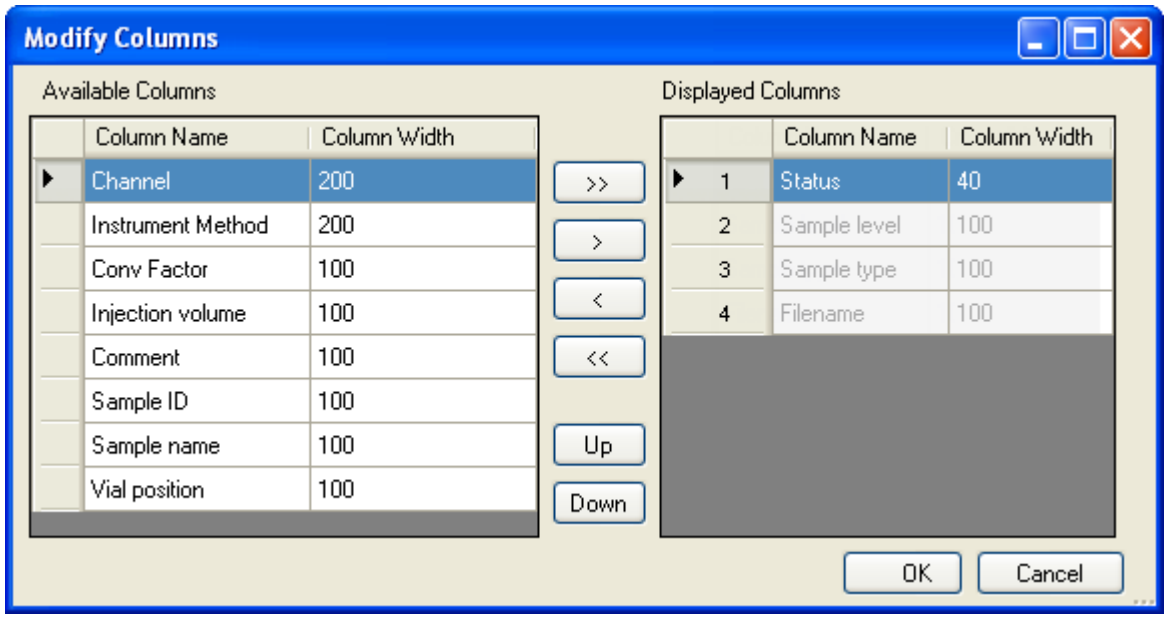
   The Status, Sample Level, Sample Type, and Filename columns can be swapped with each other, but they must always be the first four columns in the sample list.

   You cannot save these changes. When you restart the TraceFinder application, the Data Review view displays your columns in the order specified in the Modify Columns dialog box.

❖ To customize the column display

1. Right-click the Data Review sample list and choose **Modify Columns** from the shortcut menu.

   The Modify Columns dialog box opens.



Parameter	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
<	Moves the selected column to the Available Columns pane. You cannot move the Status, Sample Level, Sample Type, or Filename columns.
<<	Moves all columns except Status, Sample Level, Sample Type, and Filename to the Available Columns pane.
Up	Moves the selected column name in the Displayed Columns pane one row up in the column order. You cannot move the Status, Sample Level, Sample Type, or Filename columns.
Down	Moves the selected column name in the Displayed Columns pane one row down in the column order. You cannot move the Status, Sample Level, Sample Type, or Filename columns.

2. Use the arrow buttons to move all the columns you want to display to the Displayed Columns pane.

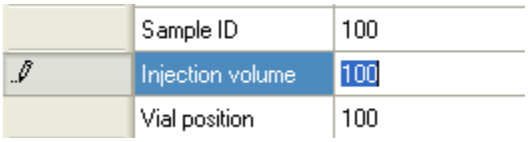
   All the columns you select are displayed after the Status, Sample Level, Sample Type, and Filename columns.

3. To arrange the order of the columns, do the following:
   a. In the Displayed Columns pane, select a column name.
   b. Use the **Up** and **Down** buttons to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Batch View sample list; the last column in the list represents the rightmost column in the Batch View sample list.

      Note You cannot move the Status, Sample Level, Sample Type, or Filename columns.

4. To change the width of a column, do the following:
   a. In the Displayed Columns pane, select the column width.



   b. Type a new value for the width.

5. When you have completed your changes, click **OK**.

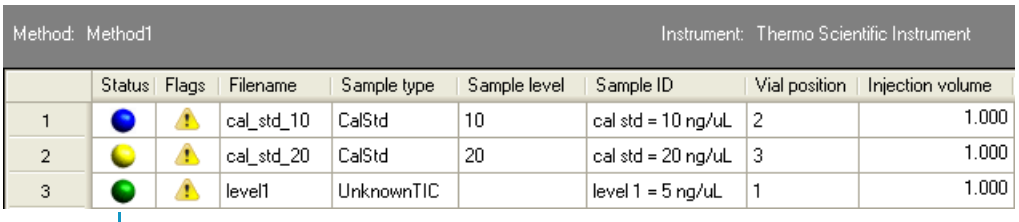
   The columns in the sample list immediately reflect your changes. The application uses these settings for all sample lists in the Data Review view.

   You can use the drag-and-drop method to temporarily reorder the columns in your sample list, but you cannot save this order. When you restart the TraceFinder application, the Data Review view displays your columns in the order specified in the Modify Columns dialog box.

Status Indicators

Status indicators show the current status of each sample during the acquisition and processing:

- Orange for samples that are currently acquiring
- Blue for samples that have not been acquired
- Yellow for samples that have been acquired and not processed
- Green for samples that have been acquired and processed

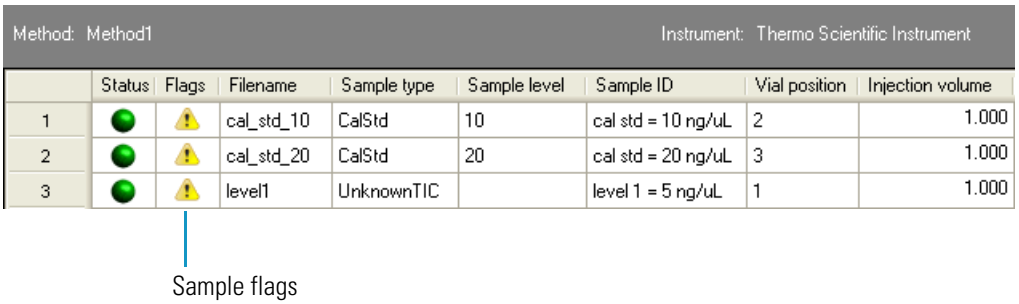


Status indicators

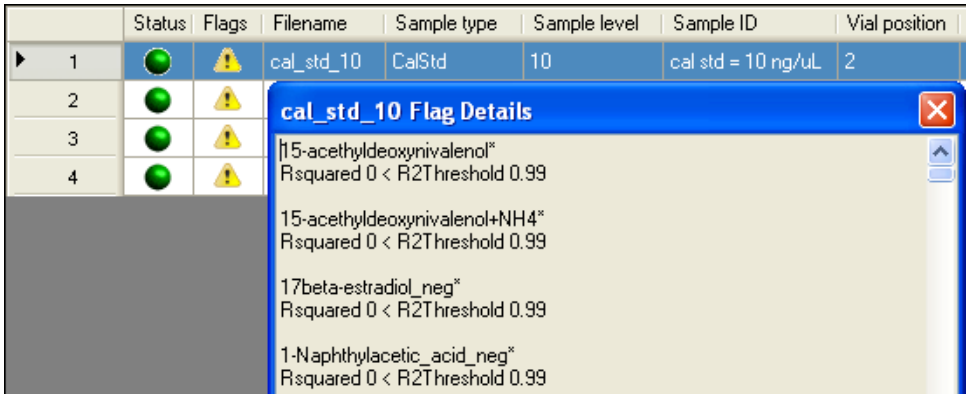
Sample Flags

The Flags column in the samples list displays a caution flag if the sample is not in compliance with the method criteria.

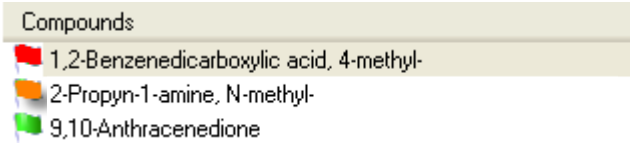
Sample caution flags remain static when you switch between compounds for chromatogram review until a change is completed, for example, when a compound is manually integrated and no longer falls outside the accepted criteria.



To display a summary of problems found in the sample, click the caution flag. The summary does not list compounds that are not found in Unknown sample types.



Compound Flags



Flags are displayed in these situations:

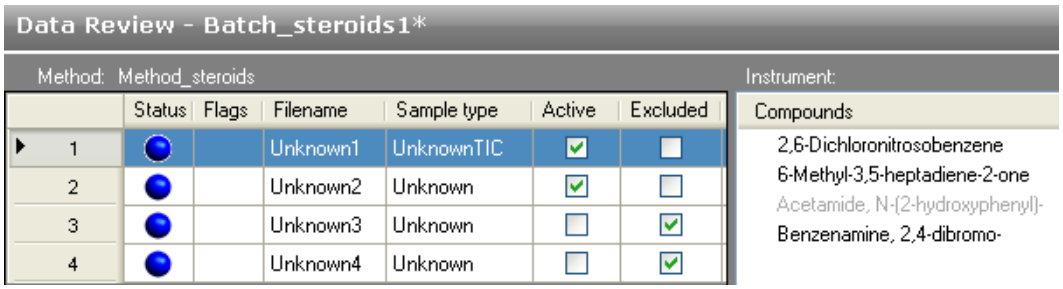
- When a compound has violated (or is activated by) any of the values set in the method. See "Editing the Flags Page" on page 159.
- For compounds that are not found.
- For compounds that are not found in Cal Std or Chk Std sample types.
- For compounds that are outside the specified ion ratio range.

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.
- No flag for compounds that have no errors or where no report options are selected.

Inactive and Excluded Compounds

Use the Active and Excluded columns to control which compounds are used for calculating the calibration curve and for reporting.



Use the following procedures:

- To make a sample active or inactive
- To exclude a calibration point

❖ To make a sample active or inactive

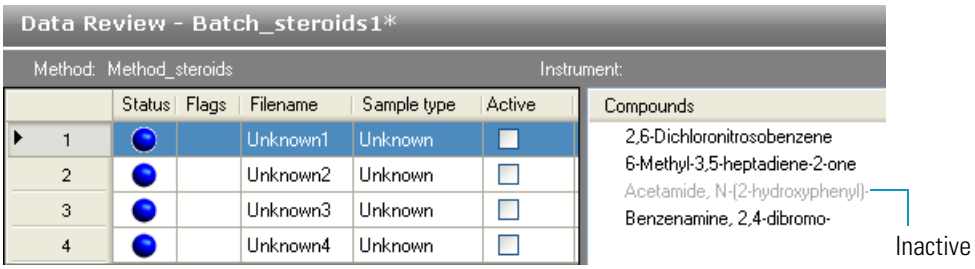
1. Select the sample in the samples list.

   All compounds in the selected sample are displayed in the Compounds pane. Inactive compounds are grayed out.

2. In the Compounds pane, select the compound whose active/inactive status you want to change.

3. In the samples list, 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 samples list, select the **Excluded** check box for the sample.

Use the horizontal scroll bar at the bottom of the table to scroll to the Excluded column.

When a value is no longer used for calibration, it is displayed as an empty box in the graphical view of the calibration curve.

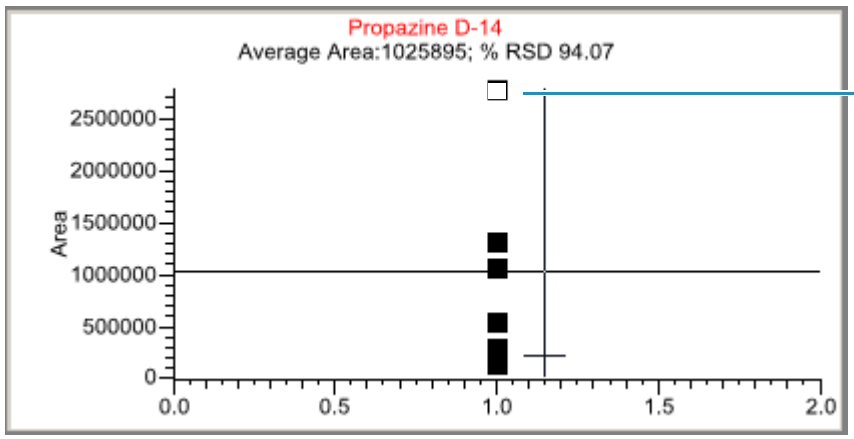


Figure 75. Samples list

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	Channel
☑	☐	N/A	N/A	N/A	Channel 1
☑	☐	N/A	N/A	N/A	Channel 3
☑	☐	N/A	N/A	N/A	Channel 1
☑	☐	N/A	N/A	N/A	Channel 3

Cells in the samples list that should not have a value, such as the 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 63. Samples list columns (Sheet 1 of 2)

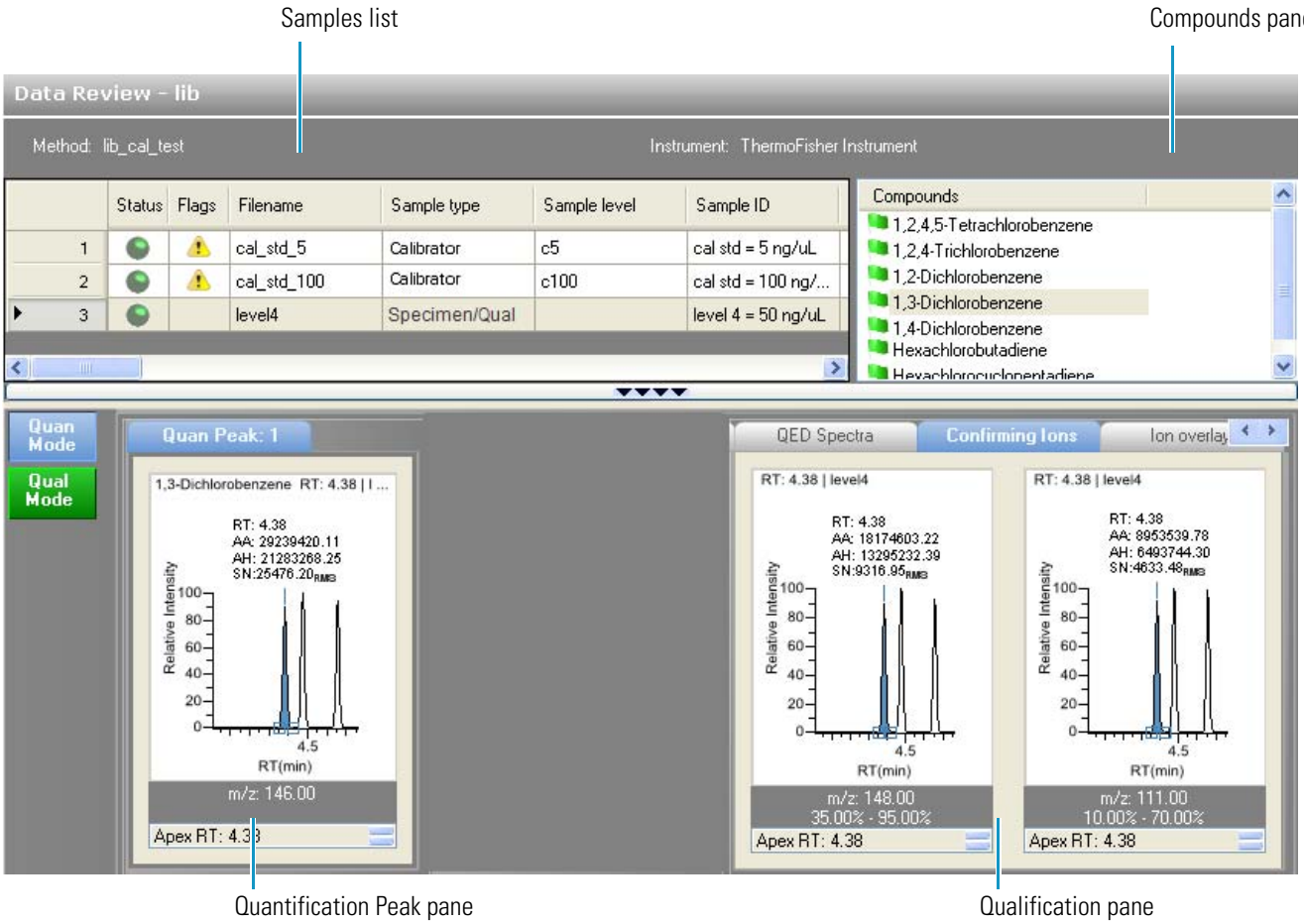
Parameter	Description
Status	• Orange for samples that are currently acquiring • Blue for samples that have not been acquired • Yellow for samples that have been acquired and not processed • Green for samples that have been acquired and processed
Flags	Displayed only when a compound within the sample has an error.
Filename	Name of the raw data file that contains the sample data.
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Environmental and Food Safety: Matrix Blank, Cal Std, Chk Std, LCS, LCSD, MDL, Method Val, MS, MSD, Unknown, Unknown/TIC, Solvent General Quantitation: Matrix Blank, Cal Std, Chk Std, Unknown, Unknown/TIC, Solvent
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. The Injection Volume value set in the master method overwrites the value in the instrument method. Range: 0.1 through 5000µL
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 displays 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 displays an asterisk (*Area).
Actual RT	Actual retention time for the compound. Retention time is the time after injection when a compound elutes and the total time that the compound is retained on the chromatograph column.

Table 63. Samples list columns (Sheet 2 of 2)

Parameter	Description
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.
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 Variance. 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.
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. This column is displayed only when you enable multiplexing.

Quan Mode

Use the Quan Mode and the associated Compounds pane to view quantitative information to complement the textual information for the selected sample. The Quan Mode displays quantitative peak and confirming ion information for selected compounds that are found in the processed samples.



In addition to the Samples list, the Quan Mode view uses the following panes:

- Compounds
- Quantification Peak
- Qualification

Compounds

The Compounds pane works with the samples list pane to display textual and graphical values for a unique file and compound combination.

Use the following procedures:

- To sort the compounds list
- To display peaks for a specific compound
- To display specific problems with a compound
- To display the internal standard for a compound

❖ To sort the compounds list

In the Compounds pane, right-click and choose one of the following sort styles from the shortcut menu:

Command	Description
Sort by flag and alphabetical	Sorts the compounds first by flag and then within each flag group, sorts the compounds alphabetically.
Sort by flag and retention time	Sorts the compounds first by flag and then within each flag group, sorts the compounds by retention time.
Sort by alphabetical	Sorts the compounds alphabetically (*1-n* followed by *a-z*).
Sort by retention time	Sorts the compounds from shorter retention time to longer retention time.

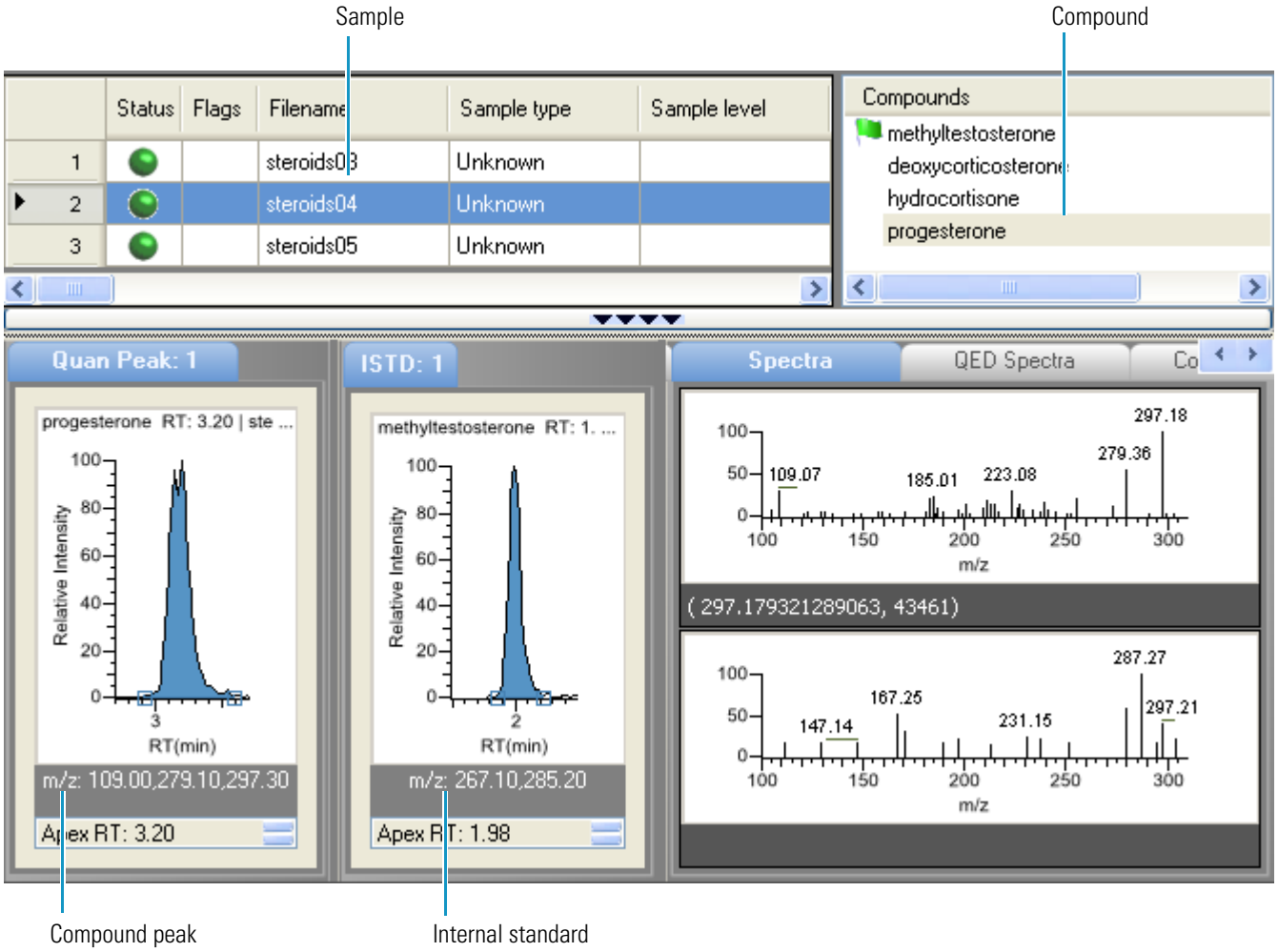
❖ To display peaks for a specific compound

1. In the samples list, select the sample.

   The Compounds pane lists all compounds specified in the method.

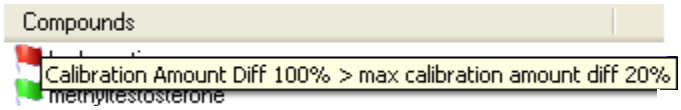
2. In the Compounds pane, select the compound in the sample.

   The Quantification Peak pane displays the peaks for the selected compound and its internal standard.



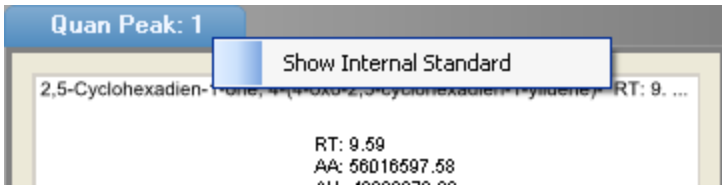
❖ To display specific problems with a compound

Hold the cursor over the flag to display the problems with the compound.



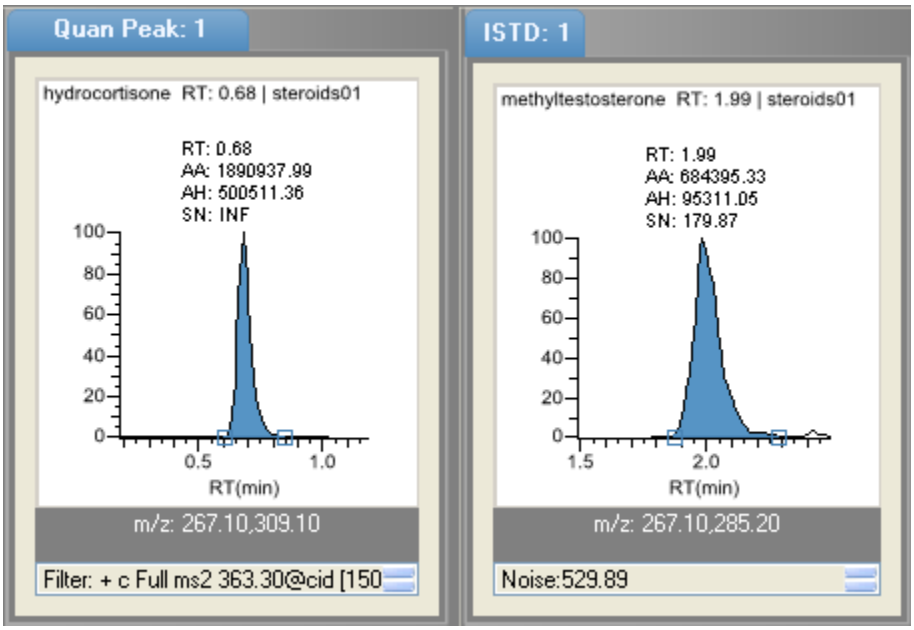
❖ To display the internal standard for a compound

1. Right-click the Quan Peak pane and choose **Show Internal Standard** from the shortcut menu.



Note By default, the ISTD pane is not displayed.

The Quantification Peak pane displays an ISTD pane with the internal standard for the selected sample and compound.



2. To hide the ISTD pane, right-click the Quan Peak or ISTD pane and choose **Hide Internal Standard** from the shortcut menu.

Quantification Peak

The Quantification Peak pane displays the compound selected in the samples list and Compound pane. 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 edited.

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

For a description of commands on the shortcut menu, see "Quantification Peak Shortcut Menu" on page 302.

❖ 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.

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 to place the peak delimiter tag 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.

Note Because a Blank Report displays only the quan mass, when you manually integrate a confirming ion, the manual integration flag in the report is displayed on the quan mass.

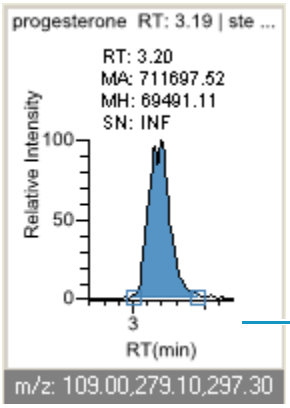
❖ To manually add a peak

1. Right-click anywhere in the Quantification Peak 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.



Manually added base points

❖ 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, each pane reflects the changes. The generated reports for these data identify the manual modifications.

Note Because a Blank Report displays only the quan mass, when you manually integrate a confirming ion, the manual integration flag in the report is displayed on the quan mass.

❖ To change the displayed information for detected peaks

1. Right-click the quantification chromatogram plot and hold 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 quantification peaks, confirming peaks, and internal standard peaks.

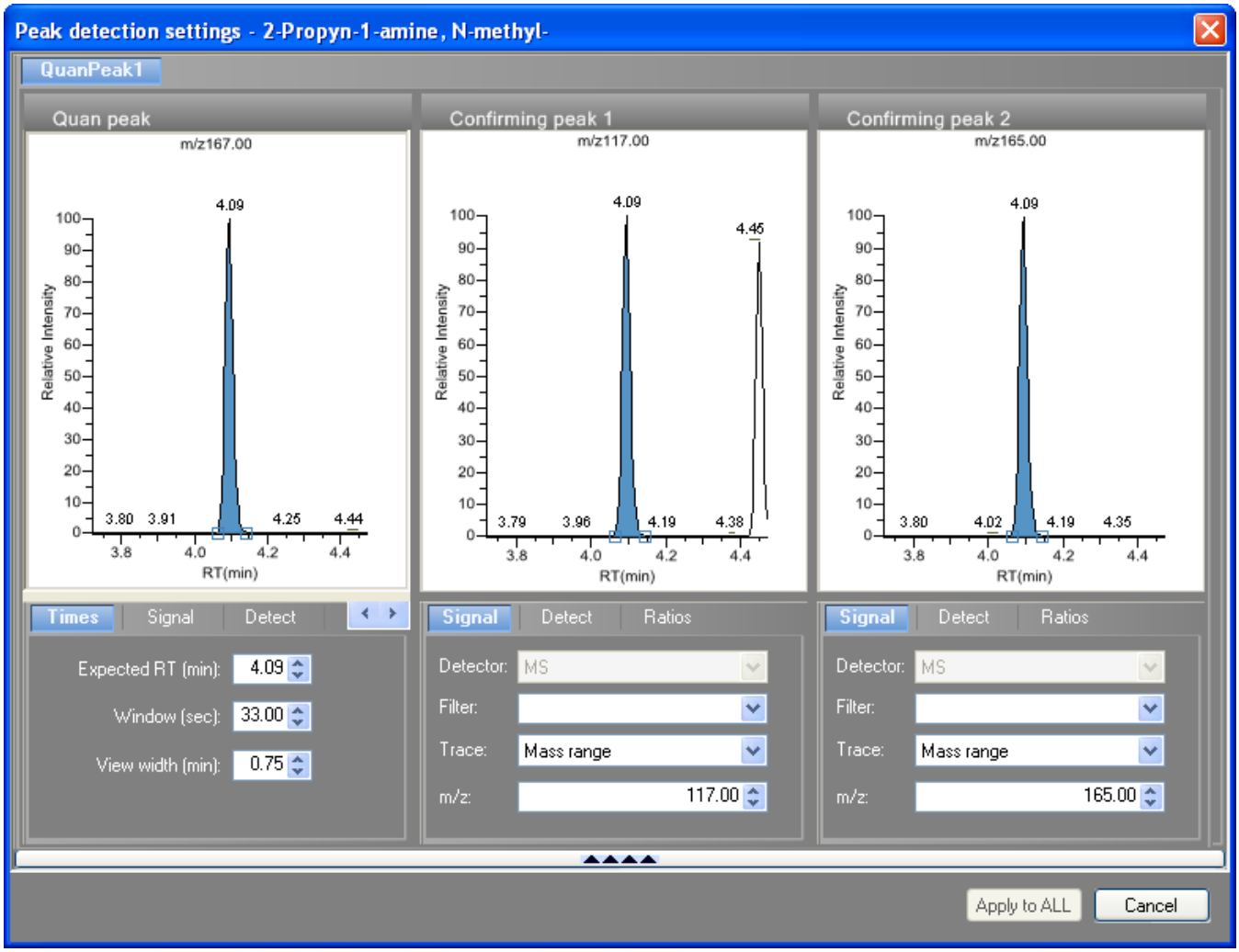
Tip The labels do not always update on all peak displays. To update all labels, select a different compound, and then reselect the compound whose labels you changed.

❖ To modify the peak detection settings

1. Right-click the chromatogram view and choose **Peak Detection Settings** from the shortcut menu.

   The Peak Detection Settings dialog box opens. Use the Peak Detection Settings dialog box to adjust detection settings that were specified in the method.

Figure 76. Peak Detection Settings dialog box



2. Edit any of the detection settings.

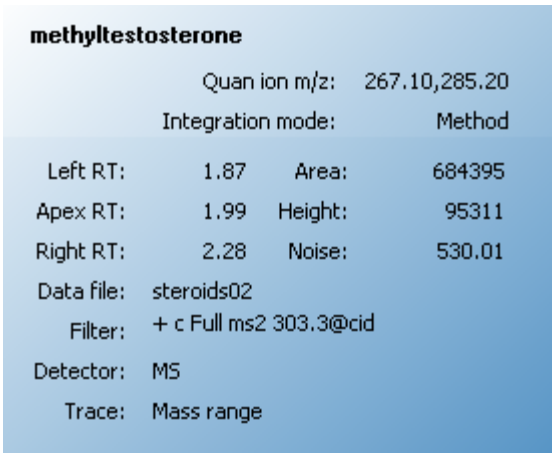
   For detailed descriptions of all detection settings, see "Detection" on page 121.

3. To save your changes to this compound in all samples in this batch, click **Apply to All**.

Quantification Peak Shortcut Menu

The Quantification Peak shortcut menu includes the following commands:

Table 64. Quantification Peak shortcut menu commands

Command	Description
Method Integration Settings	Displays method integration settings.
Manual Integration Settings	Displays manual integration settings.
Add Peak –or– Remove Peak –or– 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.

Qualification

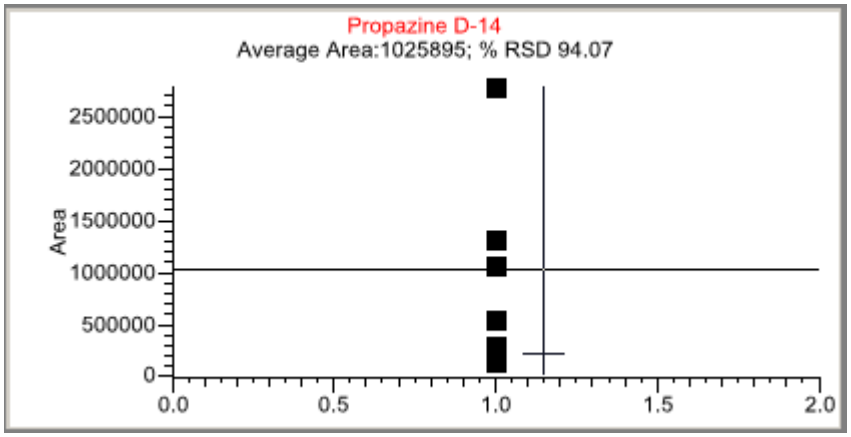
The Qualification pane displays the compound selected in the Quantification Data pane and Compounds pane.

The Qualification pane has 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.



Use the following procedures:

- To manually exclude a calibration point
- To zoom in on an area

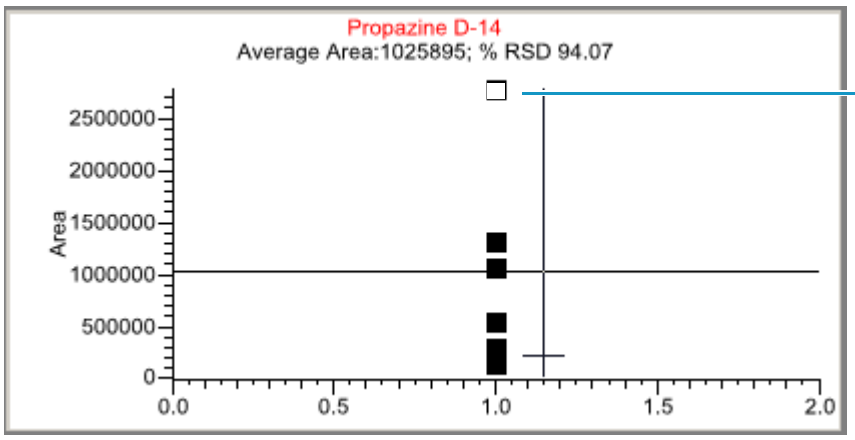
For a description of commands on the shortcut menu, see "Calibration Curve Shortcut Menu" on page 305.

❖ To manually exclude a calibration point

In the samples list, select the **Excluded** check box for the sample.

Use the horizontal scroll bar at the bottom of the table to scroll to the Excluded column.

When a value is no longer used for calibration, it is displayed as an empty box in the graphical view of the calibration curve.



❖ 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 immediately apply to the entire results set, but you save them only when you save the batch.

Calibration Curve Shortcut Menu

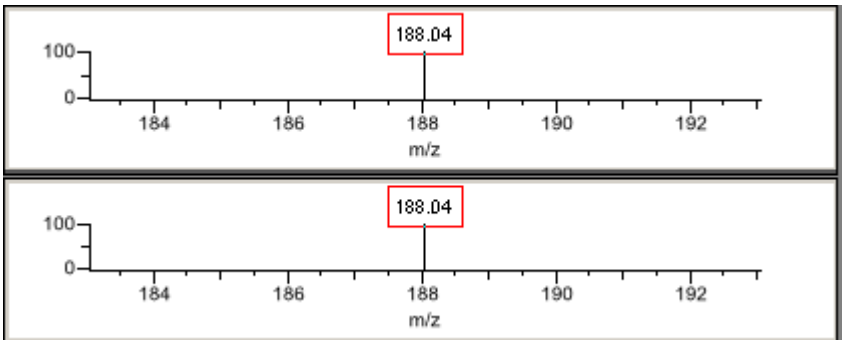
The Calibration Curve shortcut menu includes the following commands:

Table 65. Calibration Curve shortcut menu commands

Command	Description
Standard Type	Sets the standard type to External or Internal.
Calibration Curve Type	Sets the calibration curve type to one of the following: • 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 to Area or to 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

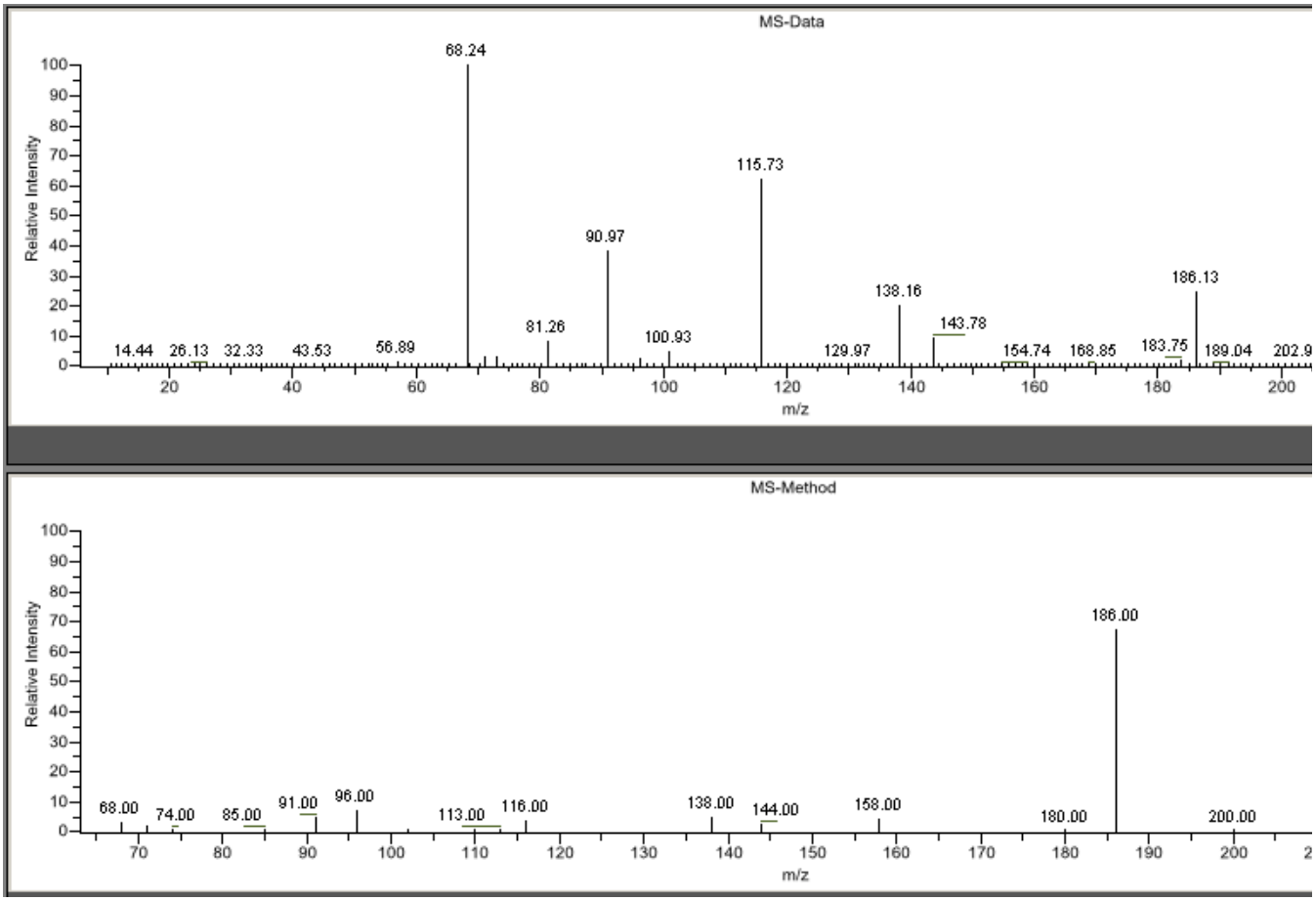
1. Drag your cursor to delineate a rectangle around an area.

   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 raw data file and the datastore match. If the sample contains no QED data, the page is blank.



❖ To zoom in on an area

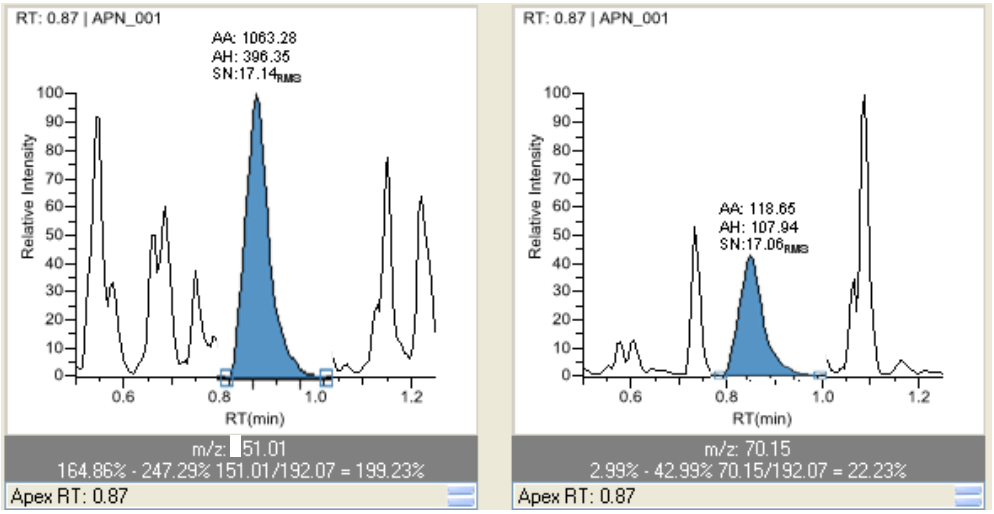
1. Drag your cursor to delineate a rectangle around an area.

   The delineated area expands to fill the view.

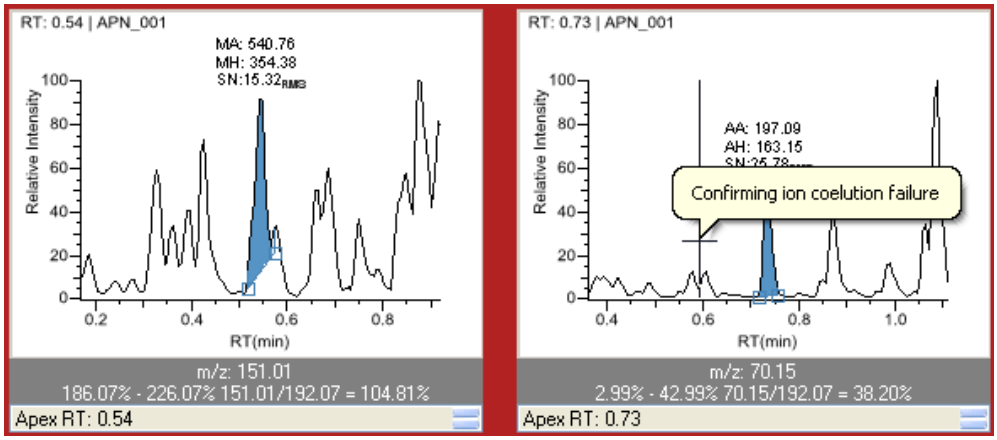
2. To restore the method default view, right-click the spectra plot and choose **Reset Scaling** from the shortcut menu.

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 311.



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

For a description of commands on the shortcut menu, see "Confirming Ions Shortcut Menu" on page 310.

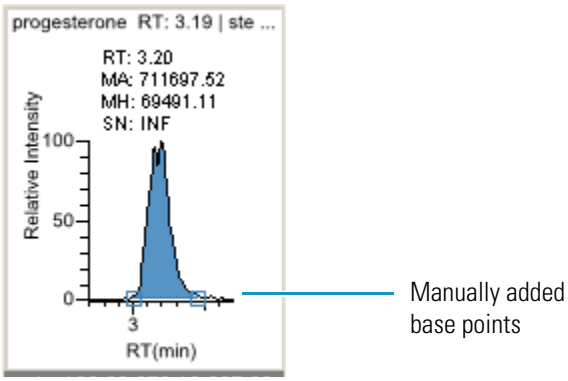
❖ To manually add a peak

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.

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 hold 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 quantification peaks, confirming peaks, and internal standard peaks.

Tip 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.

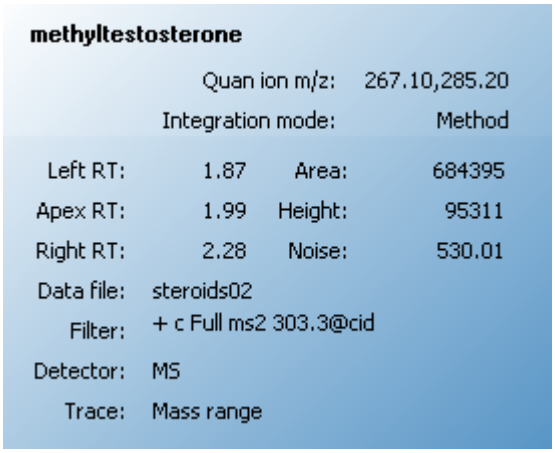
   Information in this window includes the data stream processed for this ion, consisting of a particular detector, filter (if applicable), and trace. For example, an MS detector might show a filter of "+ c Full ms [35.00-500.00]" and a Mass Range trace.

   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

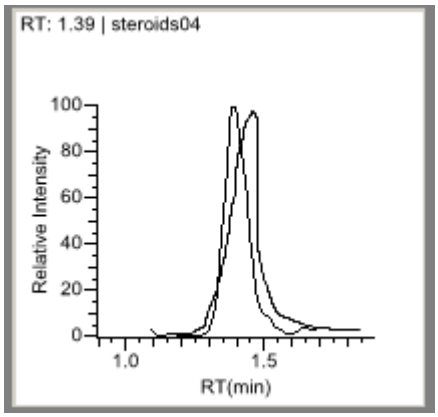
The Confirming Ions shortcut menu includes the following commands:

Table 66. Confirming Ions shortcut menu commands

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 as a percentage.
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. See "Peak Detection Settings dialog box" on page 301.

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

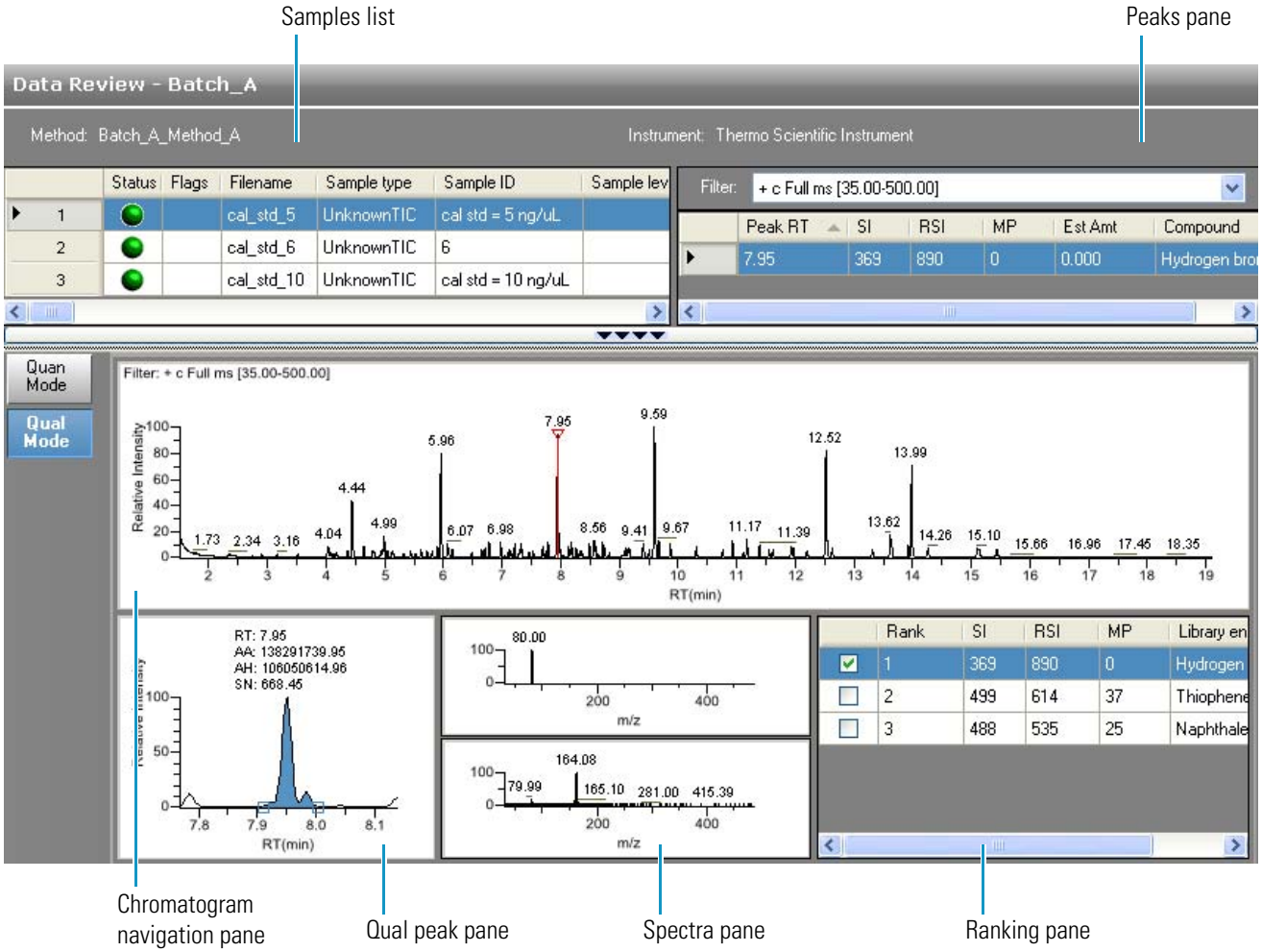
1. Drag your cursor to delineate a rectangle around the peak.

   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.

Qual Mode

Use the Qual Mode and the associated peaks pane to view qualitative information that complements the textual information for the selected Unknown/TIC sample. The Qual Mode view displays detected peaks for the selected sample. From the Qual Mode view, you can manually add peaks. The Qual Mode view is available only for Unknown/TIC sample types.



Tip To resize the panes, drag the separators that divide the panes.

In addition to the Samples list, the Qual Mode view displays data in the following panes:

- Peaks Pane
- Chromatogram Navigation Pane
- Qual Peak Pane
- Spectra Pane (Reference and Selected)
- Ranking Pane

Peaks Pane

The peaks pane works with the samples list to display graphical values for a unique sample and peak combination. For detailed descriptions parameters on the peaks pane, see "Peaks pane" on page 315.

❖ To display peaks for a specific compound

1. From the samples list, select a sample.

   Note If you choose a sample other than an Unknown/TIC sample, the TraceFinder application returns you to Quan Mode.

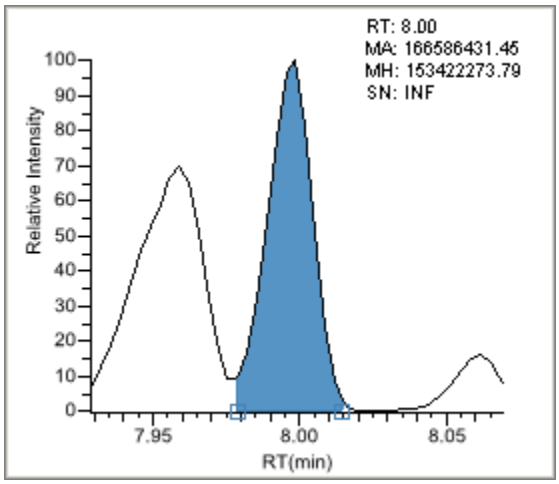
   The peaks pane lists the retention times for peaks identified in the selected sample, the values for the best match methods for each peak, and the compound match.

   The number of peaks that are listed is specified in the method. You can change the number of identified peaks in the Method Template Editor. See "Creating a Method Template" on page 188.

2. From the peaks pane, select a peak in the sample.

	Peak RT (min)	SI	RSI	MP	Library entry
	5.01	844	847	33	o-Toluidine
	5.46	892	894	98	2-Cyclohexen-1-one, 3,5,5-trimethyl-
▶	8.00	937	937	80	Acenaphthene
	8.84	259	549	0	Naphthalene, 1-methyl-
	10.94	942	943	53	Fluoranthene

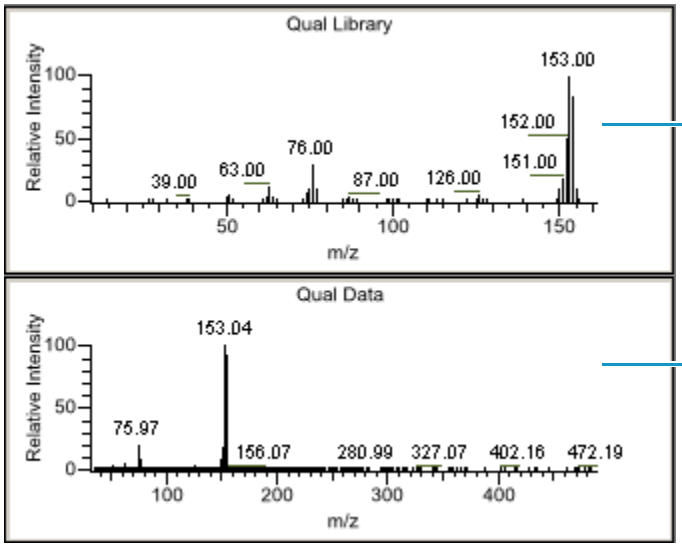
   The TraceFinder application displays the selected peak in the qual peak pane.



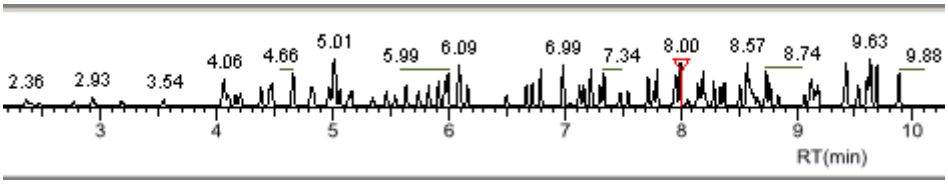
   When you select a data-dependent sample, the peak can be from either a full scan or a QED spectrum of an SRM-filtered chromatogram.

The TraceFinder application displays the Spectra pane with two sections:

- The Qual Data pane shows spectra data for the peak in the raw data file.
- The Qual Library pane shows actual spectra for the identified library compound.



The TraceFinder application locates the selected peak in the navigation chromatogram.



❖ To remove a peak

1. Select a peak in the peaks pane.
2. Right-click and choose **Remove Selected Peak** from the shortcut menu.

   The TraceFinder application removes the selected peak from the peaks list.

Note There is no undo for this action, but you can manually add a peak to redefine a removed peak. See "Chromatogram Navigation Pane" on page 316.

Figure 77. Peaks pane

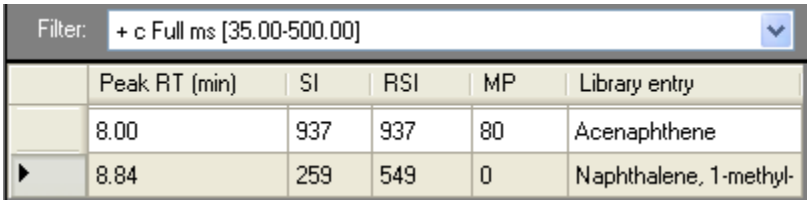
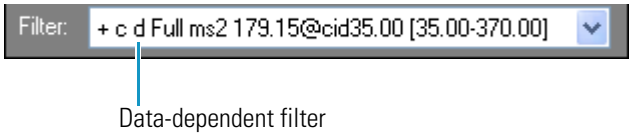


Table 67. Peaks pane parameters

Command	Description
Filter	Filter used to identify the peaks. Specified in the raw data file or the master method. When your raw data file is data-dependent, the filter indicates this with a "d":  Data-dependent filter
Peak RT (min)	Peak retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
SI	Search index method used to search the NIST library.
RSI	Reverse search index method used to search the NIST library.
MP	Match probability.
Library entry	Library compound that matches the identified peak.
Remove selected peak	Shortcut menu command that removes the selected peak from the peaks list.

Chromatogram Navigation Pane

The chromatogram navigation pane displays all peaks in the selected sample. The peak selected in the peaks pane displays a red marker.

For a description of commands on the shortcut menu, see "Chromatogram navigation pane shortcut menu commands" on page 317.

❖ To zoom in on a peak

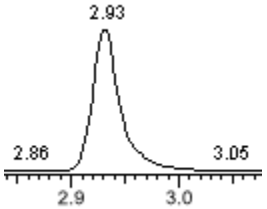
1. In the chromatogram navigation pane, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the chromatogram navigation pane and choose **Reset Scaling** from the shortcut menu.

❖ To manually add a peak

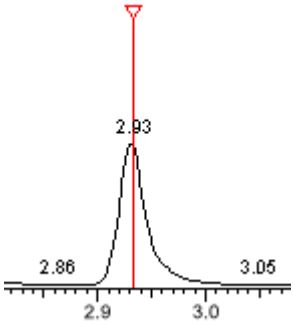
1. Zoom in to make it easier to identify the peak you want to add to the results set.



2. Right-click the chromatogram navigation pane, and choose **Add Peak** from the shortcut menu.

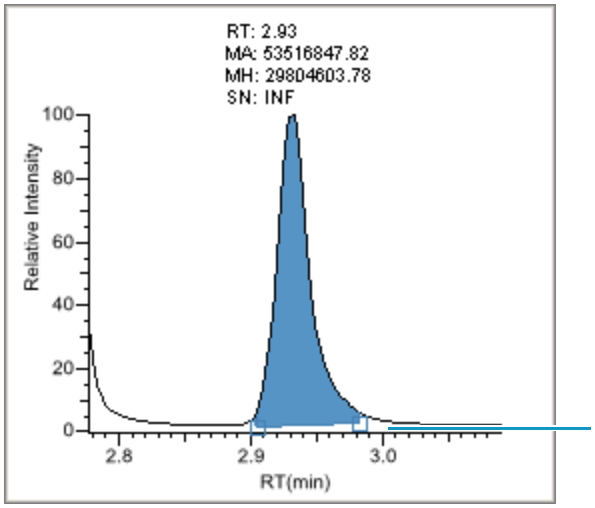
3. Click to indicate the left and right base points for the peak.

   The TraceFinder application marks the peak in the chromatogram navigation pane.



   The TraceFinder application places the peak delimiter tags at the base point locations and automatically updates the peak values in the peaks pane and qual peak pane.

Figure 78. Qual peak pane with a manually added peak



	Peak RT (min)	SI	RSI	MP	Library entry
▶	2.93	930	933	94	Phenol, 2-fluoro-
	3.18	834	845	96	Ethanamine, N-ethyl-N-nitroso-
	5.01	800	903	5	Phenol, 3-methyl-

Figure 79. Chromatogram navigation pane

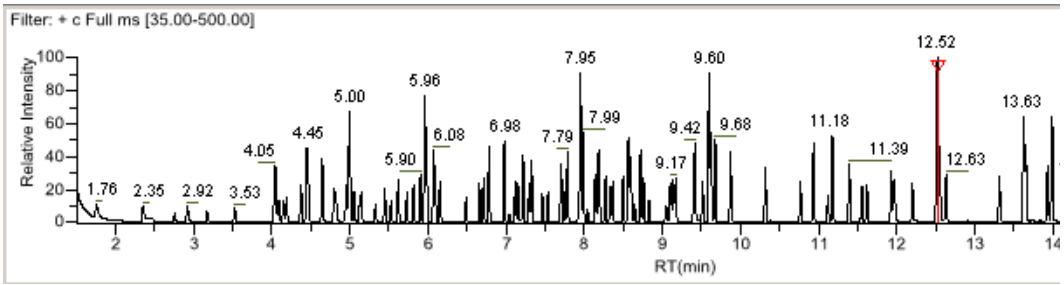


Table 68. Chromatogram navigation pane shortcut menu commands

Command	Description
Add peak	Manually adds a peak.
Reset scaling	Resets the original scaling after a zoom operation.

Qual Peak Pane

The qual peak pane displays the selected peak.

Use the following procedures:

- To zoom in on a peak
- To manually add a peak
- To remove a peak
- To switch between method and manual integration modes
- To change the displayed information for detected peaks

For a description of commands on the shortcut menu, see "Qual peak pane shortcut menu commands" on page 320.

❖ To zoom in on a peak

1. In the chromatogram plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

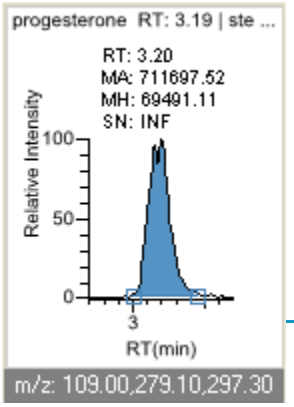
❖ To manually add a peak

1. Right-click anywhere in the qual peak 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 TraceFinder application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



Manually added base points

❖ To remove a peak

Right-click the chromatogram plot, and choose **Remove Peak** from the shortcut menu.

The TraceFinder application removes the peak displayed in the qual peak pane. All data for this peak are removed from the Qual Mode panes.

❖ To switch between method and manual integration modes

Right-click the chromatogram view and choose **Method Integration** or **Manual Integration** 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, each pane reflects the changes. The generated reports for these data identify the manual modifications.

❖ To change the displayed information for detected peaks

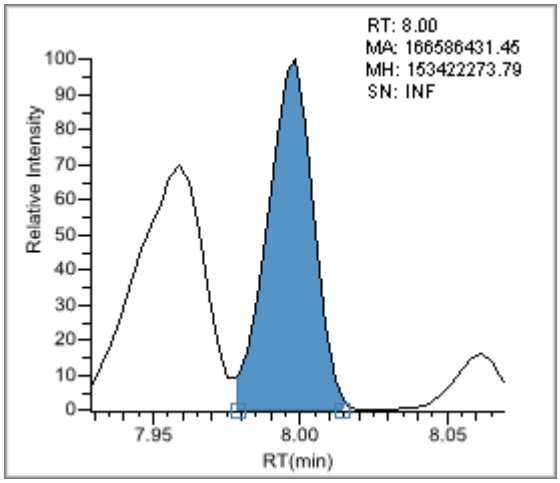
1. Right-click the chromatogram plot and hold the cursor over **Peak Labels**.
2. Choose to display labels for the peak retention time, peak height, peak area, or signal to noise.

   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 qual peaks, confirming peaks, and internal standard peaks.

Tip 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.

Figure 80. Qual peak pane



The qual peak pane shortcut menu includes the following commands:

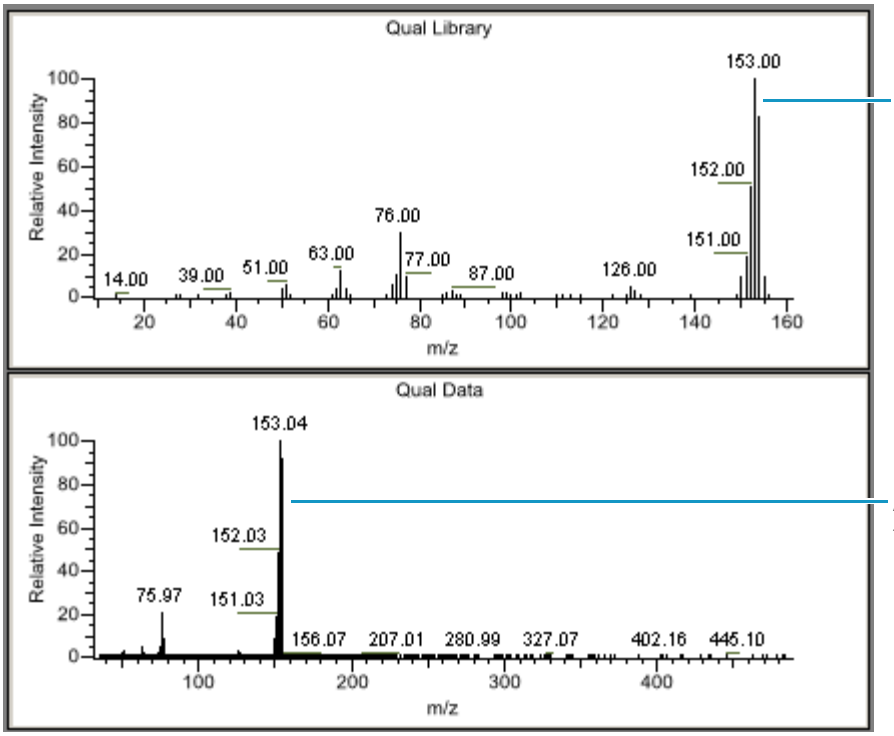
Table 69. Qual peak pane shortcut menu commands

Command	Description
Reset scaling	Resets the original scaling after a zoom operation.
Method integration	Displays method integration settings.
Manual integration	Displays manual integration settings.
Peak labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).
Remove peak	Removes the peak displayed in the Qual pane.

Spectra Pane (Reference and Selected)

The Spectra pane displays the reference spectra and the spectra for the selected sample. The top pane displays the reference spectra for the identified compound from the library; the bottom pane displays the spectra for the selected peak.

Figure 81. Spectra pane



❖ To zoom in on a peak

1. In the spectra plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

Ranking Pane

The ranking pane displays the three best library matches for the selected peak. Use this pane to select a different library entry for the peak.

When you select a library entry other than the original entry, the TIC Report and TIC Summary Report indicate this with a "P" flag:

Peak:	Retention Time	Area	Height	Inj Estimate	In-sample Est	Flag
Naphthalene, 2-chloro-	7.95	138291740	106050615	0.000	0.000	P

P flag

For a detailed description of ranking pane parameters, see "Ranking pane" on page 323.

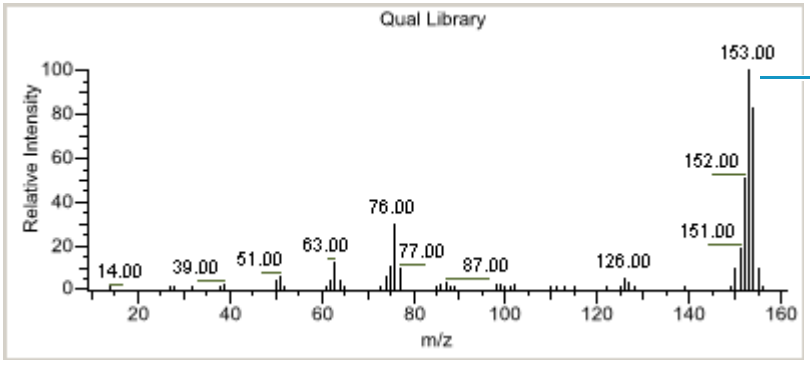
❖ To change the library entry for a selected peak

In the ranking pane, select the check box for the library entry you want to use to identify the selected peak.

- In the Spectra pane, the reference spectra change to show the spectra for the selected library entry.
- In the peaks pane, the SI, RSI, MP, and Library Entry values update to reflect the selected library entry.

	Rank	SI	RSI	MP	Library entry
☑	1	937	937	80	Acenaphthene
☐	2	865	868	11	Biphenyl
☐	3	856	856	8	Naphthalene, 2-ethenyl-

Selected library entry in the ranking pane

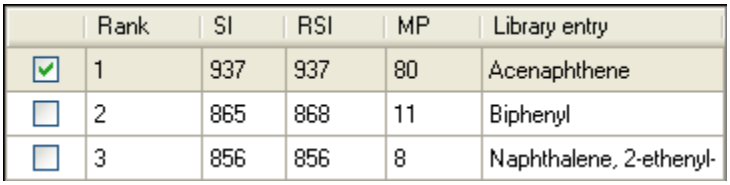


Reference spectrum for Acenaphthene

	Peak RT (min)	SI	RSI	MP	Library entry
	5.01	844	847	33	o-Toluidine
	5.46	892	894	98	2-Cyclohexen-1-one, 3,5,5-trimethyl-
▶	8.00	937	937	80	Acenaphthene
	10.94	942	943	53	Fluoranthene

Peaks pane for Acenaphthene

Figure 82. Ranking pane



	Rank	SI	RSI	MP	Library entry
☑	1	937	937	80	Acenaphthene
☐	2	865	868	11	Biphenyl
☐	3	856	856	8	Naphthalene, 2-ethenyl-

Table 70. Ranking pane parameters

Command	Description
<Check box column>	Indicates selected library entries for the selected peak.
Rank	Indicates the order of best matches between the selected peak and library entries.
SI	Search index method used to search the NIST library.
RSI	Reverse search index method used to search the NIST library.
MP	Match probability.
Library entry	Library compound that matches the identified peak.

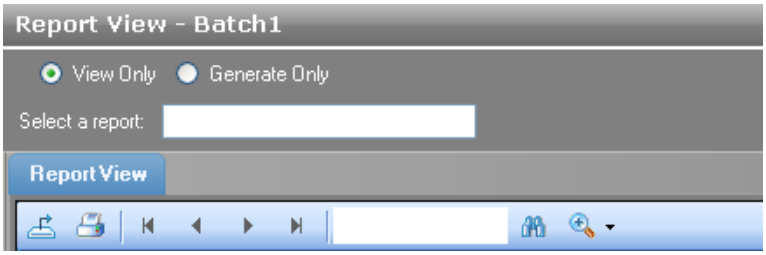
Working in Report View

Use the Report View to display or generate reports for the currently selected batch in the Data Review mode. You must process each sample in the batch before you can view or generate a sample-level report for that sample.

This section includes the following topics:

- Viewing Reports
- Generating Reports
- Working with Reports
- Working with Active View

Figure 83. Report View in Data Review mode



- View Only: Displays a PDF or Excel spreadsheet preview of the selected report type for the batch, sample, or compound. See "Viewing Reports" on page 325.

  Preview reports for all Standard report types are always available. You must generate Custom and Target Screening report types before they are available in this list.

  The Report View page displays one of the following report outputs:

  - Standard reports as PDF files
  - Custom reports in XLSM format
  - Target Screening reports as PDF files

- Generate Only: Creates all specified report output formats for the selected sample- or batch-level report. See "Generating Reports" on page 329.

❖ To open the Report View

1. Click **Data Review** in the navigation pane from any mode.
2. In the Data Review navigation pane, click **Report View**.

   The Report View for the currently selected batch opens.

Viewing Reports

Use the View Only features to view all configured standard reports and any custom or target screening reports that you have generated. After you generate a report, the application displays the report in the View Only report list.

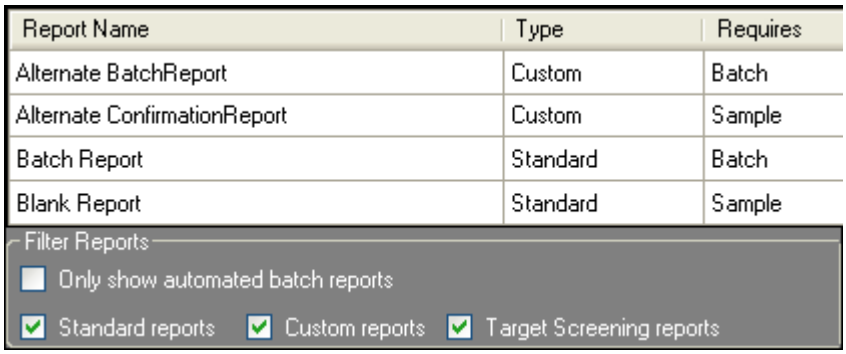
Use the following procedures:

- To select a report
- To select a sample
- To select a compound
- To select a sample and a compound

❖ To select a report

1. Select the **View Only** option.
2. Click the Select a Report box.

   The report list opens, displaying all configured report types.



   These reports reflect the Displayed Reports selections in the Configuration mode. To change the configured reports that are available in this view, see "Specifying the Reports Configuration" on page 58.

   To sort the reports, click the column headers. The application maintains this sort order each time you open the Report View for this batch.

   To help organize your reports, you can filter the list.

3. To limit the types of reports you want to display in the report list, select any combination of report filter options in the Filter Reports area.

Table 71. Filter Reports options

Option	Behavior
Only show automated batch reports	Displays only reports that have an output format specified in the Automated Batch Reports area in the Batch View. See "Editing Report Output Formats" on page 274.
Standard reports	Displays Standard report types.
Custom reports	Displays all generated Custom report types. Custom reports are not available for viewing until you have generated the report.
Target Screening reports	Displays all generated Target Screening reports. Target Screening reports are not available for viewing until you have generated the report.

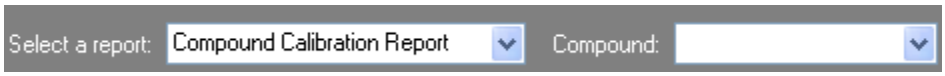
Note When you make changes to the method in the Local Method view, to the peaks in the Data Review view, or to the samples in the Batch View, you must regenerate the custom or target screening reports to see the effects of those changes.

4. Double-click the name of the report.

   The report list closes.

   - When the selected report is a batch-level report, the application displays the report on the Report View page.
   - When the selected report includes separate reports for each sample, you must select a sample file.

     Follow the procedure "To select a sample" on page 327.
   - When the selected report includes separate reports for each compound, you must select a compound.

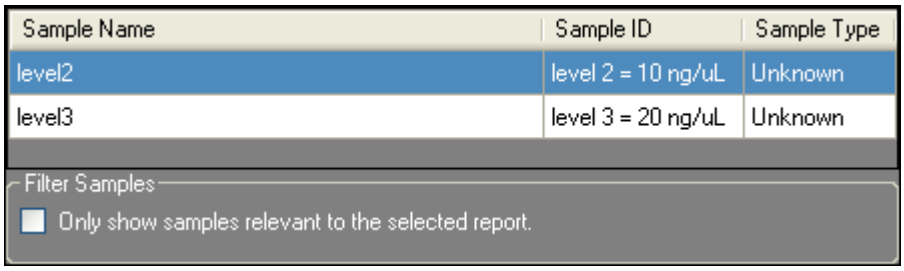
     Follow the procedure "To select a compound" on page 327.
   - When the selected report includes separate reports for each sample and each compound in the sample, you must select both a sample and a compound.

     Follow the procedure "To select a sample and a compound" on page 328.

❖ To select a sample

1. Click the Sample File box.

   The sample list displays all samples in the batch.



2. To show only samples that would be included in the selected report, select the **Only Show Samples Relevant...** check box.

   For example, if you selected the Check Standard Report, the sample list displays only Chk Std samples.

   Note Click the column headers to sort the samples. The application maintains this sort order each time you open the Report View for this batch.

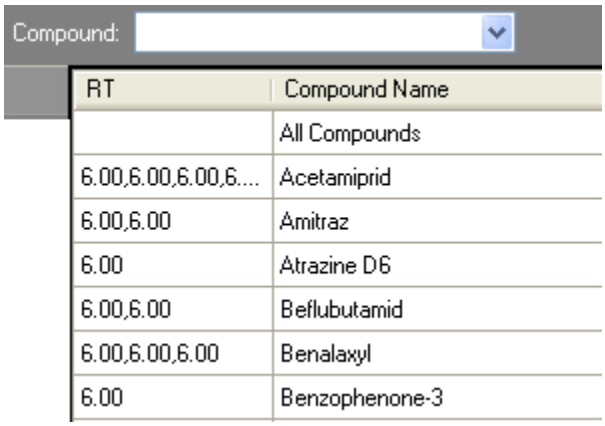
3. Double-click the name of the sample.

   The sample list closes. The Report View page displays the sample-level report.

❖ To select a compound

1. Click the Compound box.

   The compound list displays the names and retention times of all compounds in the sample.



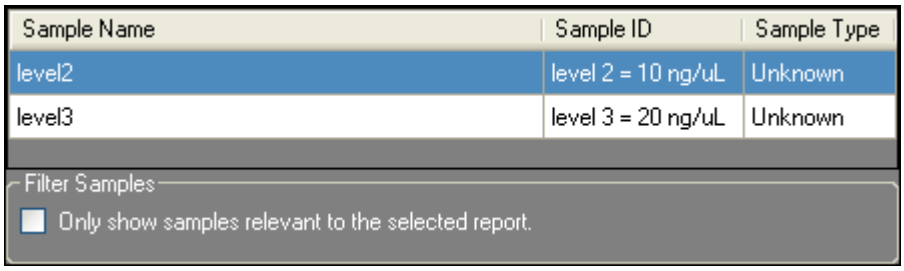
2. Double-click a single compound or **All Compounds**.

   The compound list closes. The Report View page displays the compound-level report.

❖ To select a sample and a compound

1. Click the Sample File box.

   The sample list displays all samples in the batch.



2. To show only samples that would be included in the selected report, select the **Only Show Samples Relevant...** check box.

   For example, if you selected the Check Standard Report, the sample list displays only Chk Std samples.

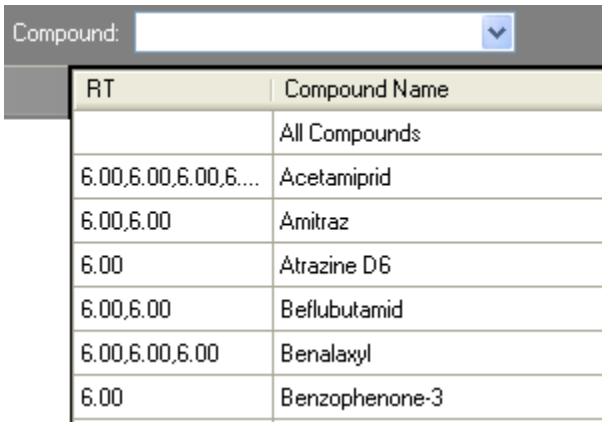
   Note Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

3. Double-click the name of the sample.

   The sample list closes.

4. Click the Compound box.

   The compound list displays the names and retention times of all compounds in the sample.



5. Double-click a single compound or **All Compounds.**

   The compound list closes.

   The Report View page displays the compound-level report for the selected sample and compound.

Generating Reports

Use the Generate Only features to create sample-level reports. You cannot use the View Only features to view custom or target screening reports until you generate the report. When you make changes to the method in the Local Method view or to the peaks in the Data Review view, you must regenerate the custom or target screening reports to see the effects of those changes.

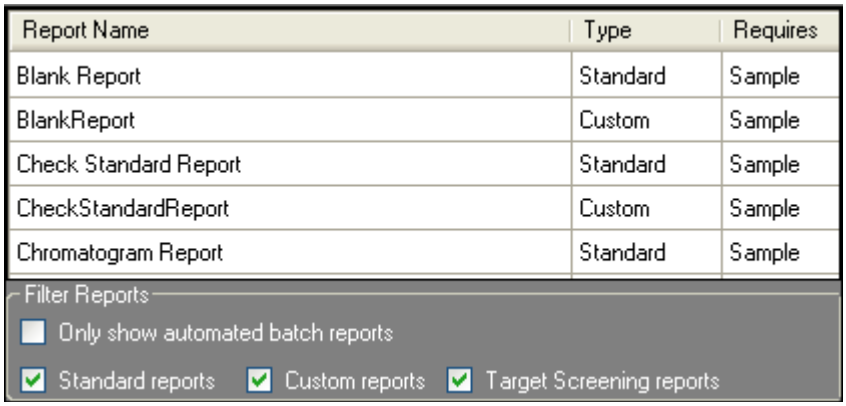
Use the following procedures:

- To select a report
- To select a sample

❖ To select a report

1. Select the **Generate Only** option.
2. Click the Select a Report box.

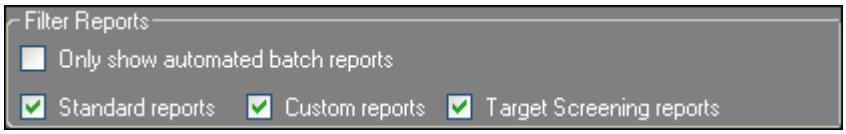
   The report list opens.



   All configured sample-level report types are displayed in the list. You cannot generate batch-level or compound-level reports from this view. To change the configured reports that are available in this view, see "Specifying the Reports Configuration" on page 58.

   If you have many reports, you can filter the list.

3. To limit the types of reports you want to display in the report list, select any combination of report filter check boxes in the Filter Reports area.



Option	Behavior
Only show automated batch reports	Displays only sample-level reports that have an output format specified in the Automated Batch Reports area in the Batch View. See "Editing Report Output Formats" on page 274. If you have only batch-level reports specified in the Batch View, selecting this option excludes all reports in the Report Name list.
Standard reports	Displays sample-level Standard report types.
Custom reports	Displays sample-level Custom report types.
Target Screening reports	Displays sample-level Target Screening report types.

Note Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

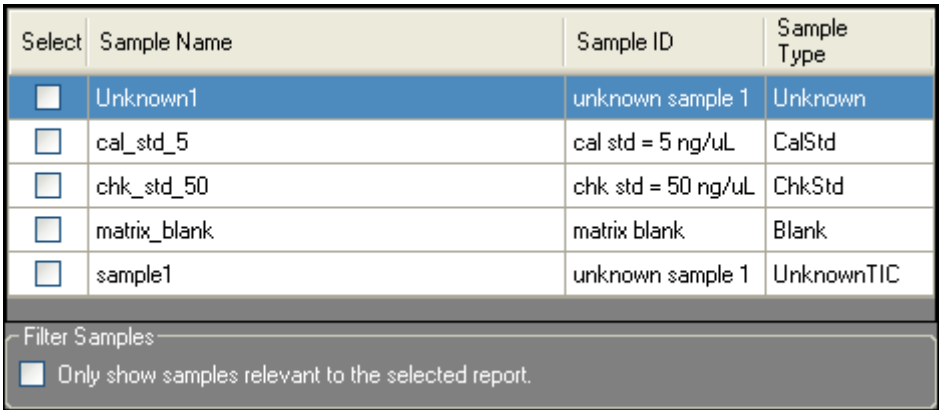
4. Double-click the name of the report.

The report list closes. You must select a sample file for the selected report.

❖ To select a sample

1. Click the Sample File box.

The sample list displays all samples in the batch.



2. To show only samples that would be included in the selected report, select the **Only Show Samples Relevant...** check box.

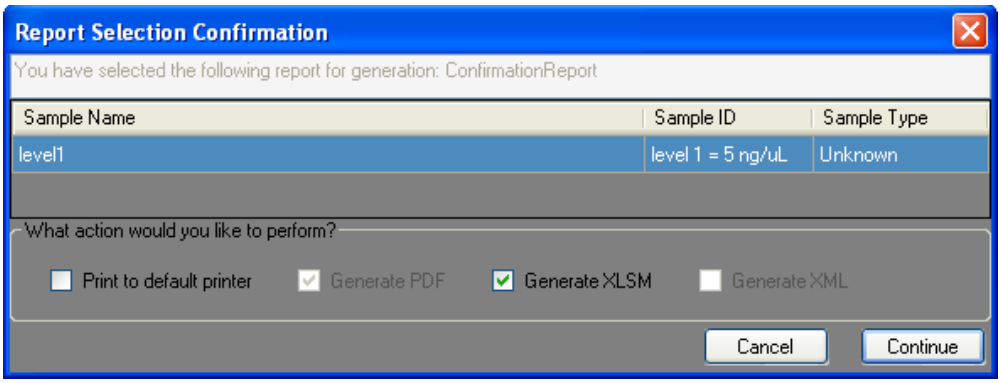
   For example, if you selected the Check Standard Report, the sample list displays only Chk Std samples.

   Note Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

3. Select the check box for each sample you want to include in the report.

4. Click **Generate**.

   The Report Selection Confirmation dialog box opens.

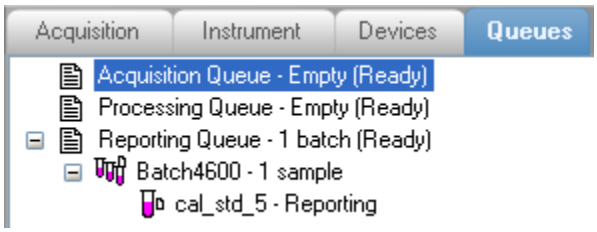


5. In the What Action Would You Like to Perform area, select the types of reports you want to create.

   Note The application automatically selects required output formats. These options are not editable.

6. Click **Continue**.

   The application submits the selected samples to the report queue.



   When you have already generated this report in the Batch View or Acquisition Mode, the new report is time-stamped to differentiate it from the original report.

7. To view the report you generated, follow the instructions in "Viewing Reports" on page 325.

Note When you make changes to the method in the Local Method view, to the peaks in the Data Review view, or to the samples in the Batch View, you must regenerate the custom or target screening reports to see the effects of those changes.

Working with Reports

Use the buttons on the Report View page to view, print, or export a report.

- A PDF report view is available for all Standard and Target Screening report types.
- An Excel Macro-Enabled Workbook report view is available for any Custom report types that you have generated with the Generate XLSM option selected.

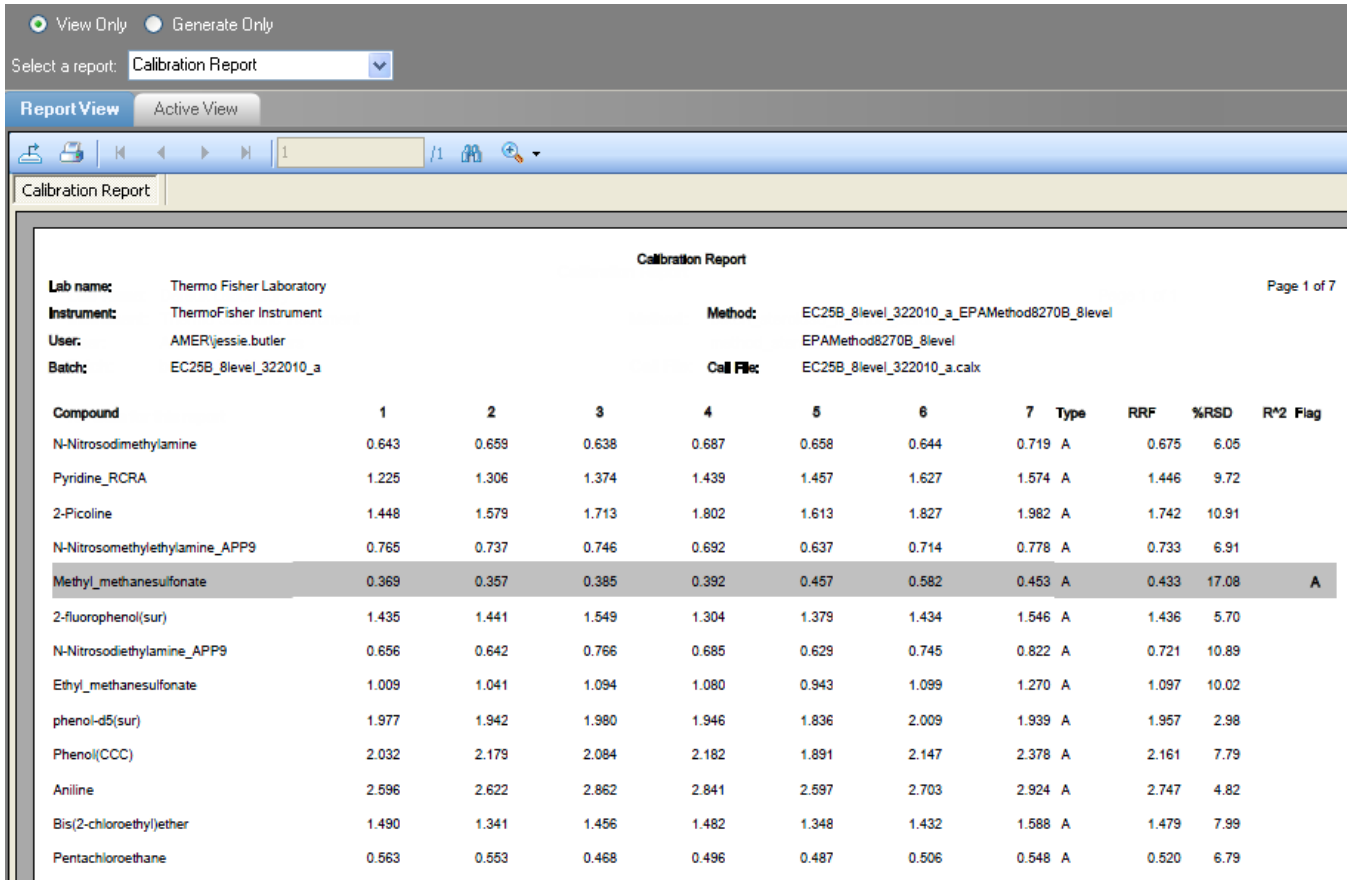
Use the following procedures:

- To print a standard or target screening report
- To export a standard report
- To search for text
- To enlarge the report text

❖ To print a standard or target screening report

1. Select the report you want to print from the Select a Report list.
2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.



Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: ThermoFisher Instrument
User: AMER\jessie.butler
Batch: EC25B_8level_322010_a
Method: EC25B_8level_322010_a_EPAMethod8270B_8level EPAMethod8270B_8level
Cal File: EC25B_8level_322010_a.calx

Page 1 of 7

Compound	1	2	3	4	5	6	7	Type	RRF	%RSD	R^2	Flag
N-Nitrosodimethylamine	0.643	0.659	0.638	0.687	0.658	0.644	0.719	A	0.675	6.05		
Pyridine_RCRA	1.225	1.306	1.374	1.439	1.457	1.627	1.574	A	1.446	9.72		
2-Picoline	1.448	1.579	1.713	1.802	1.613	1.827	1.982	A	1.742	10.91		
N-Nitrosomethylethylamine_APP9	0.765	0.737	0.746	0.692	0.637	0.714	0.778	A	0.733	6.91		
Methyl_methanesulfonate	0.369	0.357	0.385	0.392	0.457	0.582	0.453	A	0.433	17.08		A
2-fluorophenol(sur)	1.435	1.441	1.549	1.304	1.379	1.434	1.546	A	1.436	5.70		
N-Nitrosodiethylamine_APP9	0.656	0.642	0.766	0.685	0.629	0.745	0.822	A	0.721	10.89		
Ethyl_methanesulfonate	1.009	1.041	1.094	1.080	0.943	1.099	1.270	A	1.097	10.02		
phenol-d5(sur)	1.977	1.942	1.980	1.946	1.836	2.009	1.939	A	1.957	2.98		
Phenol(CCC)	2.032	2.179	2.084	2.182	1.891	2.147	2.378	A	2.161	7.79		
Aniline	2.596	2.622	2.862	2.841	2.597	2.703	2.924	A	2.747	4.82		
Bis(2-chloroethyl)ether	1.490	1.341	1.456	1.482	1.348	1.432	1.588	A	1.479	7.99		
Pentachloroethane	0.563	0.553	0.468	0.496	0.487	0.506	0.548	A	0.520	6.79		

3. Click the **Print Report** button, .

   The Print dialog box for your default printer opens.

4. Follow the typical procedure to print from your printer.

   Landscape reports automatically rotate to fit the paper.

❖ To export a standard report

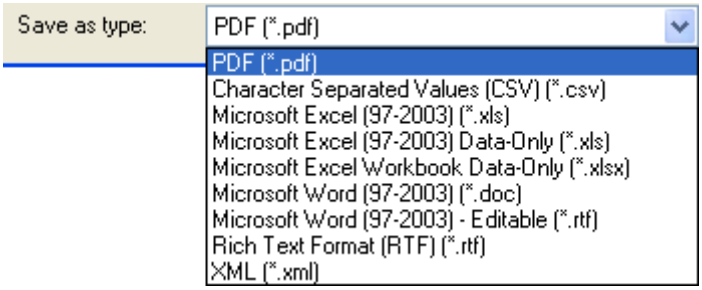
1. Select the report you want to print from the Select a Report list.
2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.

3. Click the **Export Report** button, .

   The Export Report dialog box opens.

4. Locate the folder where you want to write the report file.
5. Type a file name for the exported report file.
6. Select a file type from the Save as Type list:



7. Click **Save**.

   The TraceFinder application saves the file as the specified file type and writes the report file to the specified folder.

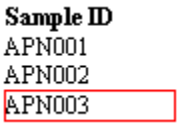
❖ To search for text

1. Select a report from the Select a Report list.
2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.
3. Click the **Find Text** button, .

   The Find Text dialog box opens.
4. Enter your text and click **Find Next**.

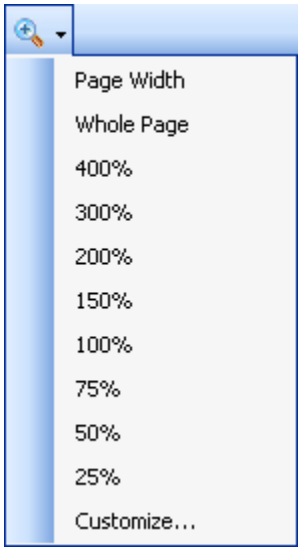
   When the TraceFinder application locates the text, it encloses the text in a red box.



❖ To enlarge the report text

1. Select a report from the Select a Report list.
2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.
3. Click the **Zoom** button, , and select a zoom scale.



Working with Active View

Use the Active View page to view quantitative data for each sample in a report. Data in the Active View are labeled with flag information. These flags are based on a comparison of the batch data to criteria defined in the master method.

❖ To display the Active View page

Click the **Active View** tab.

The Active View page displays quantitative data and QAQC error flags for each sample. See "Active View page" on page 336.

❖ 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 filter which compounds to display

Click the Showing button to display either all compounds or only compounds that are flagged for failing a QAQC test.

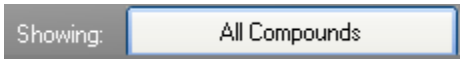


Figure 84. Active View page

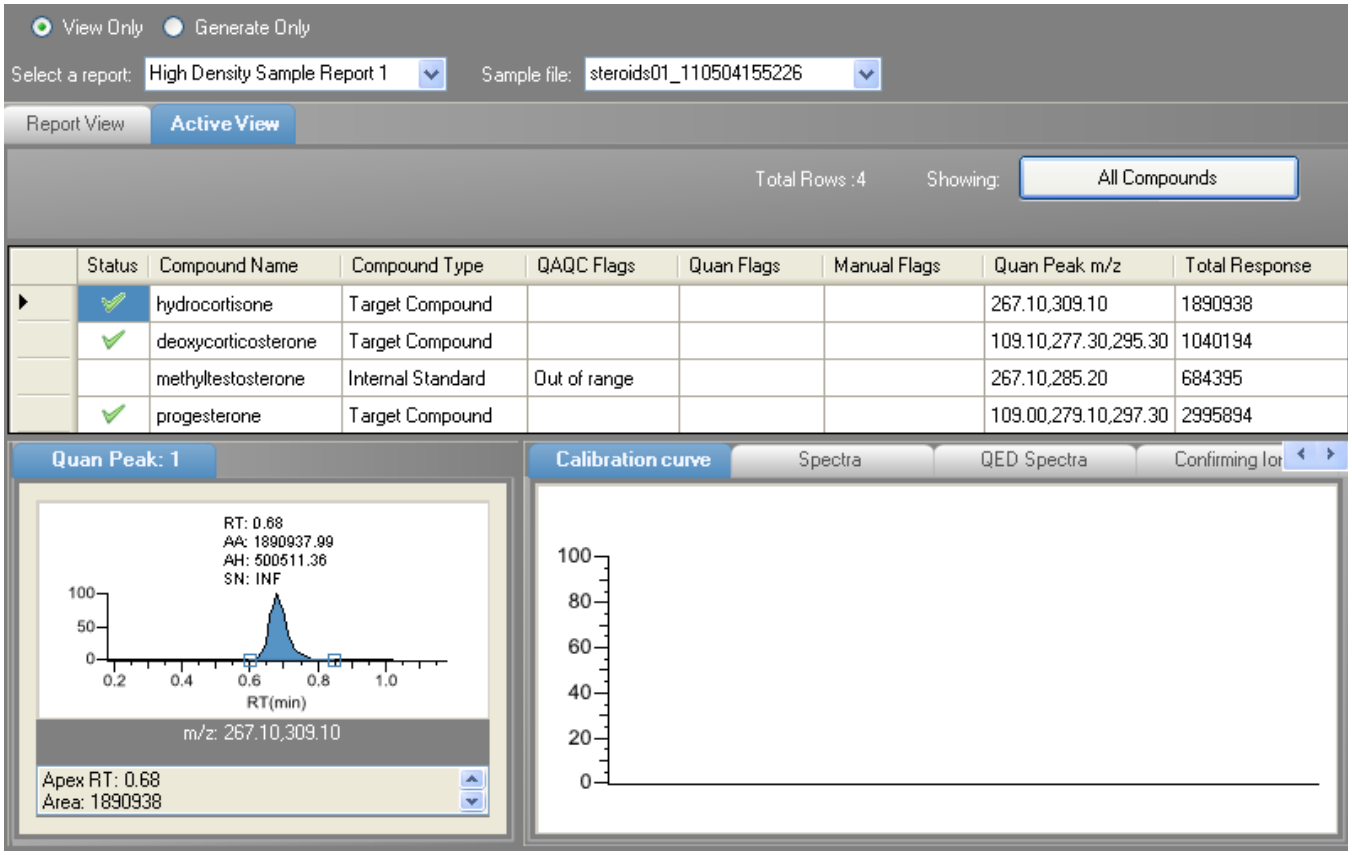


Table 72. Active View parameters (Sheet 1 of 4)

Parameter	Description
View Only	The Active View pane is available only when View Only is selected.
Select a report	Displays the report types created for the current batch.
Sample file	Used when the report type includes separate reports for each sample.
Total Rows	The number of compound rows currently displayed in the pane.
Showing	Displays all compounds or only the flagged compounds.

Table 72. Active View parameters (Sheet 2 of 4)

Parameter	Description
Column headings	Many column headings are specific to individual reports. See "Active View Report Contents" on page 340.
Status	Indicates the status of the reported compound. • A yellow check mark indicates one of the following conditions: – The compound was manually integrated. – Any of the confirming peaks was manually integrated. – The compound has quan flags. • A red check mark indicates that the QAQC checks failed. • A green check mark indicates that none of these conditions exist. When the compound is an internal standard, warnings are displayed only on the internal standard report. The Status column is blank for Manual Integration reports.
Compound Name	Alphanumeric name assigned to the compound.
Compound Type	Target Compound, Internal Standard, or Surrogate.
QAQC Flags	Indicates that the QAQC check for the sample failed. The QAQC column is not used for Manual Integration reports.
Quan Flags	• Limit of Detection (LOD) • Limit of Quantitation (LOQ) • Limit of Reporting (LOR) • Values between the limit of detection and the limit of quantitation, known as the J flag • Upper Limit of Linearity (ULOL) Quan flags do not apply to these sample types: Cal Std, Chk Std, Matrix Blank, or Solvent. The Quan Flag column is not used for Manual Integration reports.
Manual Flags	Indicates manually integrated peaks. • **M** indicates a manually integrated quan peak. • **m** indicates a manually integrated confirming peak.
Depending on the selected report, the Active View page contains any or all of the following parameters:	
Quan Peak *m/z*	Mass-to-charge ratio for the selected quantitation peak.
Total Response	The sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quan peak.
Quan peak RT	Retention time for the quan peak.
Theoretical amount	Theoretical amount of the compound. Reports N/A when not applicable.
Concentration	
Confirming *n* Mass	Mass of the confirming peak.

Table 72. Active View parameters (Sheet 3 of 4)

Parameter	Description
Confirming *n* Response	Response of the confirming peak.
Confirming *n* Manual Flag	Indicates a manually integrated confirming peak.
Confirming *n* Ion Ratio Flag	Indicates that the ion ratio is out of range.
Confirming *n* Ion Ratio	Actual ratio of the confirming ion response to the quan ion response.
Confirming *n* Range	Acceptable range for the confirming ion.
Retention Time	The time after injection when the compound elutes. The total time that the compound is retained on the column.
Quan mass	The mass-to-charge ratio used to determine the peak area and peak height of the compound.
Response	Sum of all Quan Peak Response values for the compound.
Injection concentration	Calculated amount as the sample was injected, with no conversion applied.
Injection Units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 151.
Sample Concentration	The injected concentration multiplied by the conversion factor.
Sample Units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 151.
QIon	Mass range for the quan peak.
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Manual Integration reports	
m/z	Mass-to-charge ratio for the quan peak.
Method RT	Apex retention time for the method-integrated peak.
Method Peak Height	Height of the method-integrated peak.
Method Peak Area	Area of the method-integrated peak.
Manual RT	Apex retention time for the manually integrated peak.
Manual Peak Height	Height of the manually integrated peak.
Manual Peak Area	Area of the manually integrated peak.

Table 72. Active View parameters (Sheet 4 of 4)

Parameter	Description
Internal Standard reports	
Std Response	Average of the internal standard's response as found in the calibration file.
Minimum Response	Minimum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 166.
Maximum Response	Maximum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 166.
Sample Response	Area found in the sample.
Std RT	Average retention time as found in the calibration file.
Min RT	Minimum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 166.
Max RT	Maximum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 166.
Sample RT	Retention time found in the sample.
Graphical data	
Quan Peak 1	
Calibration curve	Displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration.
Spectra	Displays a comparison of the spectra found in the data and the method reference.
QED Spectra	Displays the averaged QED spectra from the raw data file and the datastore match. If the sample contains no QED data, the page is blank.
Confirming Ions	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.

Active View Report Contents

Each standard report that uses the Active View displays values that are common to all reports:

- Common Active View report columns

In addition to the common values, the following reports display additional active view features:

- Blank Report Active View columns
- Calibration Report Active View columns
- High Density Sample Report 1 and High Density Sample Report 1 Long Active View columns
- High Density Sample Report 2 and High Density Sample Report 2 Long Active View columns
- High Density Sample Report 3 and High Density Sample Report 3 Long Active View columns
- Internal Standard Summary Report Active View columns
- Ion Ratio Failure Report Active View columns
- LCSLCSD Report Active View columns (Environmental and Food Safety only)
- Manual Integration Report Active View columns
- Method Detection Limit Report Active View columns (Environmental and Food Safety only)
- Method Validation Report Active View columns (Environmental and Food Safety only)
- MSMSD Report Active View columns (Environmental and Food Safety only)
- Quantitation Report Active View columns
- Solvent Blank Report Active View columns

Table 73. Common Active View report columns

Column	Description
Status	Indicates the status of the reported compound. • A yellow caution sign indicates one of the following conditions: – The compound was manually integrated. – Any of the confirming peaks was manually integrated. – The compound has quan flags. – The compound has a QAQC failure. • A green check mark indicates that none of these conditions exists. When the compound is an internal standard, warning flags are displayed only on the internal standard report.
Compound name	Alphanumeric name assigned to the compound.
Compound type	Target Compound, Internal Standard, or Surrogate.
QAQC flags	Indicates that the QAQC check for the sample failed. This column is not included on the Method Validation and MDL reports.
Quan flags	• Limit of Detection (LOD) • Limit of Quantitation (LOQ) • Limit of Reporting (LOR) • Values between the limit of detection and the limit of quantitation, known as the J flag • Upper Limit of Linearity (ULOL) Quan flags do not apply to these sample types: Cal Std, Chk Std, Matrix Blank, or Solvent. This column is not included on the Calibration report. This column is not included on the Calibration Curve report. This column is not included on the Method Validation, Method Detection Limit, LCS, or LCSD reports.
Manual flags	Indicates manually integrated peaks. • **M** indicates a manually integrated quan peak. • **m** indicates a manually integrated confirming peak.

Table 74. Blank Report Active View columns

Column	Description
Retention Time	Retention time for the quan mass. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Quan Mass	Mass range for the quan peak.
Response	Sum of all Quan Peak Response values for the compound.
Inj Conc	Calculated amount as the sample was injected, with no conversion applied.
Inj Units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 151.
Sample Conc	Calculated amount multiplied by the conversion factor.
Sample Units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 151.

Table 75. Calibration Report Active View columns (Sheet 1 of 2)

Column	Description
Curve Type	The type of curve used when calibrating the compound (linear, quadratic, or average response factor).
Average RF	The average response factor. Applicable if curve type is Average RF.
Average Response	The average response for the internal standard across all calibration points. Applies only to Internal Standard sample types.
A0	The value with no X. Applies only to linear and quadratic curves.
A1	The X value. Applies only to linear and quadratic curves.
A2	The X^2 value. Applies only to quadratic curves.
R^2	The minimum correlation coefficient (r^2) for an acceptable calibration (when in linear or quadratic mode).

Table 75. Calibration Report Active View columns (Sheet 2 of 2)

Column	Description
RSD	Relative standard deviation. Applies only to internal standards and targets calibrated with an average RF curve.
Level	The column specifies the level name; the field value specifies the data point used in calibration. This field can be Response Factor for external calibration, Response Ratio for internal linear or quadratic, or Relative Response Factor for Internal Average RF. There is one column for each level in the curve. If the batch uses an extended calibration, there might be more columns than calibration standards in the current batch.

Table 76. High Density Sample Report 1 and High Density Sample Report 1 Long Active View columns

Column	Description
m/z	Mass-to-charge ratio for the quan peak.
Total Response	The sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quan peak.
Quan Peak RT	Retention time for the quan peak.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.

Table 77. High Density Sample Report 2 and High Density Sample Report 2 Long Active View columns (Sheet 1 of 2)

Column	Description
m/z	Mass-to-charge ratio for the quan peak.
Total Response	Sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quan peak.
Quan Peak RT	Retention time for the quan peak.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.
Confirming 1 Mass	Mass of the confirming peak.
Confirming 1 Response	Response of the confirming peak.
Confirming 1 Manual Flag	Indicates a manually integrated confirming peak.

Table 77. High Density Sample Report 2 and High Density Sample Report 2 Long Active View columns (Sheet 2 of 2)

Column	Description
Confirming 1 Ion Ratio Flag	Indicates that the ion ratio is out of range.
Confirming 1 Ion Ratio	Actual ratio of the confirming ion response to the quan ion response.
Confirming 1 Range	Acceptable range for the confirming ion.

Table 78. High Density Sample Report 3 and High Density Sample Report 3 Long Active View columns

Column	Description
m/z	Mass-to-charge ratio for the quan peak.
Total Response	Sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quan peak.
Quan Peak RT	Retention time for the quan peak.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.
Confirming 1 Mass	Mass of the confirming peak.
Confirming 1 Response	Response of the confirming peak.
Confirming 1 Manual Flag	Indicates a manually integrated confirming peak.
Confirming 1 Ion Ratio Flag	Indicates that the ion ratio is out of range.
Confirming 1 Ion Ratio	Actual ratio of the confirming ion response to the quan ion response.
Confirming 1 Range	Acceptable range for the confirming ion.
Confirming 2 Mass	Mass of the confirming peak.
Confirming 2 Response	Response of the confirming peak.
Confirming 2 Manual Flag	Indicates a manually integrated confirming peak.
Confirming 2 Ion Ratio Flag	Indicates that the ion ratio is out of range.
Confirming 2 Ion Ratio	Actual ratio of the confirming ion response to the quan ion response.
Confirming 2 Range	Acceptable range for the confirming ion.

Table 79. Internal Standard Summary Report Active View columns

Column	Description
Std Response	Average of the internal standard's response as found in the calibration file.
Minimum Response	Minimum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 166.
Maximum Response	Maximum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 166.
Sample Response	Area found in the sample.
Std RT	Average retention time as found in the calibration file.
Min RT	Minimum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 166.
Max RT	Maximum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 166.
Sample RT	Retention time found in the sample.

Table 80. Ion Ratio Failure Report Active View columns

Column	Description
Quan Ion	The ion for quan peak.
Qual Ion	The ion for the confirming peak.
Quan Ion Response	Response of the quan ion.
Qual Ion Response	Response of the qual ion.
Ratio	The ratio of the confirming ion response to the quan ion response.
Range	The acceptable range.

Table 81. LCSLCSD Report Active View columns (Environmental and Food Safety only) (Sheet 1 of 2)

Column	Description
Spike Amount	Lab control theoretical concentration.
LCS Concentration	Lab control spike concentration.
LCS % Received	Lab control concentration percentage.
Lower Limit %	Recovery lower limit as specified in the master method. See the Limits section in "Editing the Flags Page" on page 159.
Upper Limit %	Recovery upper limit as specified in the master method. See the Limits section in "Editing the Flags Page" on page 159.

Table 81. LCSLCSD Report Active View columns (Environmental and Food Safety only) (Sheet 2 of 2)

Column	Description
LCSD Concentration	Lab control spike duplicate concentration.
LCSD % Received	Lab control spike duplicate concentration percentage.
RPD	Lab control relative percentage difference.
Max RPD	Lab control spike maximum relative percentage difference (set in method).
Number of Rec Failures	Number of recovery failures for lab control spike concentration and lab control spike concentration duplicate.
Number of RPD Failures	Number of relative percentage difference failures for lab control spike concentration and lab control spike concentration duplicate.

Note For LCSLCSD batch reports, the application displays the active view peak graphics only when you click a field pertaining to a sample, such as the LCS or LCSD concentration fields.

Table 82. Manual Integration Report Active View columns

Column	Description
m/z	Mass-to-charge ratio for the quan peak.
Method RT	Apex retention time for the method-integrated peak.
Method Peak Height	Height for the method-integrated peak.
Method Peak Area	Area for the method-integrated peak.
Manual RT	Apex retention time for the manually integrated peak.
Manual Peak Height	Height of the manually integrated peak.
Manual Peak Area	Area of the manually integrated peak.

Table 83. Method Detection Limit Report Active View columns (Environmental and Food Safety only)

Column	Description
Avg Conc	The average of the concentration for the compound across all samples.
Std Dev	The standard deviation of the concentration.
t-stat	The t-statistic value defined as the ratio of a coefficient to its standard error.
% RSD	%RSD of concentrations
MDL	Method detection limits. The calculated limit of detection.

Note For Method Detection Limit batch reports, the active view peak graphics are shown only when you click a field pertaining to a sample. These numbered fields are to the right of the MDL column.

Table 84. Method Validation Report Active View columns (Environmental and Food Safety only)

Column	Description
Avg Conc	The average of the concentration for the compound across all samples.
Theo Conc	Values for each compound that represent the expected theoretical concentration of that compound in the sample as defined in the master method. See the Meth Val section in "Editing the Flags Page" on page 159.
% Diff	The percentage difference calculated as ([MethodValidationMeanValue minus the Theo Conc] divided by the Theo Conc) multiplied by 100.
Min Conc	Calculated by (Min recovery percent * Theo Conc) divided by 100.
Max Conc	Calculated by (Max recovery percent * Theo Conc) divided by 100.
% RSD	%RSD of concentrations
Max % RSD	The maximum relative standard deviation (RSD) of the set of observed concentrations for a component across the set of method validation samples (when in average RF mode) as defined in the master method. See the Meth Val section in "Editing the Flags Page" on page 159.
Calculated Amount <*Sample Name*>	This field is reproduced for every Method Val sample.

Table 85. MSMSD Report Active View columns (Environmental and Food Safety only)

Column	Description
Unknown Concentration	Concentration of the unknown sample.
Spike Amount	Matrix spike theoretical concentration.
MS Concentration	Matrix spike concentration.
MS % Received	Matrix spike concentration percentage.
Lower Limit %	Recovery lower limit as specified in the master method. See the Limits section in "Editing the Flags Page" on page 159.
Upper Limit %	Recovery upper limit as specified in the master method. See the Limits section in "Editing the Flags Page" on page 159.
MSD Concentration	Matrix spike duplicate concentration.
MSD % Received	Matrix spike duplicate concentration percentage.
RPD	Matrix spike relative percentage difference.
Max RPD	Maximum relative percentage difference as specified in the master method. See the Lab Control section in "Editing the Flags Page" on page 159.
Number of Rec Failures	Number of matrix spike and matrix spike duplicate failures.
Number of RPD Failures	Number of relative percentage difference failures.

Note For MSMSD batch reports, the active view peak graphics are shown only when you click a field pertaining to a sample, such as Unknown, MS, or MSD concentration fields.

Table 86. Quantitation Report Active View columns (Sheet 1 of 2)

Column	Description
RT	Retention time for the peak. The time after injection when the compound elutes. The total time that the compound is retained on the column.
QIon	Mass range for the quan peak.
Response	Sum of all quan peak response values for the compound.

Table 86. Quantitation Report Active View columns (Sheet 2 of 2)

Column	Description
Injected Concentration (DE2999)	Calculated amount as the sample was injected, with no conversion applied. As each additional sample is processed, calibration data change; therefore, except for the final sample in a batch, a report in active view or report view shows different values from a physical (PDF, XML, or printed) report created at the end of processing. To avoid this discrepancy, do one of the following: • For the standard Quantitation Report or Quantitation Report - 2, observe the active or report view for only the last sample in the batch. • For the custom Quantitation Report, make the report a batch-level report.
Injected units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 151.
Sample Conc	Calculated injection amount multiplied by the conversion factor. See the Injected Concentration description.
Sample units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 151.

Table 87. Solvent Blank Report Active View columns

Column	Description
RT	Retention time for the quan peak. The time after injection when the compound elutes. The total time that the compound is retained on the column.
QIon	Mass range for the quan peak.
Response	Sum of all Quan Peak Response values for the compound.
Method	Method of evaluation defined in the method.
Upper Limit	Defined in the method.

Working in the Local Method View

A local method is a copy of a master method associated with a batch. You can edit only the local copy of the method, or you can edit the master method and overwrite the local copy with the edited master method.

In the Local Method view, you can edit the local method parameters. A local method is a copy of a master method associated with a batch. Local methods are named *BatchName_MasterMethodName*.

❖ 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.

   You can edit many of the method parameters in a local method. Editing the local method does not affect parameters in the master method.

   For detailed descriptions of method parameters, see "Working with Master Methods" on page 88.

3. Enter any local changes to the method.

4. When you have finished editing the local method, choose **File > Save**.

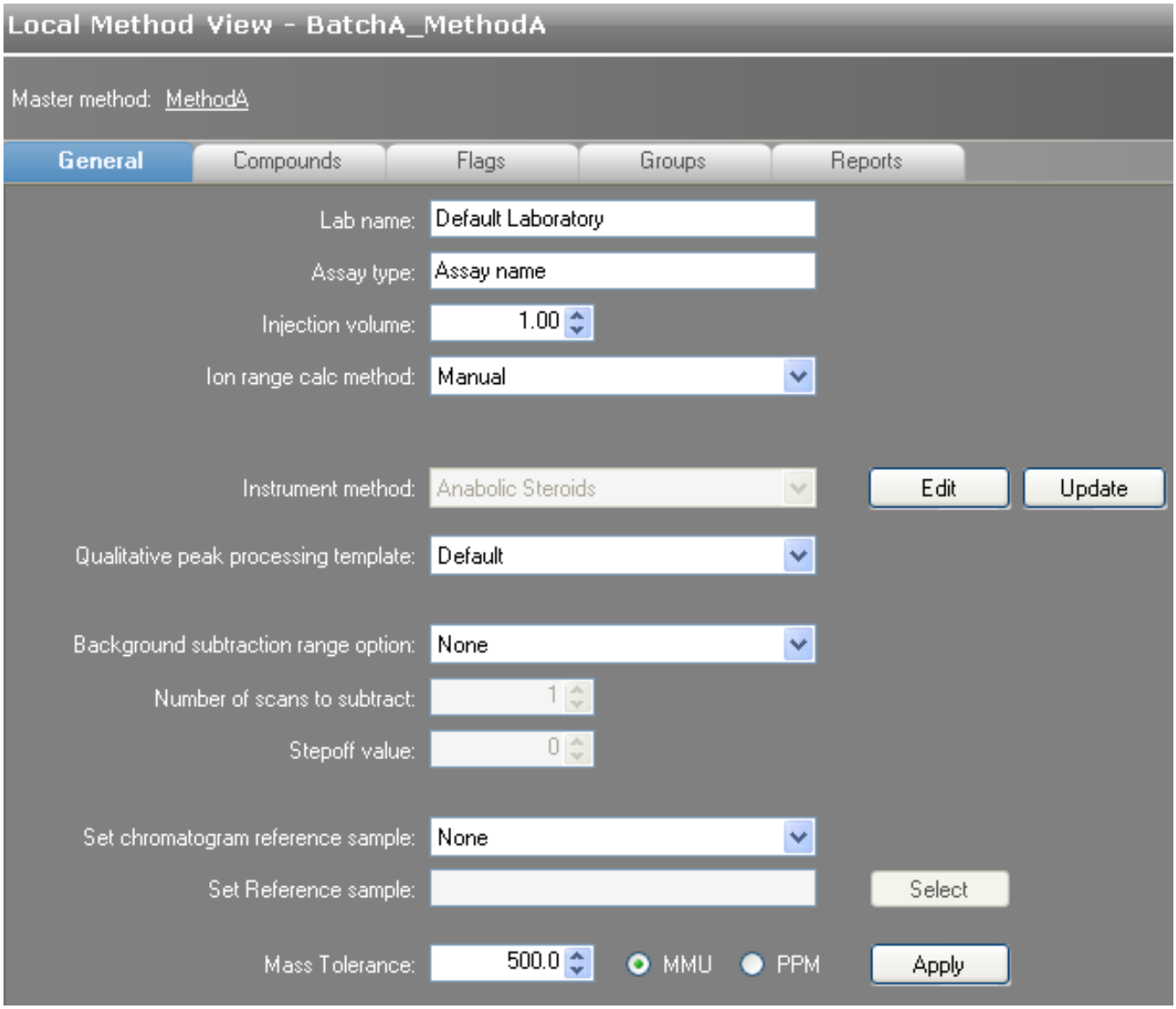
5. To process the batch or create new reports with the edited local method, return to the Batch View and submit the batch.

❖ To overwrite the local method with the master method in the Batch View

In the Batch View, click **Update**.

The application overwrites the local method with the master method of the same name. You can use this feature to overwrite an edited local method with the original master method or to overwrite the local method with an updated master method.

Figure 85. Local Method View



Reports

This appendix contains information about standard and custom reports.

Contents

- Specifying Reports
- Report Flags
- Sample Standard Reports

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 a user in the ITAdmin or LabDirector role, you can configure a list of reports that are available for Method Development or Acquisition modes.

For detailed information about configuring reports in the Configuration mode, see "Specifying the Reports Configuration" on page 58.

For detailed information about specifying reports when you create a method in the Method Development mode, see "Editing the Reports Page" on page 173.

For detailed information about viewing batch reports in the Acquisition mode, see "Selecting and Reviewing Reports" on page 233.

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 description for each of your reports. The default report description is the report name.

The TraceFinder application can generate the following types of standard reports:

- Batch Report
- Batch Report Rev 1
- Blank Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- Confirmation Report 2
- High Density Calibration Report
- 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 (Environmental and Food Safety only)
- Manual Integration Report
- Method Detection Limit Report (Environmental and Food Safety only)
- Method Report
- Method Validation Report (Environmental and Food Safety only)
- MSMSD Report (Environmental and Food Safety only)
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary Report

To view an example of each type of standard report, see "Sample Standard Reports" on page 357.

Custom Reports

For each custom report you generate, you can create a hardcopy printout or an Excel Macro-Enabled Workbook (.xlsm) output file. The default report description is the report name.

A user in the ITAdmin or LabDirector role 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
- HighDensitySampleReport4
- HighDensitySampleReport5
- QuantitationReport
- SteroidAnalysisReport

Target Screening Reports

- Target Screening Long Report
- Target Screening Summary Report

Report Flags

When generating or viewing a report, you might see one of the following quantification or calibration flags listed on the page.

Table 88. 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 89. 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 flags 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 Standard Reports

This section shows samples of the following standard report types:

- Batch Report
- Batch Report Rev 1
- Blank Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- Confirmation Report 2
- High Density Calibration Report
- 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 (Environmental and Food Safety only)
- Manual Integration Report
- Method Detection Limit Report (Environmental and Food Safety only)
- Method Report
- Method Validation Report (Environmental and Food Safety only)
- MSMSD Report (Environmental and Food Safety only)
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary 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: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Filename	Date/time	Sample ID	Sample name	Level	Sample type	Vial Pos	Inj vol	Dilution	Comment
unextracted	4/17/2008 5:05:21 PM	unextracted		N/A	Unextracted	1	1.000	1.0	
cal_1	4/17/2008 5:05:47 PM	cal 1 = 6 ng/mL		level 1	Calibrator	2	1.000	1.0	
cal_2	4/17/2008 5:06:13 PM	cal 2 = 15 ng/mL		level 2	Calibrator	3	1.000	1.0	
cal_3	4/17/2008 5:06:39 PM	cal 3 = 176 ng/mL		level 3	Calibrator	4	1.000	1.0	
hydrolysis	4/17/2008 5:07:31 PM	hydrolysis		N/A	Hydrolysis	6	1.000	1.0	
negative	4/17/2008 5:07:05 PM	negative		N/A	Negative	5	1.000	1.0	
qc_40	4/17/2008 5:07:57 PM	qc 40% = 6 ng/mL		level 40	QC	7	1.000	1.0	
qc_125	4/17/2008 5:10:17 PM	qc 125% = 18.75 r		level 125	QC	12	1.000	1.0	
solvent	4/17/2008 5:10:45 PM	solvent		N/A	Solvent	13	1.000	1.0	
specimen_1	4/17/2008 5:08:25 PM	specimen 1		N/A	Specimen/Qual	8	1.000	1.0	
specimen_2	4/17/2008 5:08:51 PM	specimen 2		N/A	Specimen	9	1.000	1.0	
specimen_3	4/17/2008 5:09:19 PM	specimen 3		N/A	Specimen	10	1.000	1.0	
specimen_4	4/17/2008 5:09:49 PM	specimen 4		N/A	Specimen	11	1.000	1.0	

Batch Report Rev 1

Batch Report Rev 1

Lab Name: Default Laboratory
Instrument: Thermo Scientific Instrument
User:
Batch: 50

Method: 50_appleMF
appleMF
Call File:

File Name	Date/Time	Sample ID	Sample Name	Level	Sample Type	Vial Pos	Inj Vol	Conv Factor	Channel
Unknown1	2/17/2011 2:57:04 AM			N/A	Unknown/TIC	CStk1-01:1	20.000	1.0	Channel 1
Unknown2	2/17/2011 3:02:33 AM			N/A	Unknown	CStk1-01:2	20.000	1.0	Channel 3
Unknown3	2/17/2011 3:06:57 AM			N/A	Matrix Blank	CStk1-01:3	20.000	1.0	Channel 1
Unknown4	2/17/2011 3:31:26 AM			N/A	Unknown	CStk1-01:4	20.000	1.0	Channel 1
Unknown5	2/17/2011 3:36:55 AM			N/A	Unknown	CStk1-01:5	20.000	1.0	Channel 3
Unknown6	2/17/2011 3:41:21 AM			N/A	Unknown	CStk1-01:6	20.000	1.0	Channel 1
Unknown7	2/17/2011 3:45:45 AM			N/A	Solvent	CStk1-01:7	20.000	1.0	Channel 3
Unknown8	2/17/2011 3:50:10 AM			N/A	Unknown	CStk1-01:8	20.000	1.0	Channel 1
Unknown9	2/17/2011 3:54:34 AM			N/A	Unknown	CStk1-01:9	20.000	1.0	Channel 3
Unknown10	2/17/2011 3:59:00 AM			N/A	Unknown	CStk1-01:10	20.000	1.0	Channel 1
Unknown11	2/17/2011 4:03:22 AM			N/A	Matrix Blank	CStk1-01:11	20.000	1.0	Channel 3
Unknown12	2/17/2011 4:07:46 AM			N/A	Unknown	CStk1-01:12	20.000	1.0	Channel 1
Unknown13	2/17/2011 4:12:10 AM			N/A	Unknown	CStk1-01:13	20.000	1.0	Channel 3
Unknown14	2/17/2011 4:16:34 AM			N/A	Unknown	CStk1-01:14	20.000	1.0	Channel 1
Unknown15	2/17/2011 4:20:58 AM			N/A	Unknown	CStk1-01:15	20.000	1.0	Channel 3
Unknown16	2/17/2011 4:25:22 AM			N/A	Unknown	CStk1-01:16	20.000	1.0	Channel 1
Unknown17	2/17/2011 4:29:46 AM			N/A	Unknown	CStk1-01:17	20.000	1.0	Channel 3
Unknown18	2/17/2011 4:34:12 AM			N/A	Unknown	CStk1-01:18	20.000	1.0	Channel 1
Unknown19	2/17/2011 4:38:34 AM			N/A	Unknown	CStk1-01:19	20.000	1.0	Channel 3
Unknown20	2/17/2011 4:42:58 AM			N/A	Unknown	CStk1-01:20	20.000	1.0	Channel 1
Unknown21	2/17/2011 4:47:22 AM			N/A	Unknown	CStk1-01:21	20.000	1.0	Channel 3
Unknown22	2/17/2011 4:51:46 AM			N/A	Unknown	CStk1-01:22	20.000	1.0	Channel 1
Unknown23	2/17/2011 4:56:10 AM			N/A	Unknown	CStk1-01:23	20.000	1.0	Channel 3
Unknown24	2/17/2011 5:00:36 AM			N/A	Unknown	CStk1-01:24	20.000	1.0	Channel 1
Unknown25	2/17/2011 5:04:59 AM			N/A	Unknown	CStk1-01:25	20.000	1.0	Channel 3
Unknown26	2/17/2011 5:09:23 AM			N/A	Unknown	CStk1-01:26	20.000	1.0	Channel 1
Unknown27	2/17/2011 5:13:47 AM			N/A	Unknown	CStk1-01:27	20.000	1.0	Channel 3
Unknown28	2/17/2011 5:18:13 AM			N/A	Unknown	CStk1-01:28	20.000	1.0	Channel 1
Unknown29	2/17/2011 5:22:35 AM			N/A	Unknown	CStk1-01:29	20.000	1.0	Channel 3
Unknown30	2/17/2011 5:27:01 AM			N/A	Unknown	CStk1-01:30	20.000	1.0	Channel 1
Unknown31	2/17/2011 5:31:23 AM			N/A	Unknown	CStk1-01:31	20.000	1.0	Channel 3

Generation Date: Thursday, February 17, 2011 7:02:59 AM

Revision: 1

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 ☐

Calibration Report

Calibration Report

Page 1 of 3

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Calibration summary

Compound	Manually integrated	Curve type	A0 y-Intercept Mean RF	A1 Slope	A2	R^2 R^2 %RSD	Flag
Int_Std		I	655596			7.51	
Drug_A		L	3.024e-2	5.471e-2		1.0000	
					Average %RSD:	3.15	

Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard; Note: Amounts displayed for internal standards represent the ISTD Response.
Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.
Manually integrated

Calibration Report

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	Method:	Drug_A_Drug_A
User:	AMER\jamie.humphries		Drug_A
Batch:	Drug_A	Cali File:	Drug_A.calx

Calibration data points

Compound	Curve type	level 1	level 2	level 3
Int_Std	I	678044	689630	599115
Drug_A	L	0.336	0.875	9.659

Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard; Note: Amounts displayed for internal standards represent the ISTD Response.
Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.
Manually integrated

Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

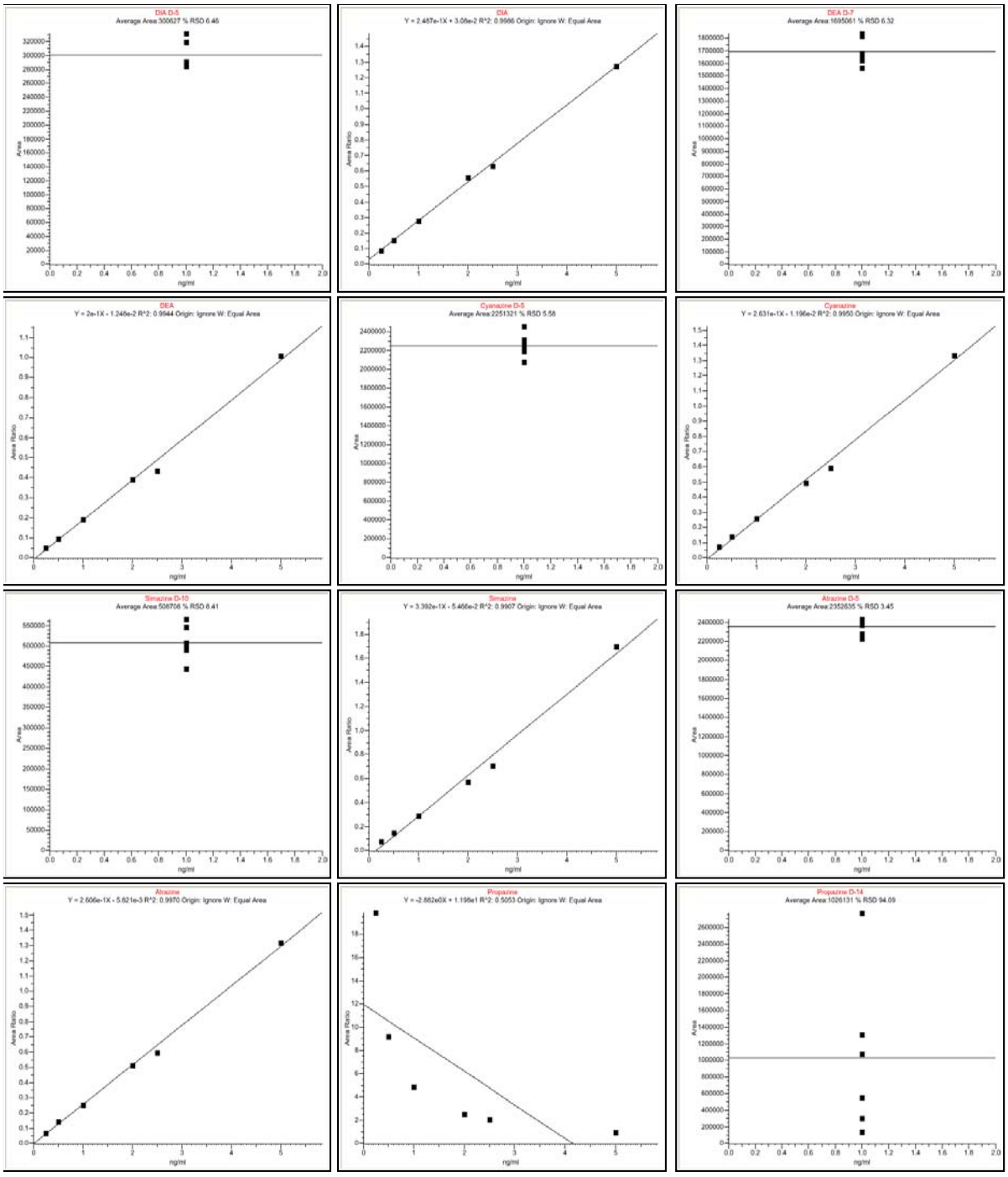
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	
3	cal 2 = 15 ng/mL	cal_2	level 2		4/17/2008 5:06:13 PM	
4	cal 3 = 176 ng/mL	cal_3	level 3		4/17/2008 5:06:39 PM	

Curve Type: A=Average RF; L=Linear; Q=Quadratic;|=Internal standard; Note: Amounts displayed for internal standards represent the ISTD Response.
Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.
Manually integrated

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



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**

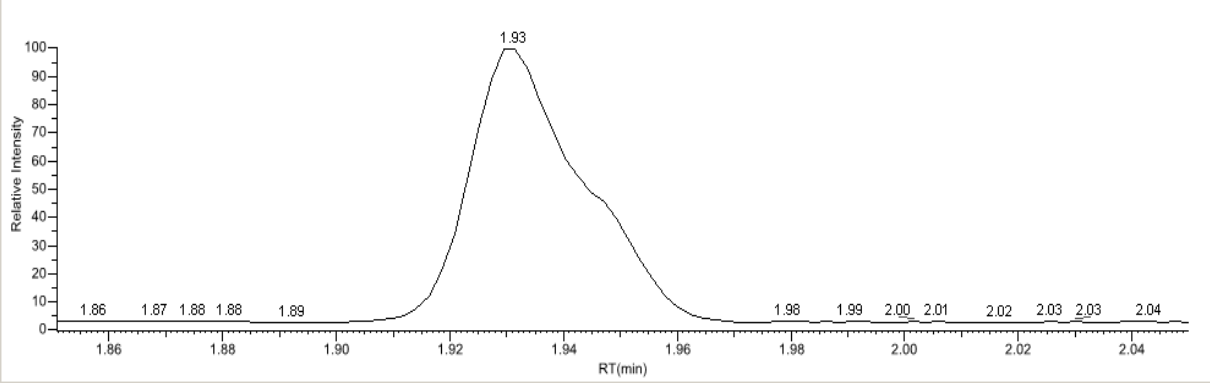
Chromatogram Report

Chromatogram Report

Page 1 of 1

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	Method:	Drug_A_Drug_A
User:	AMER\jamie.humphries		Drug_A
Batch:	Drug_A	Cali File:	Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	



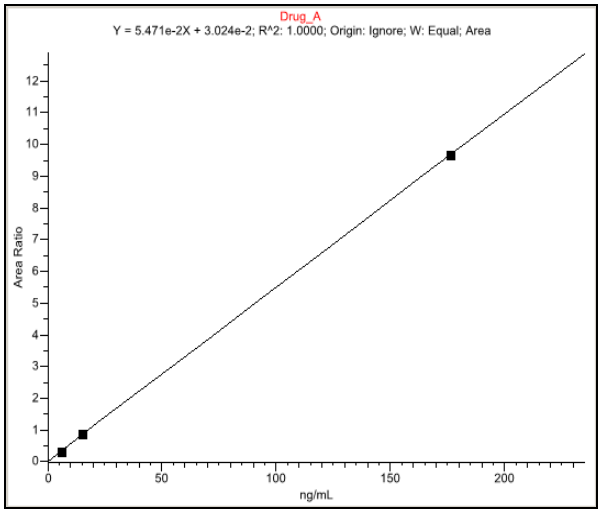
Compound Calibration Report

Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Compound Name: Drug_A



Linear
Pass

Level	Std Amount	Std Area	IS Amount	IS Area	Response ratio	Calc amt	Units
level 1	6.000	227568	15.000	678044	0.336	5.581	ng/mL
level 2	15.000	603523	15.000	689630	0.875	15.441	ng/mL
level 3	176.000	5786683	15.000	599115	9.659	175.976	ng/mL

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: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	
3	cal 2 = 15 ng/mL	cal_2	level 2		4/17/2008 5:06:13 PM	
4	cal 3 = 176 ng/mL	cal_3	level 3		4/17/2008 5:06:39 PM	

Manually Integrated:

Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount

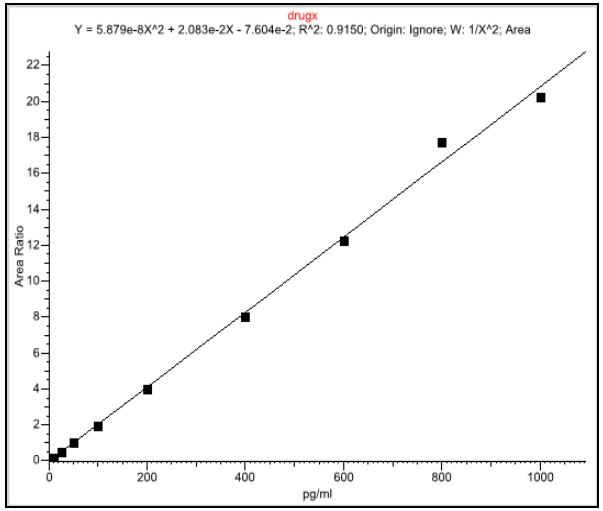
Compound Calibration Report - Alternate

Compound Calibration Report - Alternate

Lab Name: ThermoFisher Laboratory
Instrument: ThermoFisher Instrument
User: Jamie
Batch: Drux X

Method: Drux X_drugx
drugx
Cali File: Drux X.calx

Compound Name: drugx



Quadratic
Fail AR

Level	File Name	Std Amount	Std Area	IS Amount	IS Area	Response ratio	Calc Amt	Units	Min Range	Max Range	% RSD	Flags
cal 1	drugx_01	10.00	193483	100.00	982341	0.197	13.10	pg/ml	8.00	12.00	86.603	A
cal 1	drugx_02	10.00	N/F	100.00	950007	N/F	N/F	pg/ml	8.00	12.00	86.603	A
cal 1	drugx_03	10.00	183718	100.00	938286	0.196	13.04	pg/ml	8.00	12.00	86.603	A
cal 2	drugx_04	25.00	442796	100.00	945893	0.468	26.11	pg/ml	20.00	30.00	N/A	
cal 3	drugx_05	50.00	940186	100.00	941082	0.999	51.59	pg/ml	40.00	60.00	N/A	
cal 4	drugx_06	100.00	1853048	100.00	952422	1.946	97.01	pg/ml	80.00	120.00	N/A	
cal 5	drugx_07	200.00	4015027	100.00	1003046	4.003	195.67	pg/ml	160.00	240.00	N/A	
cal 6	drugx_08	400.00	8327175	100.00	1036597	8.033	388.81	pg/ml	320.00	480.00	N/A	

Manually Integrated:

Calibration Flags: D =RSD, F = Response factor, R = R Squared, A = Amount

Compound Calibration Report - Alternate

Lab Name: ThermoFisher Laboratory
Instrument: ThermoFisher Instrument
User: Jamie
Batch: Drux X

Method: Drux X_drugx
drugx
Cali File: Drux X.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
102	02	drugx_01	cal 1		5/4/1996 10:11:21 PM	STD=10 pg/ml,IS=100 pg/ml
103	03	drugx_02	cal 1		5/4/1996 10:21:24 PM	STD=10 pg/ml,IS=100 pg/ml
104	04	drugx_03	cal 1		5/4/1996 10:31:23 PM	STD=10 pg/ml,IS=100 pg/ml
105	05	drugx_04	cal 2		5/4/1996 10:41:31 PM	STD=25 pg/ml.IS=100 pg/ml
108	08	drugx_05	cal 3		5/4/1996 11:11:32 PM	STD=50 pg/ml.IS=100 pg/ml
109	09	drugx_06	cal 4		5/4/1996 11:21:33 PM	STD=100 pg/ml,IS=100 pg/ml
110	10	drugx_07	cal 5		5/4/1996 11:31:34 PM	STD=200 pg/ml,IS=100 pg/ml
111	11	drugx_08	cal 6		5/4/1996 11:41:36 PM	STD=400 pg/ml,IS=100 pg/ml
112	12	drugx_09	cal 7		5/4/1996 11:51:34 PM	STD=600 pg/ml,IS=100 pg/ml
113	13	drugx_10	cal 8		5/5/1996 12:01:38 AM	STD=800 pg/ml,IS=100 pg/ml
114	14	drugx_11	cal 9		5/5/1996 12:11:34 AM	STD=1000 pg/ml,IS=100 pg/ml

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	Method:	Drug_A_Drug_A
User:	AMER\jamie.humphries		Drug_A
Batch:	Drug_A	Cali File:	Drug_A.calx

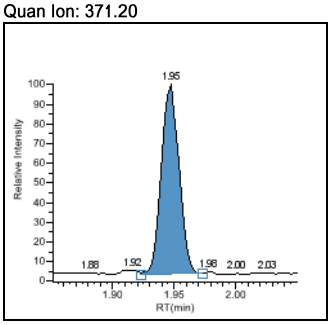
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

Drug_A

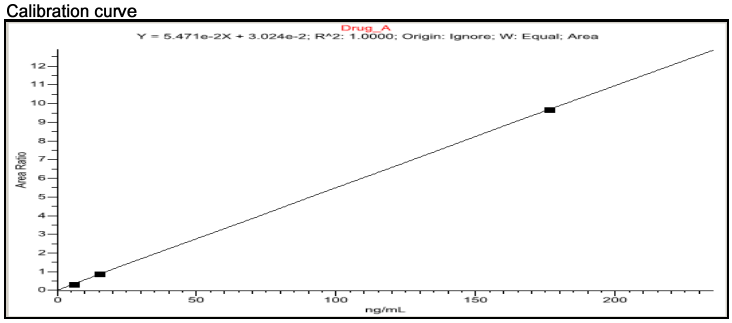
	Injected	Sample
Conc:	5.581 ng/mL	5.581 ng/mL

Retention time:	1.95
Area:	227568
Height:	226730

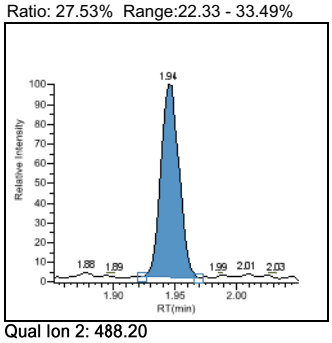
Quan Ion: 371.20



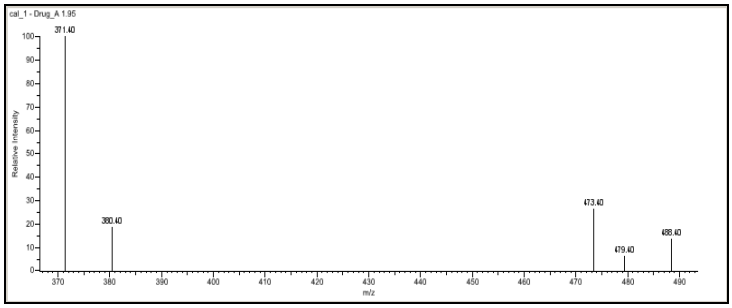
Calibration curve



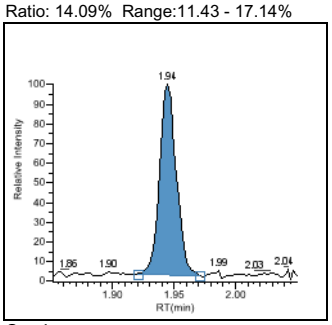
Qual Ion 1: 473.20
Ratio: 27.53% Range:22.33 - 33.49%



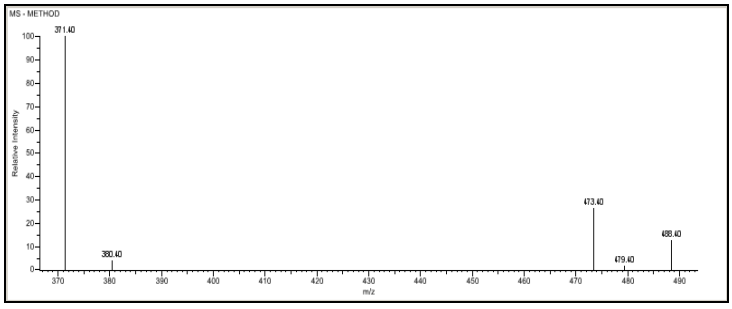
MS-Data



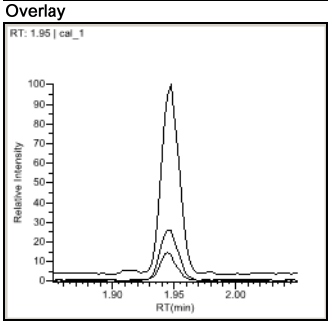
Qual Ion 2: 488.20
Ratio: 14.09% Range:11.43 - 17.14%



MS-Reference



Overlay



Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

Confirmation Report 2

Confirmation Report 2

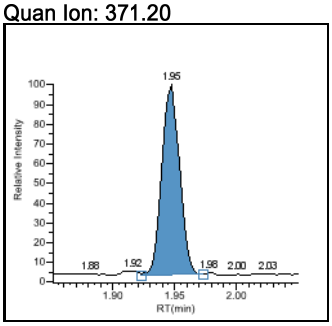
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali file: Drug_A.calx

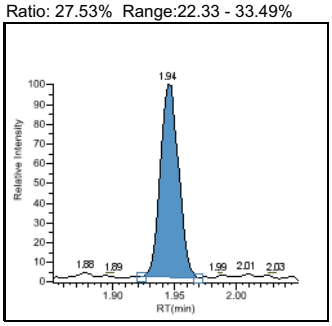
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

Compound Name: Drug_A
Injected Conc: 5.581 ng/mL
Sample Conc: 5.581 ng/mL
Retention time: 1.95
Area (Quan): 227568
Height (Quan): 226730
Qual ratio 1: Pass
Qual ratio 2: Pass

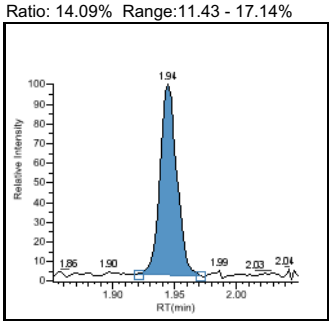
Quan Ion: 371.20



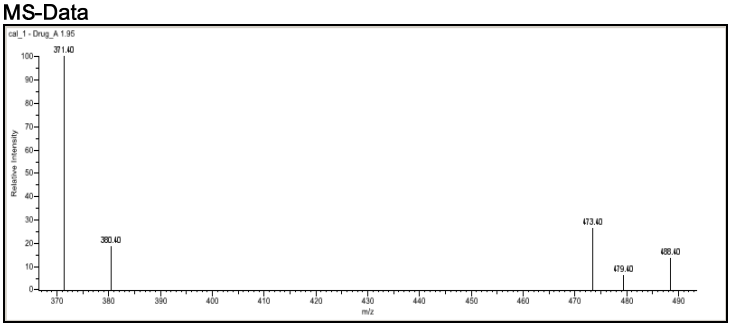
Qual Ion 1: 473.20
Ratio: 27.53% Range:22.33 - 33.49%



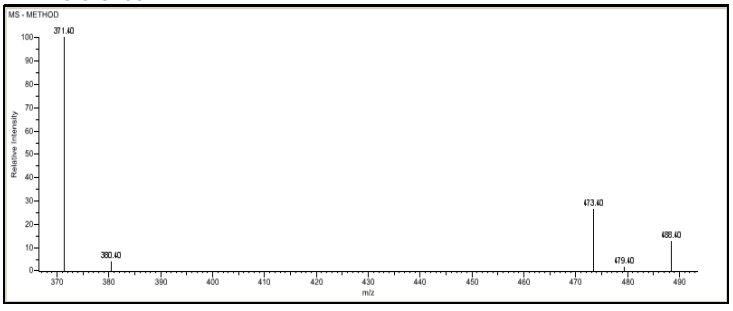
Qual Ion 2: 488.20
Ratio: 14.09% Range:11.43 - 17.14%



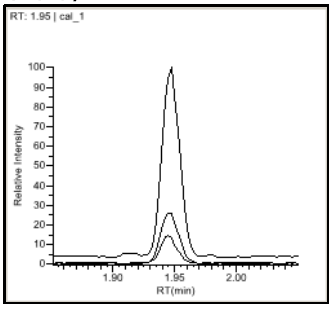
MS-Data



MS-Reference



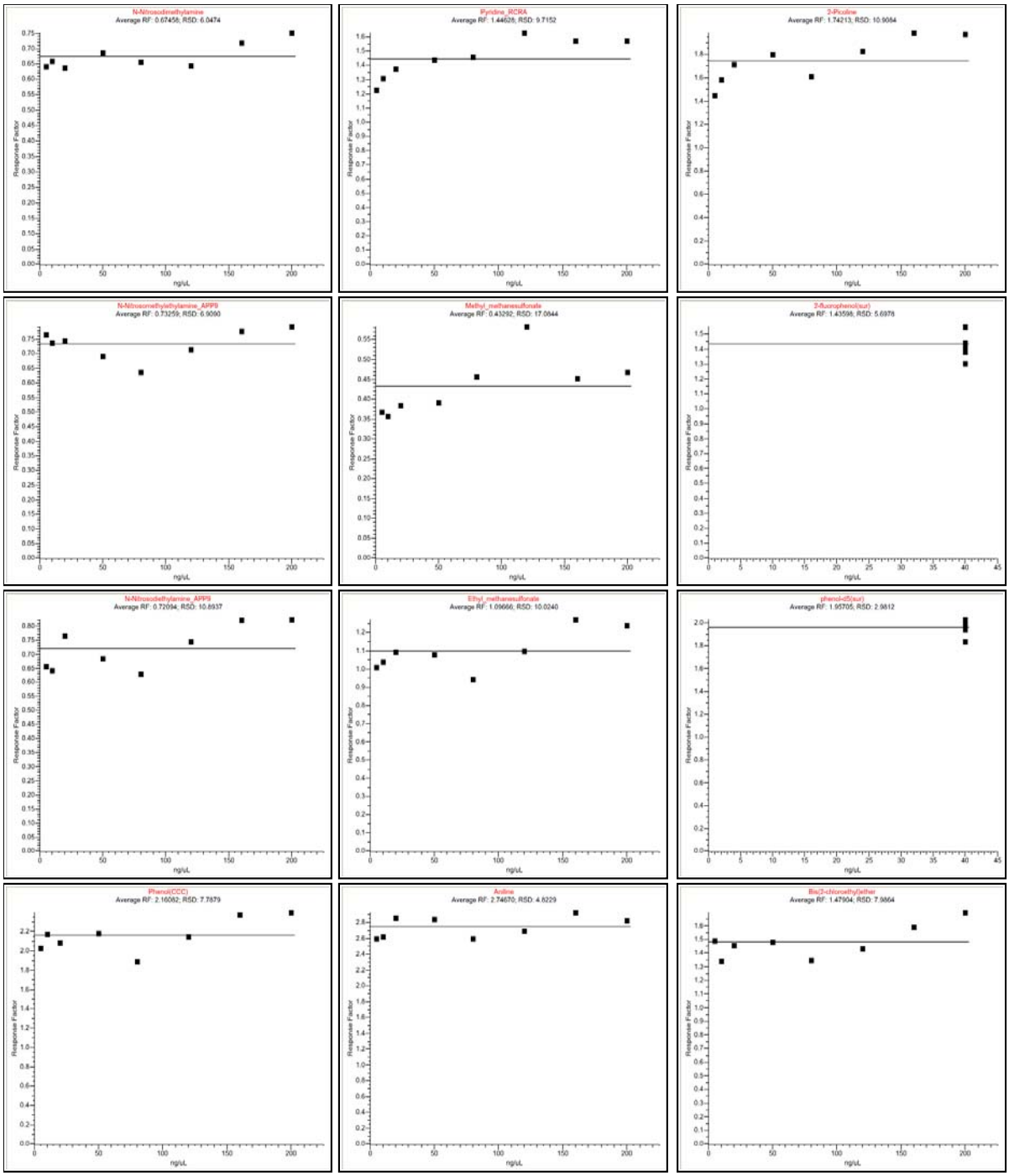
Overlay



High Density Calibration Report

High Density Calibration Report

Lab name:	Thermo Fisher Laboratory		
Instrument:	ThermoFisher Instrument	**Method:**	EC25B_8level_322010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	EC25B_8level_322010_a	**Call File:**	EC25B_8level_322010_a.calx



High Density Internal Standard Report

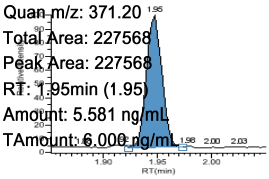
High Density Internal Standard Report

Page 1 of 1

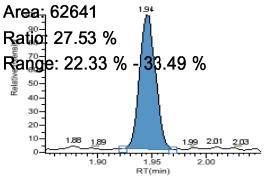
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A
Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

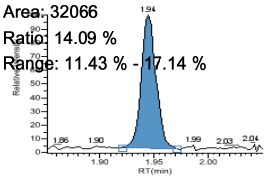
Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
Amount: 5.581 ng/mL
TAmount: 6.000 ng/mL



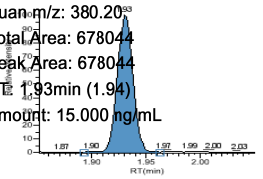
Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %



Qual m/z: 488.20
Area: 32066
Ratio: 14.09 %
Range: 11.43 % - 17.14 %



Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL



Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

High Density Internal Standard Report Long

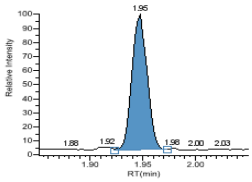
High Density Internal Standard Report Long

Page 1 of 1

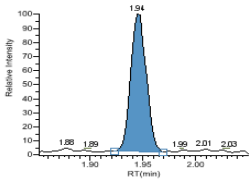
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

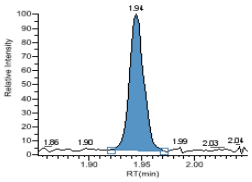
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	



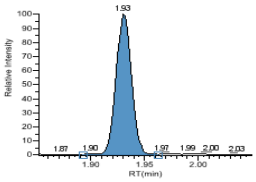
Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
Amount: 5.581 ng/mL
TAmount: 6.000 ng/mL



Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %



Qual m/z: 488.20
Area: 32066
Ratio: 14.09 %
Range: 11.43 % - 17.14 %



Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

High Density Sample Report 1

High Density Sample Report 1

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	Method:	Drug_A_Drug_A
User:	AMER\jamie.humphries		Drug_A
Batch:	Drug_A	Cali File:	Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

Int_Std Quan m/z: 380.20 Total Area: 678044 Peak Area: 678044 RT 1.93min (1.94) Amount: 15.000 ng/mL	Drug_A Quan m/z: 371.20 Total Area: 227568 Peak Area: 227568 RT 1.95min (1.95) TAmount: 6.000 ng/mL Amount: 5.581 ng/mL		

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

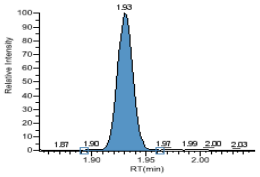
High Density Sample Report 1 Long

High Density Sample Report 1 Long

Page 1 of 1

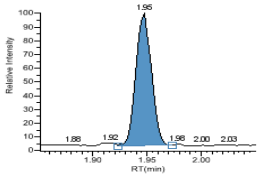
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A
Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	



Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)

Amount: 15.000 ng/mL



Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
TAmount: 6.000 ng/mL
Amount: 5.581 ng/mL

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

High Density Sample Report 2

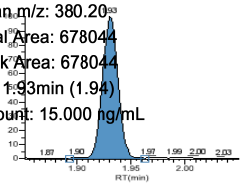
High Density Sample Report 2

Page 1 of 1

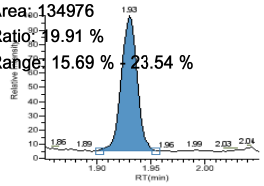
Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	Method:	Drug_A_Drug_A
User:	AMER\jamie.humphries		Drug_A
Batch:	Drug_A	Cali File:	Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

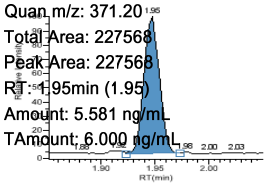
Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL



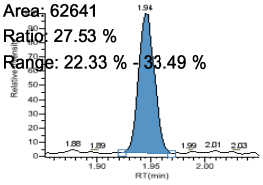
Qual m/z: 479.20
Area: 134976
Ratio: 19.91 %
Range: 15.69 % - 23.54 %



Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
Amount: 5.581 ng/mL
TAmount: 6.000 ng/mL



Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %



Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

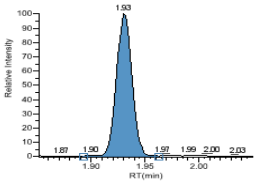
High Density Sample Report 2 Long

High Density Sample Report 2 Long

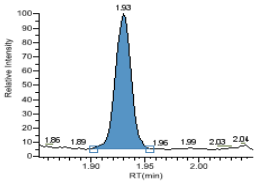
Page 1 of 1

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	Method:	Drug_A_Drug_A
User:	AMER\jamie.humphries		Drug_A
Batch:	Drug_A	Cali File:	Drug_A.calx

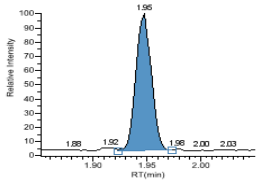
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	



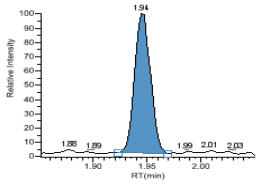
Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL



Qual m/z: 479.20
Area: 134976
Ratio: 19.91 %
Range: 15.69 % - 23.54 %



Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
Amount: 5.581 ng/mL
TAmount: 6.000 ng/mL



Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

High Density Sample Report 3

High Density Sample Report 3

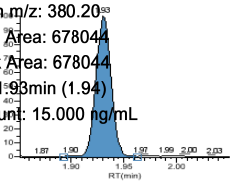
Page 1 of 1

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

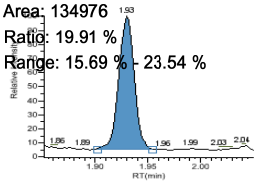
Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

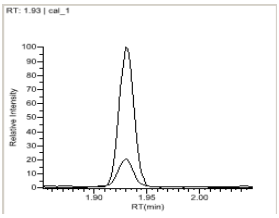
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL

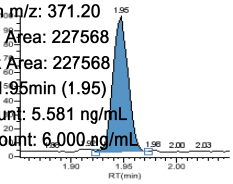


Qual m/z: 479.20
Area: 134976
Ratio: 19.91 %
Range: 15.69 % - 23.54 %

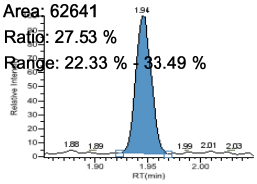




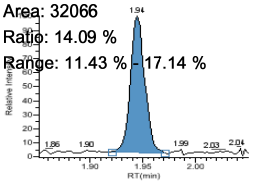
Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
Amount: 5.581 ng/mL
TAmount: 6.000 ng/mL

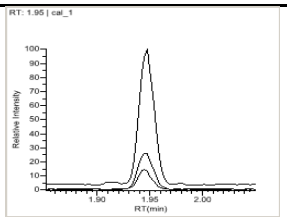


Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %



Qual m/z: 488.20
Area: 32066
Ratio: 14.09 %
Range: 11.43 % - 17.14 %





Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

High Density Sample Report 3 Long

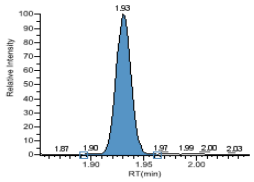
High Density Sample Report 3 Long

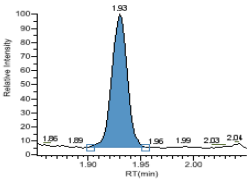
Page 1 of 1

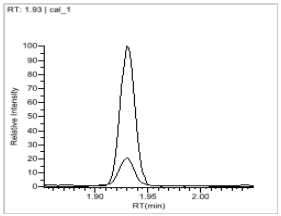
Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

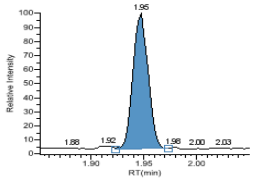


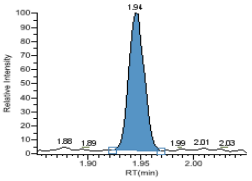


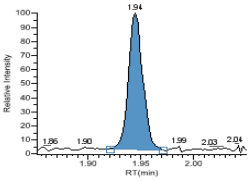


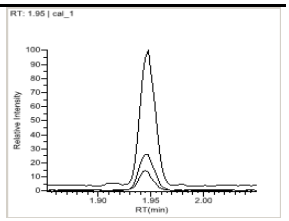
Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL

Qual m/z: 479.20
Area: 134976
Ratio: 19.91 %
Range: 15.69 % - 23.54 %









Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
Amount: 5.581 ng/mL
TAmount: 6.000 ng/mL

Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %

Qual m/z: 488.20
Area: 32066
Ratio: 14.09 %
Range: 11.43 % - 17.14 %

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

Internal Standard Summary Report

Internal Standard Summary Report

Page 1 of 1

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

Compound	Std Response	Min	Max	Sample Response
Int_Std	655596	327798(50.00%)	983394(150.00%)	678044
	Std RT	Min	Max	Sample RT
Int_Std	1.93	1.68(-0.25)	2.18(+0.25)	1.93

* = Fail Manually integrated

Ion Ratio Failure Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
9	specimen 2	specimen_2	N/A		4/17/2008 5:08:51 PM	

Compound	Response	Quan Ion	Quan Response	Qual Ion	Qual Response	Ratio	Range
Drug_A	Area	371.20	47603394	473.20	4769645	10.02	22.33-33.49
	Area	371.20	47603394	488.20	3448401	7.24	11.43-17.14

Manually integrated ☐

LCSLCSD Report (Environmental and Food Safety only)

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

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 I
Tray1:9	SampleID002	500ppt-002	QC	D002	6/26/2007 9:47:43 PM	New Dilutions 6/26/2007 I
Tray1:3	SampleID002	Cal002	c2	D002	6/26/2007 6:09:47 PM	New Dilutions 6/26/2007 I
Tray1:15	SampleID008	5ppb-001	N/A	D008	6/27/2007 12:54:35 AM	New Dilutions 6/26/2007 I
Tray1:8	SampleID008	500ppt-001	QC	D008	6/26/2007 9:16:35 PM	New Dilutions 6/26/2007 I

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**

Manually integrated

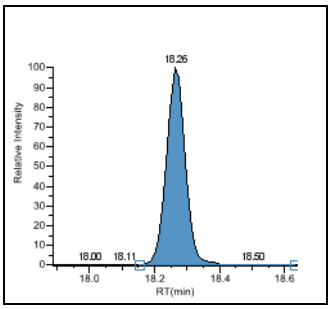
Manual Integration Report

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

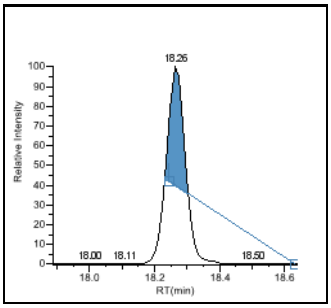
Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:4	SampleID003	Cal003	c3	D003	6/26/2007 6:40:58 PM	New Dilutions 6/26/2007 I

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

Method Detection Limit Report (Environmental and Food Safety only)

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: Drug_A_Drug_A — Page number: Page 1 of 11
Master method name: Drug_A
Current calibration file: Drug_A.calx
Assay type: Drug_A — Ion range calc method: Average
Inj vol: 1.000
Instrument method: 20x

Compound Identification:

Compound	Quan mass	RT	Window	View width	Use as reference	Reference compound
Int_Std	380.20	1.94	10.00	0.40	Yes	
Drug_A	371.20	1.95	10.00	0.40	No	Int_Std

Method Report

Method name: Drug_A_Drug_A — Page number: Page 2 of 11
Master method name: Drug_A
Current calibration file: Drug_A.calx
Assay type: Drug_A — Ion range calc method: Average
Inj vol: 1.000
Instrument method: 20x

Compound Calibration:

Compound	Response	Calibration	Curve type	Weighting	Origin	Units	ISTD Name	ISTD Units
Drug_A	Area	Internal	Linear	Equal	Ignore	ng/mL	Int_Std	ng/mL

Method Report

Method name: Drug_A_Drug_A — Page number: Page 3 of 11
Master method name: Drug_A
Current calibration file: Drug_A.calx
Assay type: Drug_A — Ion range calc method: Average
Inj vol: 1.000
Instrument method: 20x

QAQC Limits:

Compound	LOD	LOQ	Cutoff	ULOL	Carryover
Drug_A	1.500	1.500	15.000	1000.000	1000.000

Method Report

Method name: Drug_A_Drug_A — Page number: Page 4 of 11
Master method name: Drug_A
Current calibration file: Drug_A.calx
Assay type: Drug_A — Ion range calc method: Average
Inj vol: 1.000
Instrument method: 20x

Groups:

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 5 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x				

Report options:

Quan report options

Report concentration:	Always
Decimal places to be reported:	3
Show chromatogram on Quantitation report:	True
Display valid compounds only	False

Qual options

Sort Qual results by:	Search Index
Enable limiting peaks:	False
Limit Peaks to :	

User interface options

Shade row when sample is outside of evaluation criteria:	False
Separate ion overlay display :	True
Use alternative calibration report format:	False
Display quan flags and legend	True

ToxLab Forms settings

Quan flags

Flag values below LOD:	True
Flag values below LOQ:	True
Flag values above Cutoff:	True
Flag values above ULOL:	True
Flag values above Carryover:	True
Flag values between LOD and LOQ:	True

Calculated amount option

Calculate concentration as:	Truncated

Tune time tracking options

Enable tune time tracking:	False
Tune file lifetime (hrs):	N/A

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 6 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x				

QAQC Calibration

Compound	Max RSD (%)	Min RF	R^2 threshold	Max amt diff (%)
Drug_A	20.00	0.00	0.990	20.000

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 7 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x				

QAQC QC Check:

Compound	Max RF diff (%)	Min RF
Drug_A	20.00	0.000

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 8 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x				

QAQC Negative:

Compound	Criterion	Max value
Drug_A	% of LOD	1.500

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 9 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x				

QAQC ISTD:

Compound	Min recovery (%)	Max recovery (%)	Min RT (-min)	Max RT (+min)
Int_Std	50.00	150.00	0.25	0.25

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 10 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x				

QAQC Solvent Blank:

Compound	Method	Upper Limit %
Int_Std	None	
Drug_A	Quan Ion RT	0

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 11 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x				

QAQC Hydrolysis:

CompoundName	EvaluationMethod	LowerLimit	UpperLimit
Drug_A	Range	15.000	23.000

Method Validation Report (Environmental and Food Safety only)

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 (Environmental and Food Safety only)

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

Manually integrated ☐

Quantitation Report

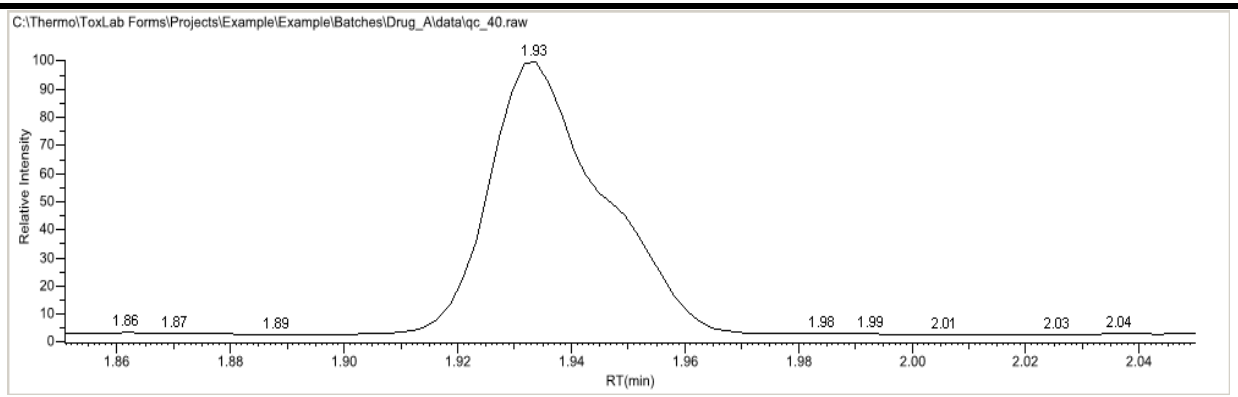
Quantitation Report

Page 1 of 1

Lab name: Thermo Fisher Laboratory
Instrument Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
7	qc 40% = 6 ng/mL	qc_40	level 40		4/17/2008 5:07:57 PM	



Internal Standards	RT	Qion	Response	Curve Type	Average RF/ Response	Injected Conc	Units	Calculated Conc	Units	Flags
Int_Std	1.93	380.20	639922	Average RF	0.000	15.000	ng/mL	15.000	ng/mL	

Target Compounds	RT	Qion	Response	Curve Type	Average RF/ Response	Injected Conc	Units	Calculated Conc	Units	Flags
Drug_A	1.95	371.20	215541	Linear	0.336	5.603	ng/mL	5.603	ng/mL	

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

Manually integrated

Quantitation Report - 2

MS Integ Params:	cal_test	**Quant Time:**	6/24/2010 10:55:46 AM
Quant Method:	Breakdown report1_cal_test	**Data File:**	level2
Title:	Assay name	**Acq On:**	2/22/2008 9:37:36 AM
Last Update:	6/24/2010 4:32:35 PM	**Sample:**	
Data Acq Method:	simulator7	**Comment:**	
Operator:	DGT4K5D1\ThermoFisher	**Vial:**	2
Instr:	Thermo Scientific Instrument	**Multiplr:**	1.000
Response Via:	Breakdown report1.calx	**Quant Results File:**	C:\Thermo\EnviroLab Forms\Projects\Default\Default\Batches\Breakdown report1\Data\level2.rsx

Internal Standards

Compound Name	RT	Qion	Response	Conc	Units	Dev (min)	Flags
10 Naphthalene-d8	5.96	136.00	55923713	40.00	ng/uL	0.00	
16 Acenaphthene-d10	7.95	164.00	31181554	40.00	ng/uL	0.00	
19 Phenanthrene-d10	9.60	188.00	59349974	40.00	ng/uL	0.00	
21 Chrysene-d12	12.53	240.00	35937685	40.00	ng/uL	0.01	
22 Perylene-d12	13.99	264.00	31490138	40.00	ng/uL	0.00	

Surrogates

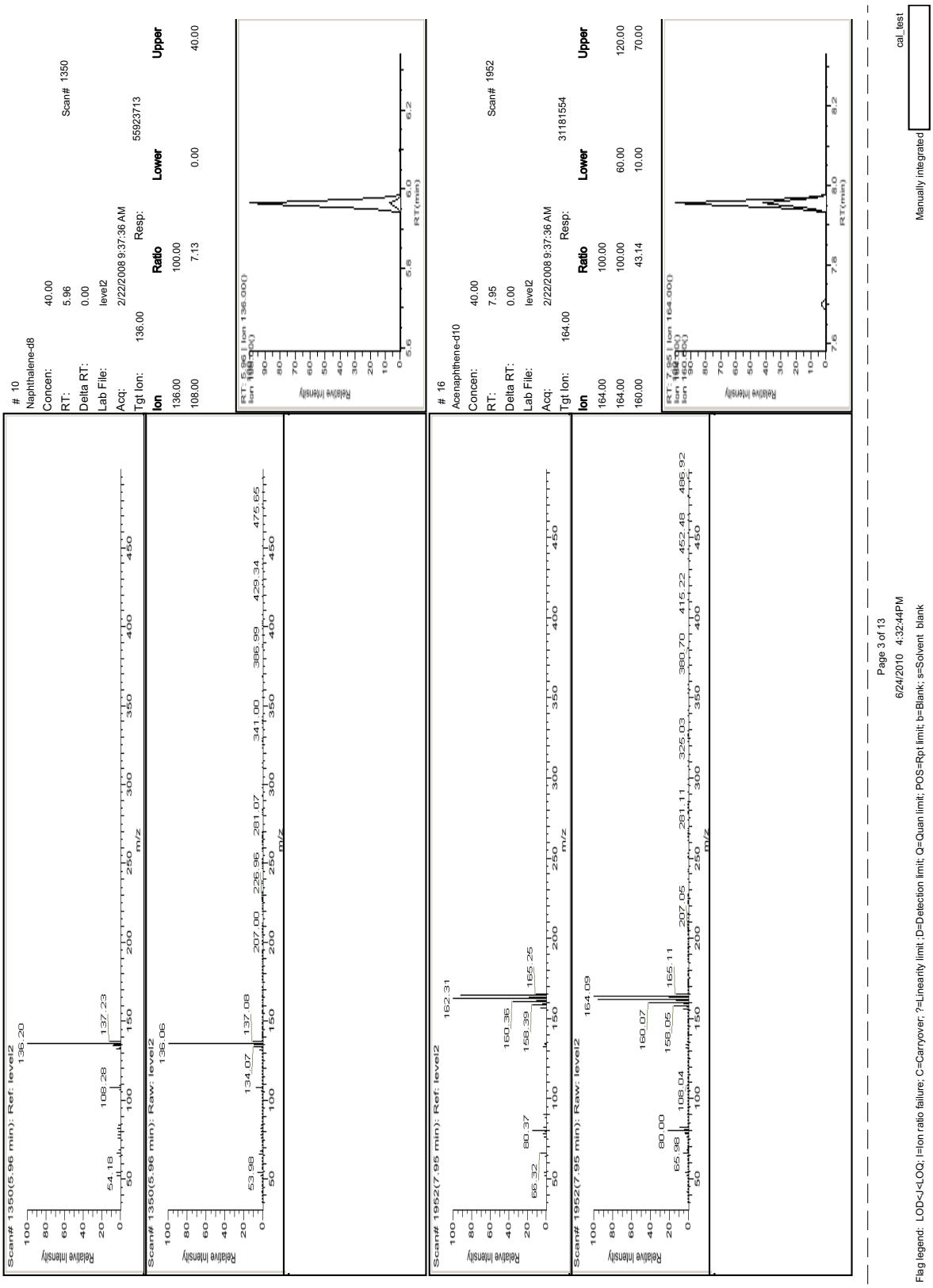
Compound Name	RT	Qion	Response	Conc	Units	Dev (min)	Spike Amt	Recovery	Flags
13 1,2,4,5-Tetrachlorobenzene	6.98	216.00	4472645	10.32	ng/uL	0.00	1.00	1031.69	

Target Compounds

Compound Name	RT	Qion	Response	Conc	Units	Dev (min)	Flags
1 2-Fluorobiphenyl	2.49	172.00	42	30.00	ng/uL	-0.01	I
2 Pentachloroethane	4.09	167.00	1863192	N/A	ng/uL	0.00	
3 1,3-Dichlorobenzene	4.38	146.00	5835082	N/A	ng/uL	0.00	
4 1,4-Dichlorobenzene-d4	4.45	152.00	15043882	N/A	ng/uL	0.00	
5 1,4-Dichlorobenzene	4.47	146.00	6053754	N/A	ng/uL	0.00	
6 1,2-Dichlorobenzene	4.47	146.00	6078986	N/A	ng/uL	-0.02	
7 Hexachloroethane	5.06	201.00	1894687	0.00	ng/uL	0.01	
8 Nitrobenzene-d5	5.13	82.00	3737881	10.27	ng/uL	-0.01	
9 1,2,4-Trichlorobenzene	5.91	180.00	4644534	9.97	ng/uL	0.01	
11 Hexachloropropene	6.10	213.00	2526300	10.18	ng/uL	0.00	
12 Hexachlorobutadiene	6.16	225.00	2056801	10.07	ng/uL	0.00	
14 Hexachlorocyclopentadiene	6.98	237.00	2004237	10.14	ng/uL	0.00	
15 2-Chloronaphthalene	7.33	162.00	13334992	10.01	ng/uL	0.00	
17 Pentachlorobenzene	8.14	250.00	3306626	10.10	ng/uL	0.00	
18 Hexachlorobenzene	9.17	284.00	2673192	9.85	ng/uL	-0.01	

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Manually integrated


Quantitation Report - 2
10
Naphthalene-d8
Concen: 40.00
RT: 5.96
Delta RT: 0.00
Lab File: level2
Acq: 2/22/2008 9:37:36 AM
Tgt Ion: 136.00
Resp: 55923713
Scan# 1350
Ion Ratio Lower Upper
136.00 100.00
108.00 7.13 0.00 40.00
16
Acenaphthene-d10
Concen: 40.00
RT: 7.95
Delta RT: 0.00
Lab File: level2
Acq: 2/22/2008 9:37:36 AM
Tgt Ion: 164.00
Resp: 31181554
Scan# 1952
Ion Ratio Lower Upper
164.00 100.00
164.00 100.00 60.00 120.00
160.00 43.14 10.00 70.00
Scan# 1350(5.96 min): Ref: level2
Scan# 1350(5.96 min): Raw: level2
Scan# 1952(7.95 min): Ref: level2
Scan# 1952(7.95 min): Raw: level2
Relative Intensity
m/z
RT(min)
Manually integrated
cal_test
Page 3 of 13
6/24/2010 4:32:44PM
Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Solvent Blank Report

Solvent Blank Report

Page 1 of 1

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER\jamie.humphries
Batch: Drug_A

Method: Drug_A_Drug_A
Drug_A
Cali File: Drug_A.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
13	solvent	solvent	N/A		4/17/2008 5:10:45 PM	

Internal Standards	RT	QIon	Response	Method	Upper Limit	
Int_Std	1.92	380.20	746596	None		

Target Compounds	RT	QIon	Response	Method	Upper Limit	
Drug_A	1.93	371.20	1071	Quan Ion RT	0	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 1

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**

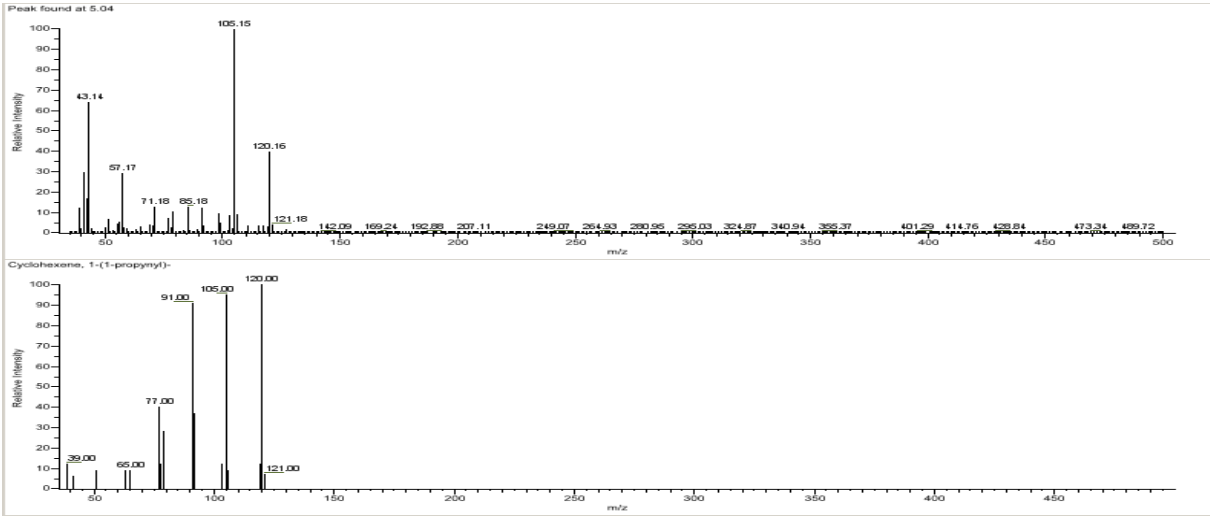
TIC Report

Lab name: Thermo Fisher Laboratory
Instrument: ThermoFisher Instrument
User: AMER\jessie.butler
Batch: March48270B_8level_342010_a
Method: March48270B_8level_342010_a_EPAMethod8270B_8l
EPAMethod8270B_8level
Cali File: EC25B_8level_322010_a_March48270B_8level_34201

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

Peak:	Retention time	Area	Height	Inj. estimate	In-sample est.	Flag
Cyclohexene, 1-(1-propynyl)-	5.04	243538856	71816093	104.902	104.902	

Compound	CAS number	Library	Entry	Match prob.	Search Index	Rev. search index	Formula	Weight
Cyclohexene, 1-(1-propynyl)-	1655056	mainlib	82371	0	623	845	C9H12	120



Manually integrated

Flag legend: P = Library entry selected manually

TIC Summary Report

TIC Summary Report

Lab name: Thermo Fisher Laboratory

Instrument: ThermoFisher Instrument
User: AMER\jessie.butler
Batch: March48270B_8level_342010_a
Method: March48270B_8level_342010_a_EPAMethod8270B_8level
EPAMethod8270B_8level
Call File: EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

Internal standards

Internal standard	ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units
1,4-DICHLOROBENZENE-D4_(IS)	1	5.59	92863341	40.000	ng/uL	40.000	ng/uL
NAPHTHALENE-D8_(IS)	2	7.04	305413673	40.000	ng/uL	40.000	ng/uL

Qualitatively-identified compounds

Compound	Uses ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units	Flag
Cyclohexene, 1-(1-propynyl)-	1	5.04	243538856	104.902	ng/uL	104.902	ng/uL	
Decane	1	5.38	307929153	132.638	ng/uL	132.638	ng/uL	
Undecane	1	6.27	231391187	99.670	ng/uL	99.670	ng/uL	
2,6-Dimethyldecane	2	8.39	309626174	40.552	ng/uL	40.552	ng/uL	
Eicosane	2	11.08	391448222	51.268	ng/uL	51.268	ng/uL	

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.

- Use the Fill Down command for the Filename, Sample Name, Sample ID, and Vial Position columns.
- Use the Copy Down command for the Sample Type, Vial Position, Injection Volume, Conv Factor, Sample Level, and Comment columns.

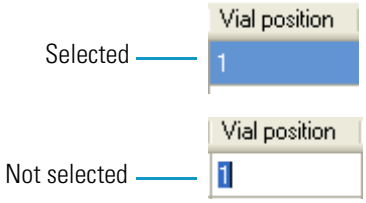
Use the following procedures:

- To automatically copy column values
- To automatically enter sequential column values
- To use Copy Down or Fill Down for a range of samples

❖ 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.

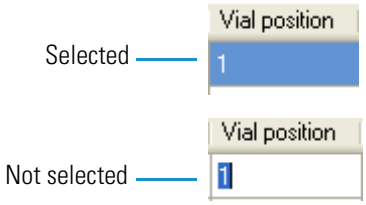
❖ To automatically enter sequential column values

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.



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.

   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

When you use the Fill Down command for the Vial Position column with an autosampler configured, 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:B1
A:B2
A:B3
A:B4
A:B5
A:B6

❖ 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:

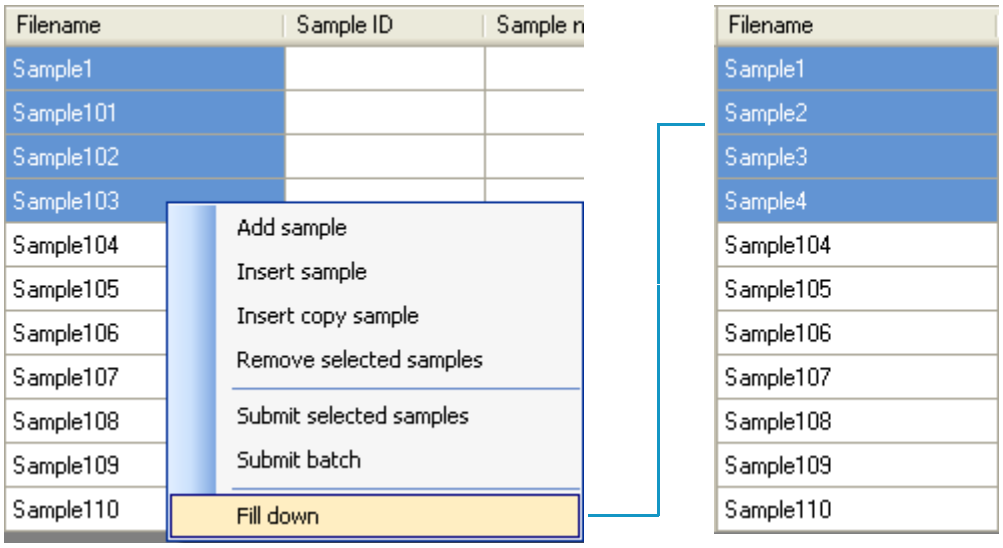
   Drag your cursor to select a contiguous group of sample values.

   –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.



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 button, , in the column header.

   For each column, a list of filterable criteria is displayed. In all columns, your filter choices are All, Blanks, and NonBlanks. 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.

   The Enter Filter Criteria dialog box opens. See "Enter Filter Criteria" on page 408.

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 86. Enter Filter Criteria dialog box

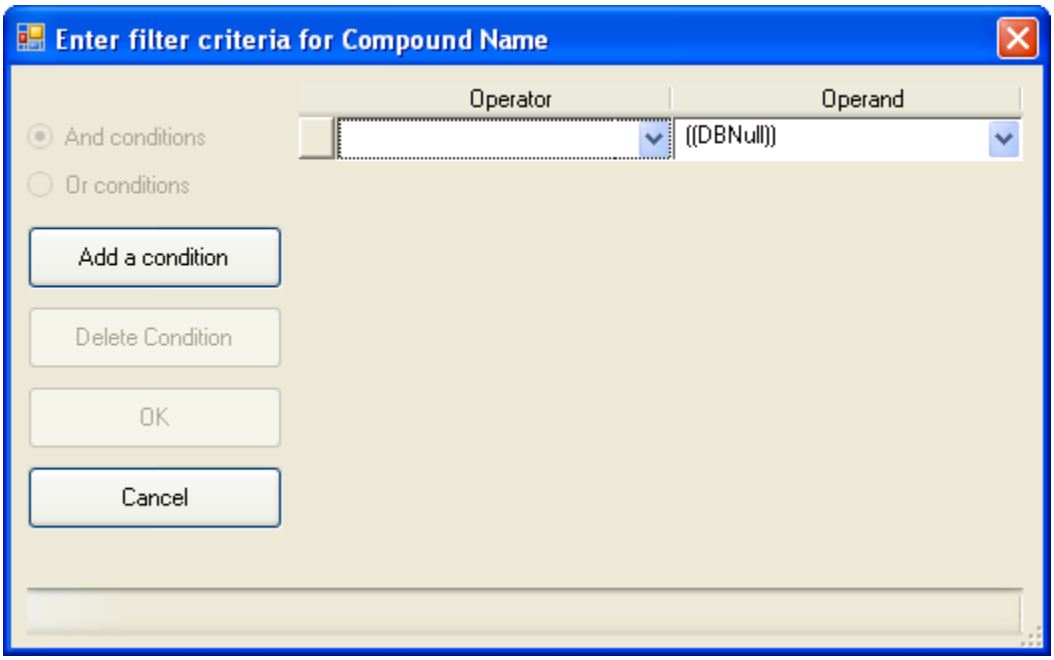


Table 90. Enter Filter Criteria dialog box parameters

Parameter	Description
And conditions	Requires meeting all filter criteria.
Or conditions	Requires meeting any of the specified filter criteria.
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.

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