

Thermo

TraceFinder

User Guide

Software Version 3.3
Optimized for General Quantitation

XCALI-97728 Revision A May 2015



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Preface

This guide describes how to use the Thermo TraceFinder™ 3.3 application with compatible Thermo Scientific™ GC/MS and LC/MS analytical instruments.

Contents

- [Related Documentation](#)
- [License Activation](#)
- [Special Notices](#)
- [Contacting Us](#)

Related Documentation

The TraceFinder application includes complete documentation. In addition to this guide, you can also access the following documents as PDF files from the data system computer:

- *TraceFinder User Guide*
- *TraceFinder Administrator Console User Guide*
- *TraceFinder Acquisition Quick Reference Guide*
- *TraceFinder Analysis Quick Reference Guide*
- *TraceFinder Shortcut Menus Quick Reference Guide*

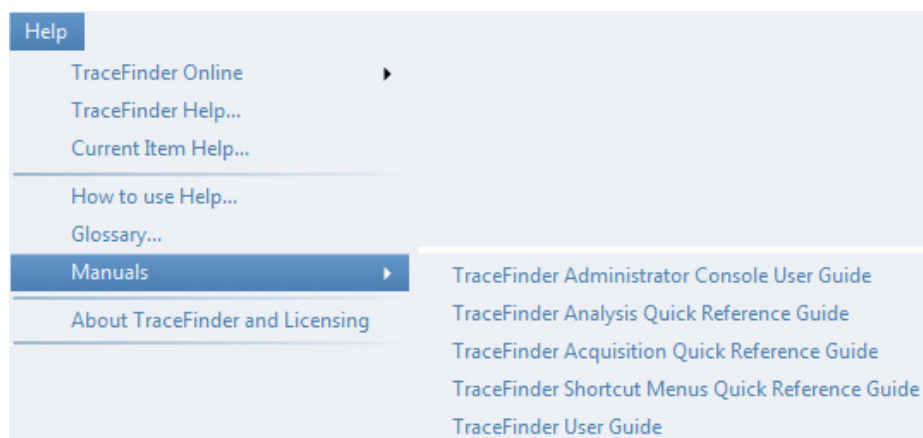
❖ To view TraceFinder documents using the Start menu

From the Microsoft™ Windows™ taskbar, choose **Start > All Programs > Thermo TraceFinder > Manuals**.

❖ **To open TraceFinder Help and access related documents from the application**

1. Open the TraceFinder application and choose **Help > TraceFinder Help**.
 - To find a particular topic, use the Contents, Index, or Search panes.
 - To create your own bookmarks, use the Favorites pane.
2. To view the operator manual, user guide, or one of the quick reference guides, choose **Help > Manuals > PDF file**.

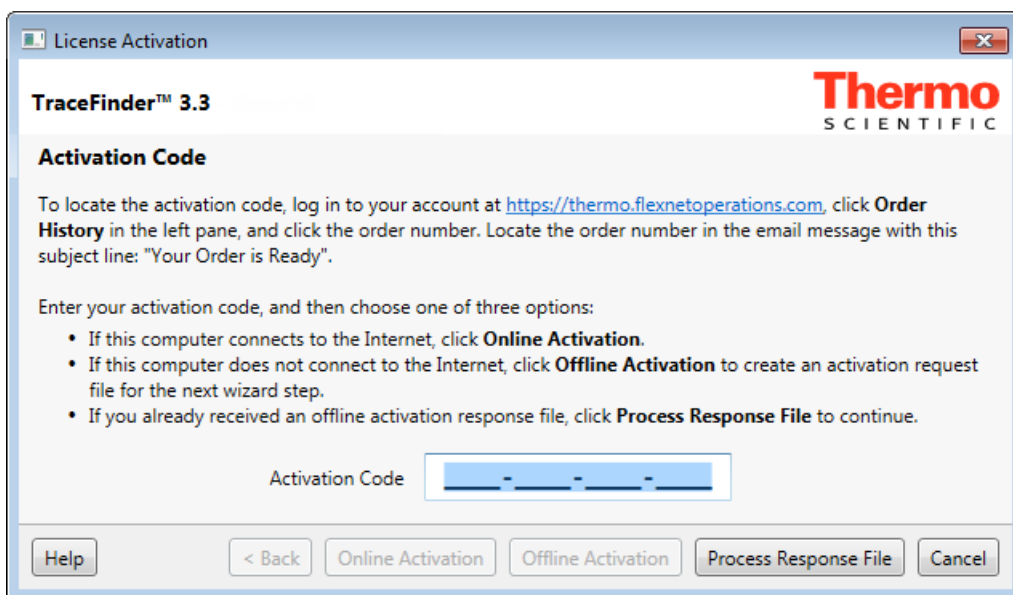
Figure 1. PDF files available from the Help menu



The PDF file of the selected document opens in a new window.

License Activation

When you first start the TraceFinder application, a dialog box displays the number of days remaining in your 120-day free evaluation license. If your evaluation license has expired, the License Activation wizard opens.



Note You can open the License Activation wizard at any time during your evaluation period by choosing Help > About TraceFinder and Licensing from the TraceFinder menu and then clicking Activate. If you already have a permanent license, a message tells you that your product is fully licensed.

Two types of licenses are available:

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

The evaluation version is full-featured and automatically expires 120 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 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 software download and licensing questions, contact support at ThermoMSLicensing@thermo.com.

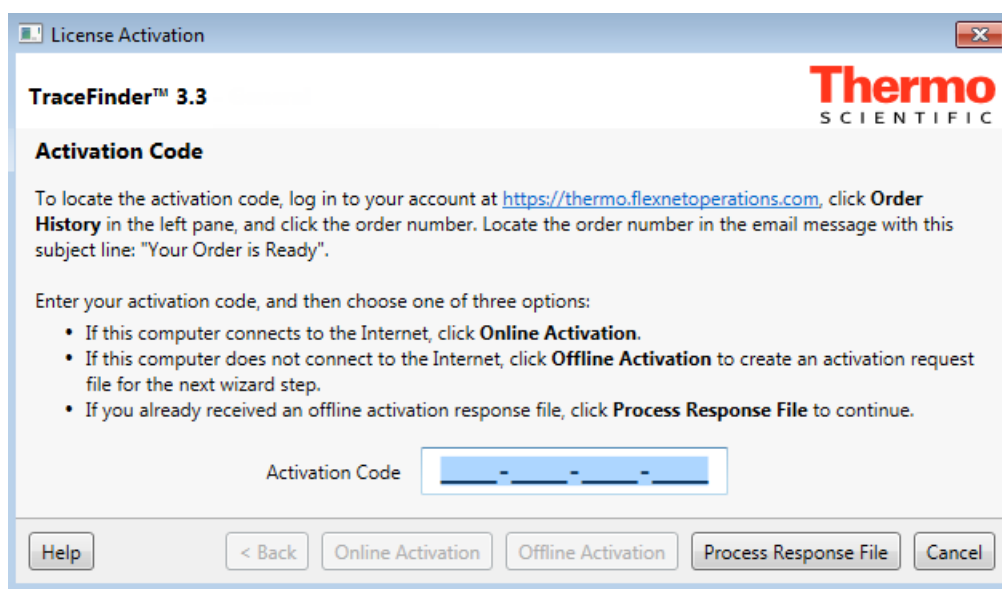
IMPORTANT The 120-day evaluation license includes both the basic TraceFinder 3.3 features and the unknown screening features. When you purchase a permanent license, you have the option of purchasing the unknown screening features. Your permanent license might not include the unknown screening features.

Use the License Activation wizard to activate or deactivate the license for the application. To activate the license, you must have an activation code from Thermo Fisher Scientific. You must deactivate the license before you transfer it to another computer.

❖ **To start the license activation or deactivation process**

1. Open the application.
2. Choose **Help > About TraceFinder and Licensing** to display the License Activation wizard.
3. Click **Activate (Deactivate)** to start the activation or deactivation process, as applicable.

The License Activation wizard opens.



4. Follow the instructions in the License Activation wizard.

For additional instructions, click **Help** in the wizard.

Special Notices

Make sure you follow the special notices that appear in boxes.

This guide uses 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.

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	(U.S.) 1 (561) 688-8731	(U.S.) 1 (561) 688-8736
	us.customer-support.analyze@thermofisher.com 	us.techsupport.analyze@thermofisher.com 

Contact us	Customer Service and Sales	Technical Support
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2. Click **Contact Us**, select the **Using/Serviceing a Product** option, and then type the product name.
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- Complete a survey at www.surveymonkey.com/s/PQM6P62.

Introduction

This chapter describes general features of the TraceFinder application.

Contents

- [About the TraceFinder Application](#)
- [TraceFinder Summary of Features](#)
- [TraceFinder Workflow](#)
- [Reporting Features](#)

About the TraceFinder Application

The TraceFinder application targets the general quantitation market. It supports a focused quantification workflow for specific nonbioanalytical laboratory use, instrument control, and method development functionality. TraceFinder is the primary application for the TSQ Quantum™ XLS triple quadrupole mass spectrometers.

The application can export mass data in the Acquisition List to XML format so that other systems' applications, such as for the TSQ 8000, TSQ Quantum™, ISQ, and Q Exactive™, can import the files into their databases.

The application can import the following file types:

- Sample lists in .csv or .xml format

See [“Defining a Sample List”](#) on page 360.

- Processing (.pmd) and instrument (.meth) method files from the Xcalibur™ data system

For detailed information about creating quantitative processing methods, see [Chapter 5, “Using the Method Development Mode for Quantitation Methods.”](#)

For detailed information about creating target screening processing methods, see [Chapter 6, “Using the Method Development Mode for Target Screening Methods.”](#)

For detailed information about creating unknown screening processing methods, see [Chapter 7, “Using the Method Development Mode for Unknown Screening Methods.”](#)

For detailed information about creating instrument methods, see [“Working with Instrument Methods”](#) on page 108.

- Compounds from files that use the database (.xml or .cdb) format
See [“Working with the Compound Database”](#) on page 74.
- Batches, methods, or templates from the TraceFinder 2.0, 2.1, 3.0, 3.1, or 3.2 applications.
See [“Converting Legacy Data”](#) on page 20.

The 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 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 data system suite with specific instructions that enable scientific instruments to perform data acquisition.
- Processing method (.pmd): A proprietary file format for the Xcalibur data system 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.
- Compound database (.cdb): The file type for TraceFinder or ExactFinder™ compound database data.
- Library (.db): A library used for target screening.

TraceFinder Directory Structure

The application creates folders for batches, methods, and templates in the ...\\TraceFinderData directory. Within each batch folder, the application creates folders for data, methods, and reports.

You can create batches in the TraceFinderData\\3.3\\Projects folder, or you can create subfolders within the Projects folder for your batches. You can create as many subfolders as you want for your batches, but you cannot create a batch within another batch folder.

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

Figure 2. Example batch directory structure

Name	Date modified	Type	Size
Data	3/21/2014 2:10 PM	File folder	
Methods	3/21/2014 12:38 PM	File folder	
Reports	3/21/2014 12:38 PM	File folder	
BatchData.btd	3/21/2014 2:10 PM	BTD File	655 KB
Equan_batch1.log	3/21/2014 2:10 PM	Text Document	10 KB

TraceFinder Summary of Features

The TraceFinder system provides a workflow-oriented approach to high-throughput quantitation, using tools that 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 general quantitation applications. The application has a fully automated acquisition mode and a manual data analysis mode. You can use the data acquisition system to create and submit batches and monitor real-time review of results.

The application uses a comprehensive processing method to provide improved handling of ion ratio calculations, reviewing, and reporting. In addition, it can compare the mass spectra and integrate the processes of data review and reporting.

Key features include the following:

- Role-based authorization for Security, LabDirector, ITAdmin, Supervisor, Technician, and QAQC (quality assurance) roles

- Administrator Console for user security, role-based permissions, and data repositories
- Configuration console for report configuration, detection and acquisition defaults, adduct definitions, screening library selection, and customized columns and flags
- Method Development mode for editing instrument methods, setting processing and error flag parameters, and setting reporting options
- Acquisition mode that guides you in creating batches and running samples
- Analysis mode with batch views, data review, local method views, and reporting views
- Database-capable method development
- Quantification workflows
- Target screening workflows
- Unknown screening workflows
- Spreadsheet-based report designer

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 application is structured with a typical laboratory workflow in mind. You create 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 laboratory. When you are ready to run a particular type of sample, select the appropriate method and begin.

When using the 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 the following:

- How the raw data is acquired and processed
- How the error checking information evaluates the results
- How the results appear in reports

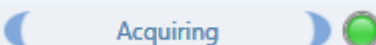

2. Create and submit a batch using the Acquisition wizard.

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 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 upper right corner of the TraceFinder window. This area displays a green, yellow, or red status light and a description of any activity in the queues, as in this example:

Apple_0_81_01  Acquiring 

The status light (in any color) might include an exclamation mark.

- An exclamation mark on a green status light, , might indicate that the instrument method contains the wrong source (for example, APCI instead of HESI).
- An exclamation mark on a red status light, , might indicate that a vial is missing and the batch was forced to stop.

Click the status light to display details of the error.

4. Evaluate the data in the Analysis mode.

The Analysis 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 Analysis mode.

Use the Report View to view or print the reports for the current 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 following types of reports meet the requirements of various methods and global regulatory agencies, helping to track the performance of LC and GC systems and methods.

Standard Report Types

- Ad Hoc Tune Report
- Batch Report
- Blank Report
- Breakdown 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 Long
- High Density Sample Report 1 Long
- Intelligent Sequencing Report
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- QC Summary Report

- Quantitation Report
- Quantitation Report - 2
- Sample Report
- Solvent Blank Report
- Standard Addition Report
- Surrogate Recovery Report
- Target Screening Height Density Sample Report
- Target Screening Height Density Sample Report 2
- Target Screening Summary Report
- TIC Report
- TIC Summary Report
- Tune Report
- Unknown Screening Summary Report

Use the features in the Report Designer to create custom report types. See [Chapter 12, “Using the Report Designer.”](#)

Getting Started

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

Contents

- [Installing the TraceFinder Application](#)
- [Installing the NIST and QED Libraries](#)
- [Launching the NIST Library Browser](#)
- [Launching a Qualitative Explorer](#)
- [Converting Legacy Data](#)
- [Choosing a Mode or Console](#)

Installing the TraceFinder Application

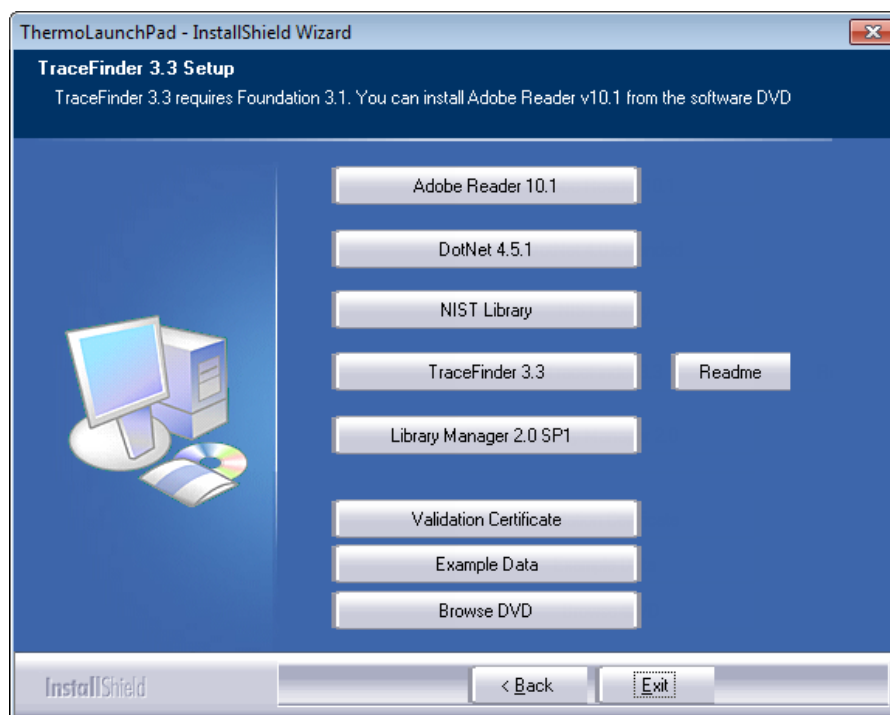
To initially install the TraceFinder 3.3 application, follow the instructions in the *TraceFinder Installation Guide*. Later, you might need to reinstall the application or other features using the InstallShield Wizard.

Follow these instructions to reinstall, start, and log in to the application.

❖ To reinstall the TraceFinder application

1. From the Thermo Foundation Instrument Configuration window, remove all instruments.
2. From the Windows Control Panel, uninstall the application and then uninstall all Thermo instrument drivers.
3. Insert the TraceFinder CD, and install both the TraceFinder 3.3 application and the NIST™ library as follows:
 - a. Open the TraceFinder launcher and click **Next**.

The InstallShield Wizard opens.



- b. Click **TraceFinder 3.3**, and follow the instructions in the InstallShield Wizard.

The installer verifies that you have the appropriate versions of the Thermo Foundation™ platform and Xcalibur data system and updates them if necessary.

- c. At the prompt, click **Yes** to completely remove any previously installed applications.
- d. Open the TraceFinder launcher again and click **Next**.
- e. Click **TraceFinder 3.3**, and follow the instructions in the InstallShield Wizard.

IMPORTANT For the application to properly install, you might be prompted to uninstall Foundation platform. Do the following:

1. Click **Yes**, and then when prompted to restart your computer, click **OK**.

The wizard continues the TraceFinder installation.

2. When prompted to install Thermo Foundation, click **Yes**, and then when prompted to restart your computer, click **OK**.

The wizard continues the installation.

- f. When prompted, choose to install either the **GC** or **LC** version of the software.
- g. When the installation is complete, open the TraceFinder launcher again and click **Next**.
- h. When prompted to restart your computer, select the **Yes** option and click **Finish**.

3. (Optional) After your system restarts, open the TraceFinder launcher again, click **Next**, and install any of the following:
 - a. Click **NIST Library** and follow the instructions to install it.
 - b. Click **Example Data**.

The application installs example compound databases, instrument methods, and batch data.
 - c. Click **Library Manager 2.0** and follow the instructions to install the Thermo Library Manager application.
4. Install the appropriate device drivers, and configure the instruments in the Thermo Foundation Instrument Configuration window.

You can now start the TraceFinder application.

❖ **To start the TraceFinder application**

1. Configure your instruments.

You must close the TraceFinder application before you can configure your instruments.

2. Double-click the **TraceFinder** icon on your desktop, or choose **Start > All Programs > Thermo TraceFinder 3.3 > TraceFinder 3.3 General Quan**.

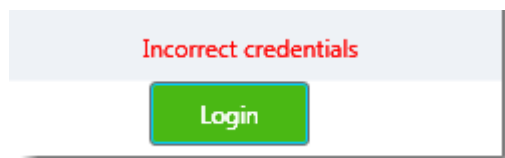
By default, user security is not activated and the application does not require a password. To activate user security, refer to the *TraceFinder Administrator Console User Guide*.

❖ **To log in to the TraceFinder application (when user security is activated)**

Note Before you can log in to the application when user security is activated, a system administrator must set up a user account for you.

1. Enter your user name in the TraceFinder login window. See “[TraceFinder login window](#)” on [page 13](#).
2. Enter your password.

If your user name or password does not match, the system reports this error:



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

3. Click **Login**.

The TraceFinder login window opens. See [TraceFinder main window](#).

2 Getting Started

Installing the TraceFinder Application

Figure 3. TraceFinder main window, showing the Analysis mode for a quantitation batch

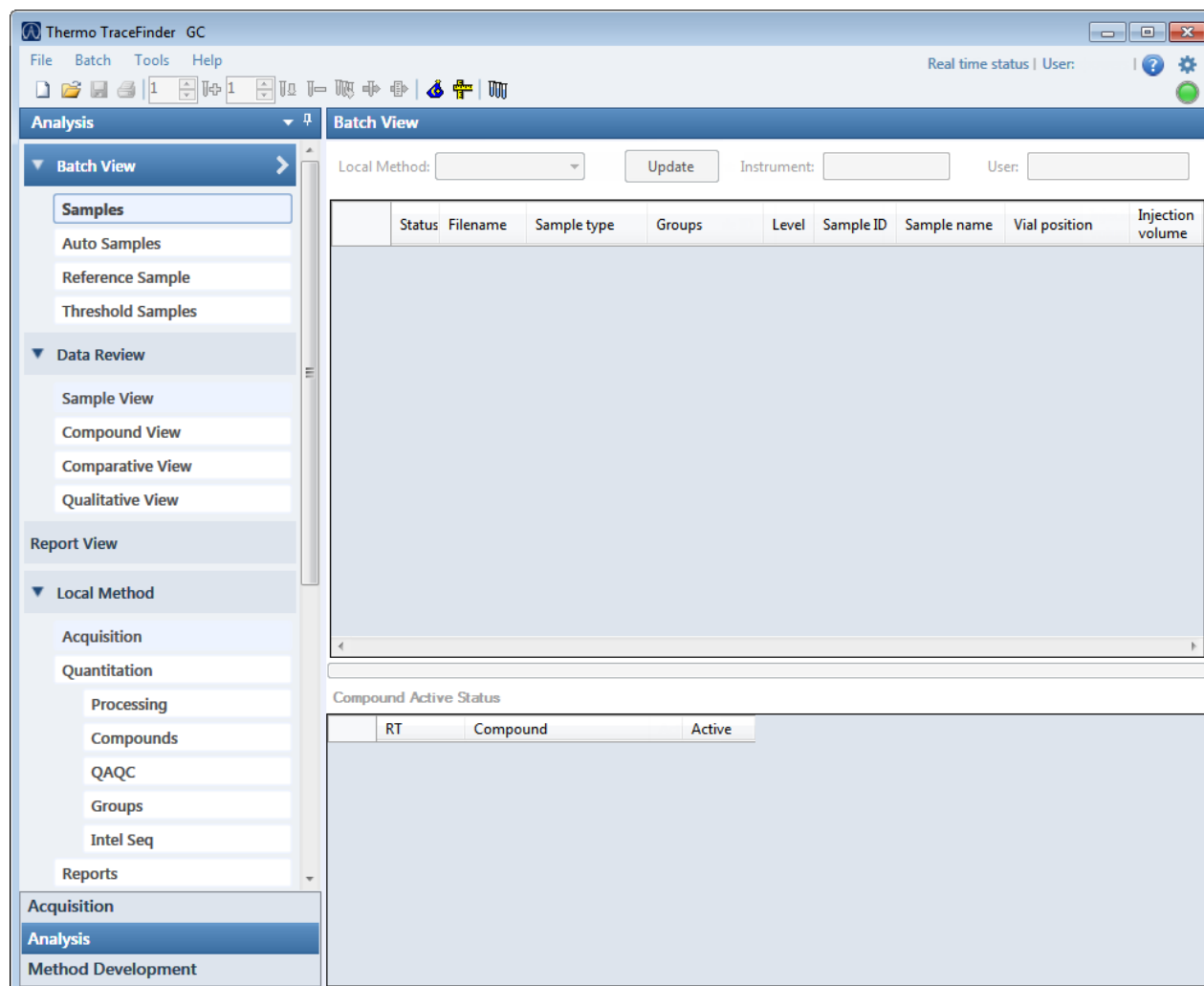


Table 1. TraceFinder main window features (Sheet 1 of 2)

Parameter	Description
Modes	
Acquisition	See Chapter 8, “Using the Acquisition Mode.”
Analysis	See Chapter 9, “Using the Analysis Mode for Quantitation Batches.” See Chapter 10, “Using the Analysis Mode for Target Screening Batches.” See Chapter 11, “Using the Analysis Mode for Unknown Screening Batches.”
Method Development	See Chapter 4, “Using the Common Features of the Method Development Mode.” See Chapter 5, “Using the Method Development Mode for Quantitation Methods.” See Chapter 6, “Using the Method Development Mode for Target Screening Methods.” See Chapter 7, “Using the Method Development Mode for Unknown Screening Methods.”

Table 1. TraceFinder main window features (Sheet 2 of 2)

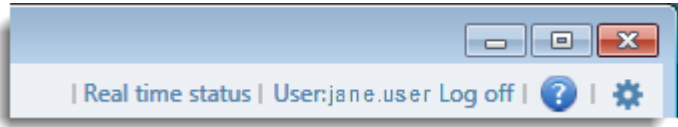


Parameter	Description
Additional Features	A TraceFinder window with user security for a user in the default LabDirector role has these functions. 
Real Time Status	Opens the Real Time Status pane for the current acquisition. The acquisition progress is displayed within the current mode window.
<i>CurrentUserName</i>	Displays the name of the current user.
Log Off	Logs off the current user and displays the login screen. This function is available only when user security is activated.
Help 	Opens the TraceFinder Help.
Application Configuration 	Opens the Configuration console where you can configure several options for using the application. See Chapter 3, “Using the Configuration Console.”

Figure 4. TraceFinder login window

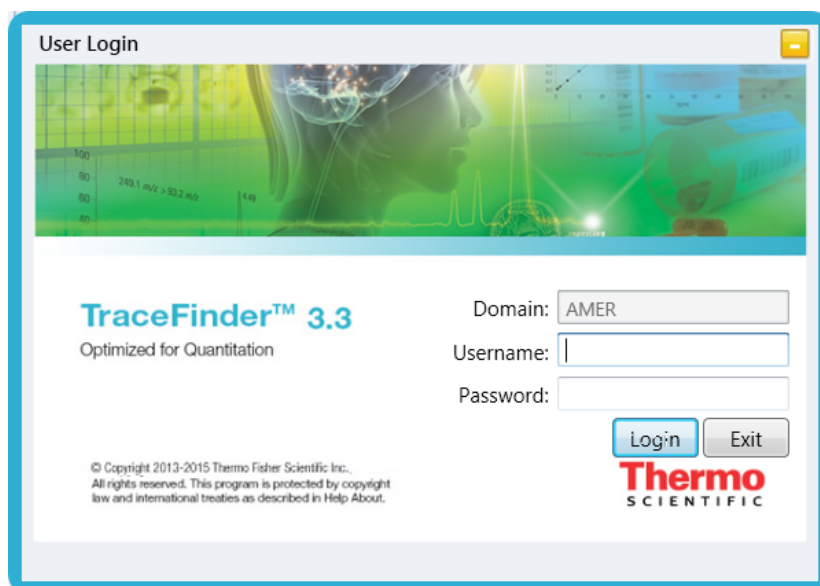


Table 2. Login window parameters

Parameter	Description
Domain	The authentication method.
Username	The user’s assigned user name.
Password	The assigned password for the user name.
Login	Verifies the user name and password, and opens the application.
Exit	Closes the TraceFinder login window.

Installing the NIST and QED Libraries

When you are using triple quadrupole instruments, such as the TSQ Quantum XLS, follow these instructions to install the NIST and QED libraries.

❖ To install the NIST library


1. Open the TraceFinder launcher, and click **Next**.
2. Click **NIST Library**.

The NIST 08 MS Search and AMDIS Setup wizard opens.

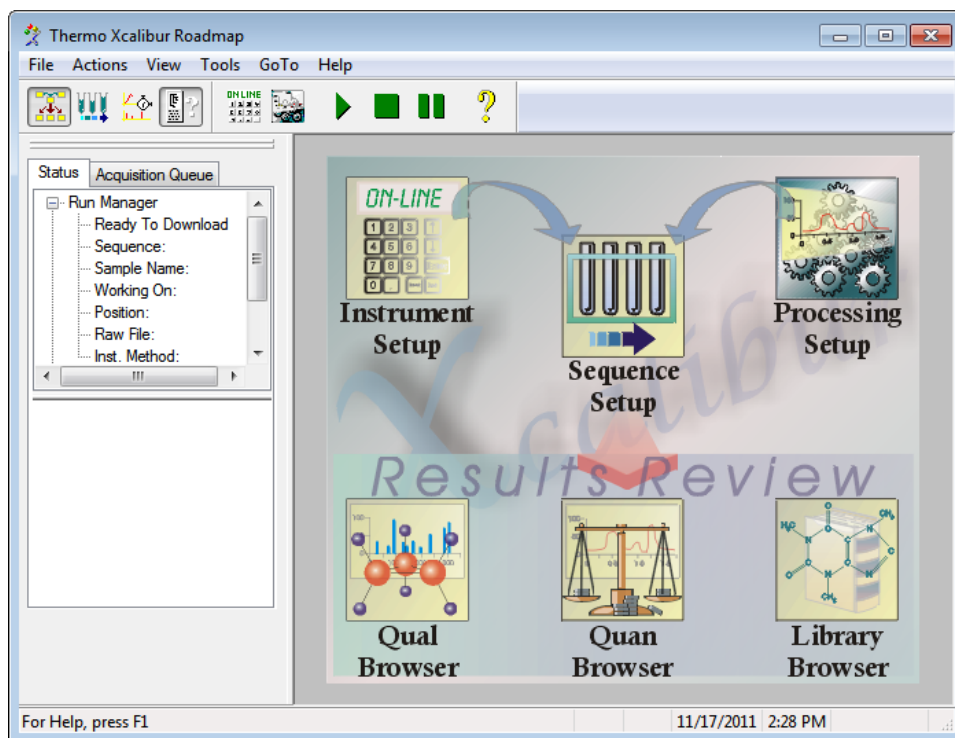
3. Follow the instructions in the setup wizard.
4. When the wizard prompts you to select a destination folder, select **C:\Program Files\NISTMS**.
5. Continue to follow the instructions in the wizard until the setup is complete.

Note The application installs the NIST 2008 library; however, it also supports the NIST 2011 and NIST 2014 libraries.

❖ To install the QED library

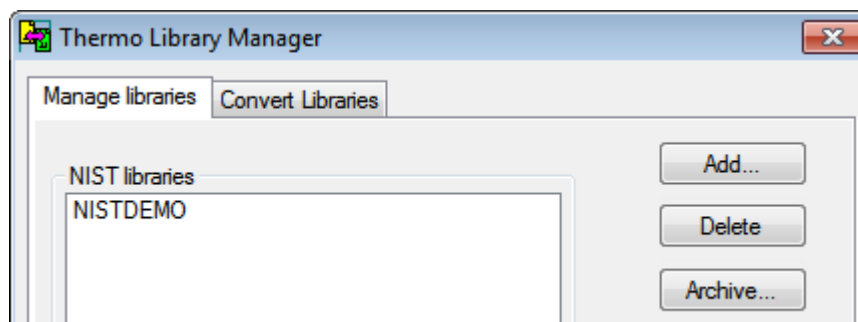
1. On your desktop, double-click the **Xcalibur** icon, .

The Thermo Xcalibur Roadmap opens.



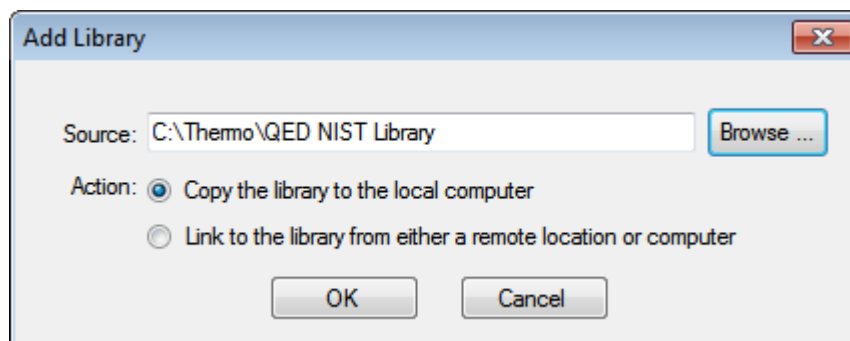
2. Choose **Tools > Library Manager** from the main menu.

The Thermo Library Manager dialog box opens, showing the NIST Libraries list.



3. Click **Add**.

The Add Library dialog box opens.

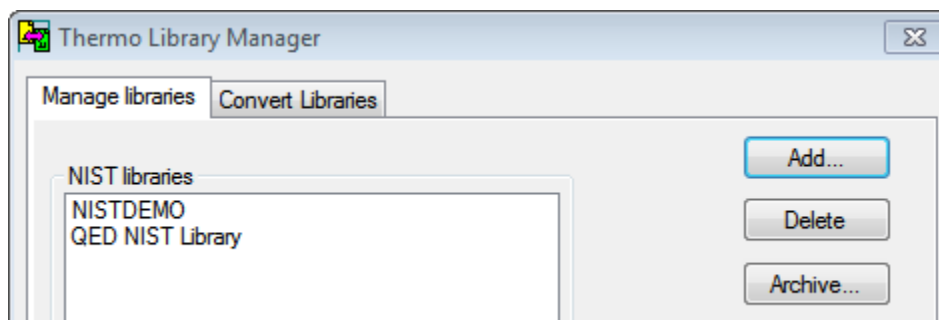


4. Click **Browse**, and locate your QED library in the C:\Thermo folder.
5. Click **OK**.

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

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

The Xcalibur data system adds the QED library to the NIST Libraries list in the Library Manager dialog box.

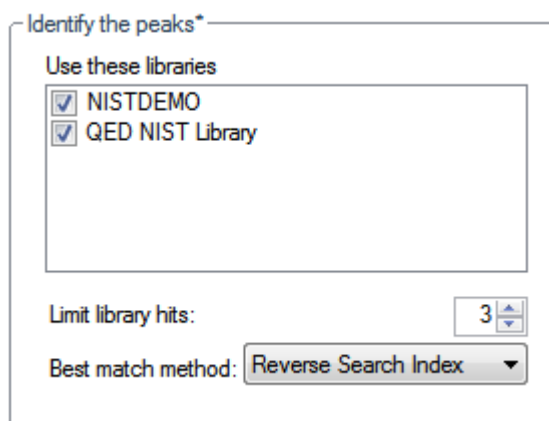


2 Getting Started

Installing the NIST and QED Libraries

7. Click **Exit** in the Thermo Library Manager dialog box.
8. To confirm the library installation, do the following:
 - a. Start the application.
 - b. Click **Method Development** in the navigation pane.
 - c. Click **Method View** in the Method Development navigation pane.
 - d. Choose **File > New > Method Template** from the main menu.

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

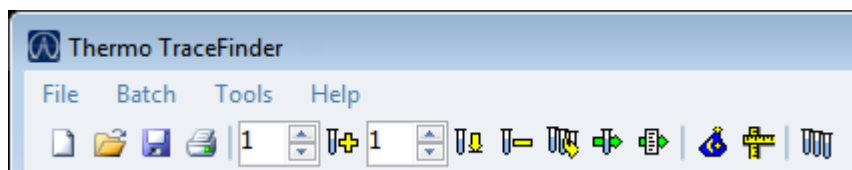


Launching the NIST Library Browser

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

❖ **To open the NIST library browser**

Choose **Tools > Launch Library Browser** from the TraceFinder main menu.



The NIST MS Search window opens.

#	Src.	Name
1	L	Caffeine
2	L	Theobromine
3	L	Xanthine
4	L	Vitamin C

(Spec. List) Caffeine

Name: Caffeine
 Formula: C₈H₁₀N₄O₂
 MW: 194 CAS#: 58-08-2 NIST#: 290714 ID#: 1 DB: Spec. List
 Other DBs: Fine, TSCA, RTECS, EPA, USP, HODOC, NIH, EINECS, IRDB
 Comment: NIST Mass Spectrometry Data Center, 1998.
 10 largest peaks:
 194 999 | 109 721 | 55 439 | 67 438 | 82 328 |
 42 138 | 193 135 | 195 103 | 110 92 | 81 81 |
 Synonyms:
 1,1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-
 Estimated non-polar retention index (n-alkane scale):
 Value: 1795 iu
 Confidence interval (Nitrogen-containing): 83(50%) 356(95%) iu

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

Launching a Qualitative Explorer

Use a qualitative explorer application to display chromatograms and spectra, detect chromatogram peaks, search libraries, simulate spectra, subtract background spectra, apply filters, add text and graphics, create and save layouts, and view instrument parameters as they changed during the acquisition.

Your TraceFinder application is configured to use one of the following applications:

- Thermo Scientific FreeStyle
- Thermo Xcalibur Qual Browser

Thermo Scientific FreeStyle

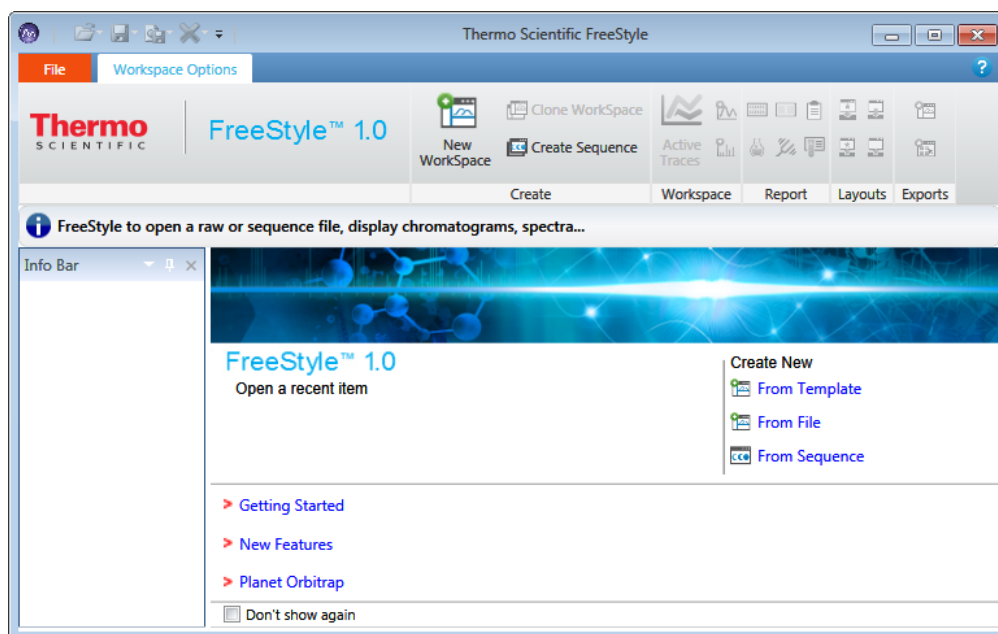
IMPORTANT The FreeStyle™ application is available only when you configure it as your default qualitative explorer in the Configuration Console. See [Chapter 3, “Using the Configuration Console.”](#)

❖ To open the FreeStyle window

Choose **Tools > Launch Qual Explorer** from the TraceFinder main menu.

The Thermo Scientific FreeStyle application opens.

Figure 5. FreeStyle main window



For detailed instructions about using the FreeStyle application, click the **Help** icon, , in the FreeStyle window.

Thermo Xcalibur Qual Browser

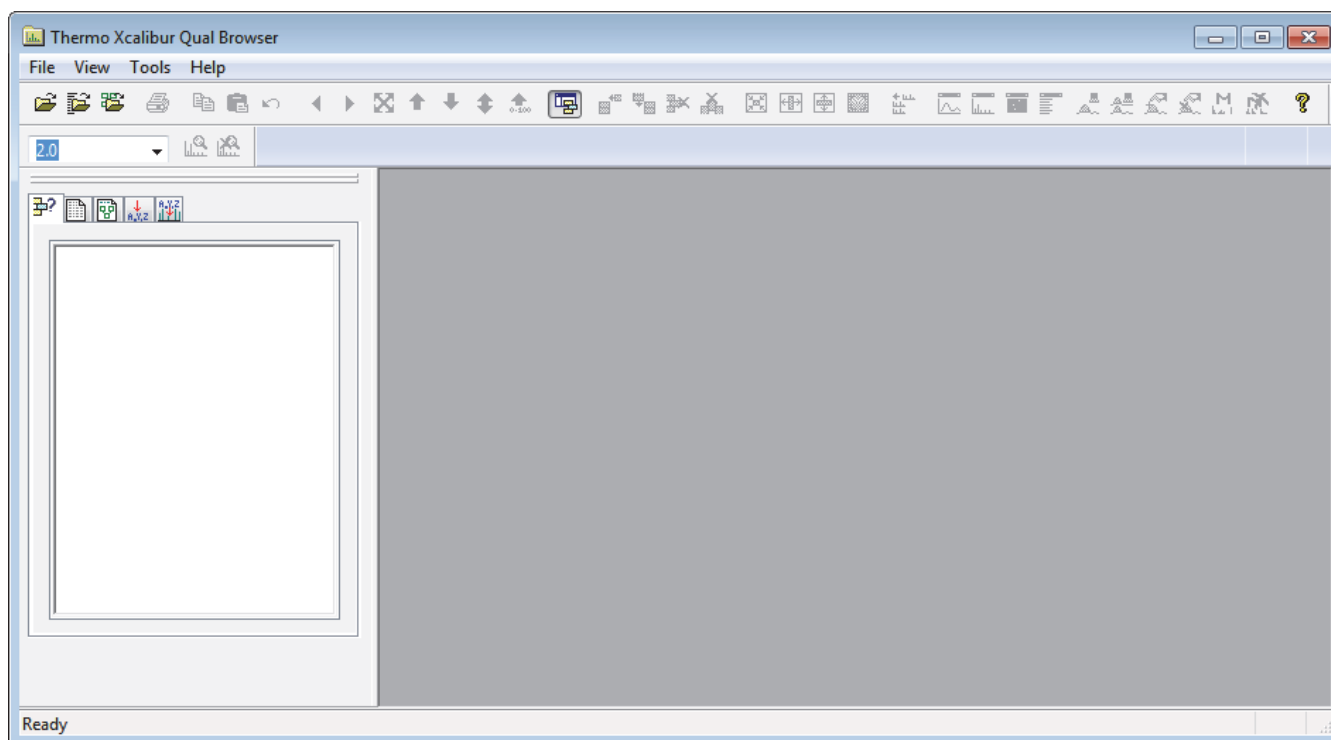
IMPORTANT The Qual Browser application is available only when you configure it as your default qualitative explorer in the Configuration Console. [Chapter 3, “Using the Configuration Console.”](#)

❖ **To open the Qual Browser window**

Choose **Tools > Launch Qual Explorer** from the TraceFinder main menu.

The Thermo Xcalibur Qual Browser application opens.

Figure 6. Qual Browser main window



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

Converting Legacy Data

Use the TraceFinder Legacy Data Converter to convert methods, batches, method templates, batch templates, or compound databases (CDBs) from the source versions to compatible TraceFinder 3.3 target configurations.

- You can convert legacy methods, batches, or method templates from TraceFinder versions 2.1, 3.0, 3.1, or 3.2.
- You can convert legacy batch templates from TraceFinder versions 3.0, 3.1, or 3.2.
- You can convert legacy compound databases from Thermo ToxFinder™ version 1.0 or from TraceFinder versions 3.0, 3.1, or 3.2.
- You can convert data from TraceFinder version 3.3 for general quantitation to another installed configuration of TraceFinder 3.3.

Version Compatibility

This table shows which source versions of methods, batches, method templates, batch templates, or compound databases are compatible with TraceFinder 3.3 target configurations.

Table 3. Version compatibility

Source	TraceFinder 3.3 target			
	General	EFS ^a	Clinical Research	Forensic Toxicology
TraceFinder 3.3 General		✓	✓	✓
TraceFinder 3.2 General		✓	✓	✓
TraceFinder 3.2 EFS		✓		
TraceFinder 3.2 Clinical Research			✓	✓
TraceFinder 3.2 Forensic Toxicology			✓	✓
TraceFinder 3.1 General		✓	✓	✓
TraceFinder 3.1 EFS		✓		
TraceFinder 3.1 Clinical Research			✓	✓
TraceFinder 3.1 Forensic Toxicology			✓	✓
TraceFinder 3.0 General	✓	✓	✓	✓
TraceFinder 3.0 EFS		✓		
TraceFinder 3.0 Clinical Research			✓	✓
TraceFinder 3.0 Forensic Toxicology			✓	✓
TraceFinder 2.1 General	✓	✓	✓	✓
TraceFinder 2.1 EFS		✓		
TraceFinder 2.1 Clinical Research			✓	✓
TraceFinder 2.1 Forensic Toxicology			✓	✓

^a Environmental and Food Safety

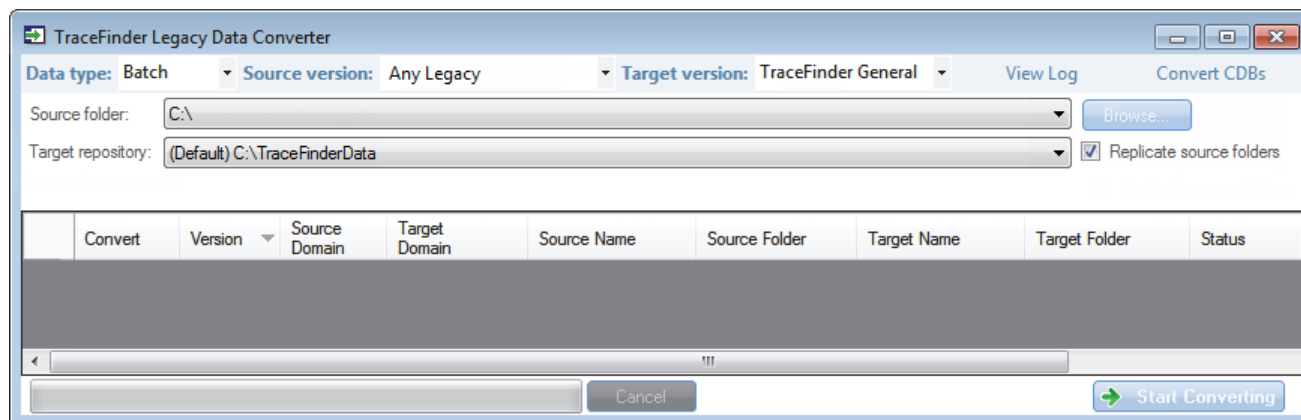
See the following topics:

- [Converting Methods](#)
- [Converting Batches](#)
- [Converting Method Templates](#)
- [Converting Batch Templates](#)
- [Converting Compound Databases](#)

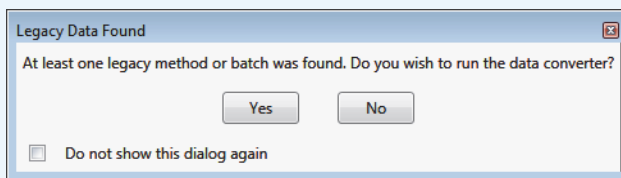
❖ **To open the TraceFinder Legacy Data Converter**

Choose **Tools > Launch Legacy Data Converter** from the TraceFinder main menu.

The TraceFinder Legacy Data Converter window opens.



Note When you open the application, the system checks for any legacy data and prompts you to open the Legacy Data Converter.



Converting Methods

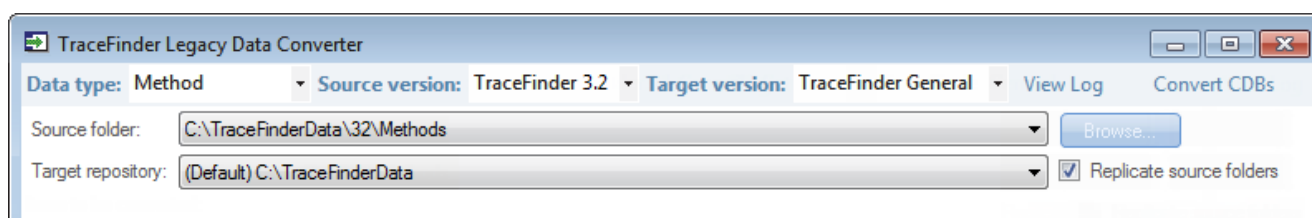
Use the data converter to convert legacy methods to TraceFinder 3.3 methods.

❖ To convert a method

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

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

The following example shows that you can convert methods from the TraceFinder 3.2 General configuration to the current General configuration. For a complete list of version compatibilities, see “[Version Compatibility](#)” on [page 20](#).



2. In the Source Version list, select the version of the method that you will convert.

Note When you select Any Legacy, the Legacy Data Converter examines all possible methods in the source folder, regardless of version.

The conversion table displays the methods in the Methods folder for the selected source version. The application verifies that the method file is in the .mmx file format.

3. To convert a method that is not in the default list, do the following:
 - a. Click **Browse** and locate a different source method folder.

You can select a specific method folder or a folder that contains multiple methods.

- b. Click **OK** in the Browse for Folder dialog box.

The application displays the selected method folder in the conversion table.

When you select a folder that contains multiple method folders, the application displays all the methods.

4. In the Target Version list, select the version that you are converting to.

The list displays only TraceFinder configurations with compatible data. See “[Version Compatibility](#)” on [page 20](#).

5. (Optional) In the Target Name column, change the default new name for each method that you want converted.

When you populate the conversion table, the application checks each method to see if a method with this name exists in the target repository.

- If the method name already exists in the target repository, the default new name appends “_1” to the original name.
- If the method name does not exist in the target repository, the application keeps the original method name.

IMPORTANT The conversion cannot overwrite an existing file name. If the new name is identical to an existing method file, the conversion will not work. When you manually enter a new name, you must verify that the name does not already exist.

6. Select the **Convert** check box for each method that you will convert, and click



The application confirms that all methods to be converted use the .mmx file format.

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 a method is successfully converted, the application writes the converted file to the specified target repository.

Note If a method conversion is unsuccessful, the Status column displays “Conversion failed.” The log file contains details about the failed conversion.

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

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

Figure 7. Sample log file for converting a method

```
===== Start Converting Method from Any Legacy to TraceFinder General =====
--- Converting master method from 'Method_Apple1'
--- Creating master method
--- Importing properties of object 'OuanMethodData' from
XML file 'C:\TraceFinderData\3.2\Methods\Method_Apple1001\Metho
--- Saving master method
--- Copying instrument method
--- Successfully converted master method from 'Method_Apple1'
to 'C:\TraceFinderData\3.3\Methods\Method_Apple1\Method_Apple1.mmx'
-----
===== Conversion completed. 1 total, 1 successful, 0 failed. =====
```

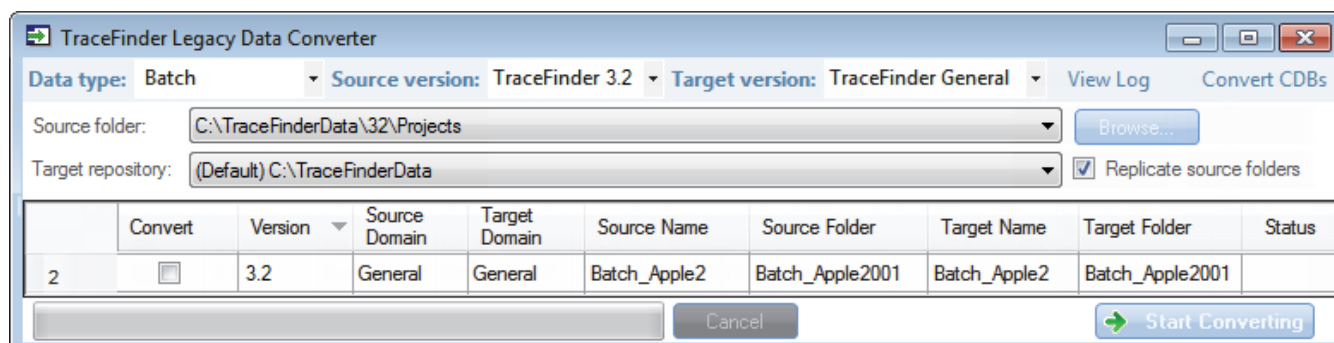
Converting Batches

Use the data converter to convert legacy batches to TraceFinder 3.3 batches.

❖ To convert a batch

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

The following example shows that you can convert batches from the TraceFinder 3.2 General configuration to the current General configuration. For a complete list of version compatibilities, see “[Version Compatibility](#)” on [page 20](#).



2. In the Source Version list, select the version of the batch that you will convert.

Note When you select Any Legacy, the Legacy Data Converter examines all possible batches in the source folder, regardless of version.

The conversion table displays all batches in the Projects folder for the selected source version.

3. In the Target Version list, select the version that you are converting to.

The list displays only TraceFinder configurations with compatible data. See “[Version Compatibility](#)” on [page 20](#).

4. 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.

5. (Optional) In the New Name column, change the default new name for each batch that you want converted.

When you populate the conversion table, the application checks each batch to see if a batch with this name exists in the target repository.

- If the batch name already exists in the target repository, the default new name appends “_1” to the original name.
- If the batch name does not exist in the target repository, the application keeps the original batch name.

IMPORTANT The conversion cannot overwrite an existing file name. If the new name is identical to an existing batch folder, the conversion will not work. When you manually enter a new name, you must verify that the name does not already exist.

6. Select the **Convert** check box for each batch that you will convert, and click



The application confirms that all batches to be converted use the .btx file format.

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 a batch is successfully converted, the application writes the converted batch to the ...TraceFinderData\3.3\Projects folder and uses either the original project and subproject names or the new names that you entered.

Note If a batch conversion is unsuccessful, the Status column displays “Conversion failed.” The log file contains details about the failed conversion.

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

Figure 8. Sample log file for converting a batch

```

===== Start Converting Batch from Any Legacy to TraceFinder General =====
--- Converting batch from 'C:\TraceFinderData\32\Projects\Batch_Apple1\BatchData.btd
--- archiving legacy batch Batch_Apple1 as Batch_Apple1001
Loading data from source batch database
--- Copying raw file
    from 'C:\TraceFinderData\32\Projects\Batch_Apple1001\Data\Apple_0_81_01.raw'
    to 'C:\TraceFinderData\3.3\Projects\Batch_Apple1\Data\Apple_0_81_01.raw'
[W !!! Cannot find source chrospec file 'C:\TraceFinderData\32\Projects\Batch_Apple1001
--- ----- Completed sample import -----
--- Importing local method for 'Batch_Apple1'
--- Importing properties of object 'QuanMethodData'
    from XML file 'C:\TraceFinderData\32\Projects\Batch_Apple1001\Methods\Method_
--- Saving local method data for 'Batch_Apple1_Method_Apple1'
--- Copying reference files method
--- Copying instrument method
--- Saving batch data for 'Batch_Apple1'
--- Successfully converted batch from 'Batch_Apple1' to 'C:\TraceFinderData\3.3\Projects'
-----
===== Conversion completed. 1 total, 1 successful, 0 failed. =====
  
```

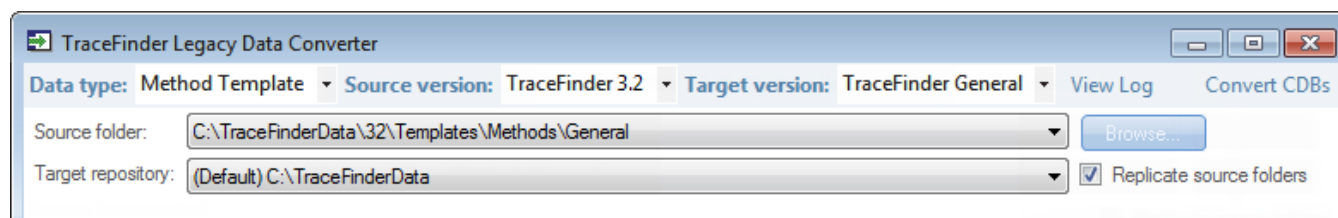
Converting Method Templates

Use the data converter to convert legacy method templates to TraceFinder 3.3 method templates.

❖ To convert a method template

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

The following example shows that you can convert method templates from the TraceFinder 3.2 General configuration to the current General configuration. For a complete list of version compatibilities, see “[Version Compatibility](#)” on [page 20](#).



2. In the Source Version list, select the version of the method template that you will convert.

Note When you select Any Legacy, the Legacy Data Converter examines all possible method templates in the source folder, regardless of version.

The conversion table displays the method templates in the Templates folder for the selected source version. The application verifies that the method template file is in the .pmtx file format.

3. To convert a method template that is not in the default list, do the following:

- a. Click **Browse** and locate a template folder.
You can select a specific template folder or a folder that contains multiple templates.
- b. Click **OK** in the Browse for Folder dialog box.

The application displays the selected folder in the conversion table.

When you select a folder that contains multiple method template folders, the application displays all the method templates.

4. In the Target Version list, select the version that you are converting to.

The list displays only TraceFinder configurations with compatible data. See “[Version Compatibility](#)” on [page 20](#).

5. (Optional) In the Target Name column, change the default name for each method template that you want converted.

When you populate the conversion table, the application checks each method template to see if a method template with this name exists in the target repository.

- If the method template name already exists in the target repository, the default new name appends “_1” to the original name.
- If the method template name does not exist in the target repository, the application keeps the original method template name.

IMPORTANT The conversion cannot overwrite an existing file name. If the new name is identical to an existing method template file, the conversion will fail. When you manually enter a new name, you must verify that the name does not already exist.

6. Select the **Convert** check box for each method template that you will convert, and click



The application confirms that all method templates to be converted use the .pmtx file format.

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 specified target repository.

Note If a template conversion fails, the Status column displays “Conversion failed.” The log file contains details about the failed conversion.

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

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

Figure 9. Sample log file for converting a method template

```

=== Start Converting Method Template from Any Legacy to TraceFinder General ===
--- Converting method template from 'Default'
--- Importing properties of object 'ProcMethodTemplateData' from
    XML file 'C:\TraceFinderData\32\Templates\Methods\General\FALSEDefault001.m
--- Saving the method template
--- Successfully converted method template from
    'C:\TraceFinderData\32\Templates\Methods\General\Default.pmtx'
```

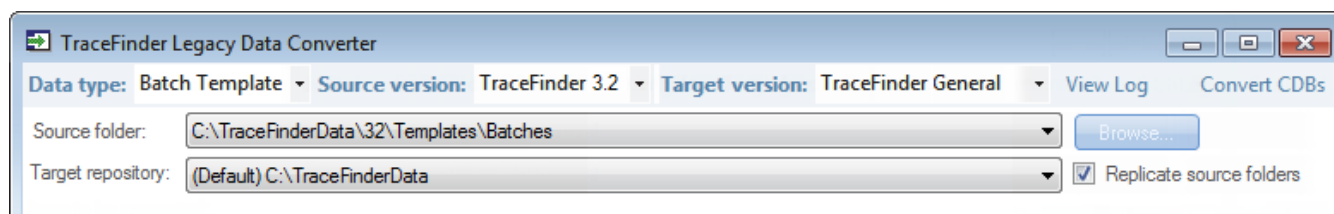
Converting Batch Templates

Use the data converter to convert legacy batch templates to TraceFinder 3.3 batch templates.

❖ To convert a batch template

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

The following example shows that you can convert batch templates from the TraceFinder 3.2 General configuration to the current General configuration. For a complete list of version compatibilities, see “[Version Compatibility](#)” on page 20.



2. In the Source Version list, select the version of the batch template that you will convert.

Note When you select Any Legacy, the Legacy Data Converter examines all possible batch templates in the source folder, regardless of version.

The conversion table displays the batch templates in the Templates folder for the selected source version.

3. To convert a batch template that is not in the default list, do the following:
 - a. Click **Browse** and locate a template folder.
You can select a specific batch template folder or a folder that contains multiple batch templates.
 - b. Click **OK** in the Browse for Folder dialog box.

The application displays the selected folder in the conversion table.

When you select a folder that contains multiple batch template folders, the application displays all the batch templates.

4. In the Target Version list, select the version that you are converting to.

The list displays only TraceFinder configurations with compatible data. See “[Version Compatibility](#)” on page 20.

5. (Optional) In the New Name column, change the default new name for each batch template that you want converted.

When you populate the conversion table, the application checks each batch template to see if a batch template with this name exists in the target repository.

- If the batch template name already exists in the target repository, the default new name appends “_1” to the original name.

- If the batch template name does not exist in the target repository, the application keeps the original batch template name.

IMPORTANT The conversion cannot overwrite an existing file name. If the new name is identical to an existing batch template file, the conversion will fail. When you manually enter a new name, you must verify that the name does not already exist.

6. Select the **Convert** check box for each batch template that you will convert, and click



The application confirms that all batch templates to be converted use the .btx file format.

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 ...\\TraceFinderData\\3.3\\Templates\\Batches folder.

Note If a template conversion fails, the Status column displays “Conversion failed.” The log file contains details about the failed conversion.

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

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

Figure 10. Sample log file for a failed batch template conversion

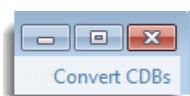
```
===== Start Converting Batch Template from TraceFinder 3.2 General to TraceFin
Archiving legacy batch template Apple as Apple_TF31
-- Converting batch template from 'C:\\TraceFinderData\\32\\Templates\\Batches\\Apple\\Ba
-----
===== Conversion completed. 1 total, 0 successful, 1 failed. =====
```

Converting Compound Databases

Use the data converter to convert legacy compound databases to TraceFinder 3.3 compound databases.

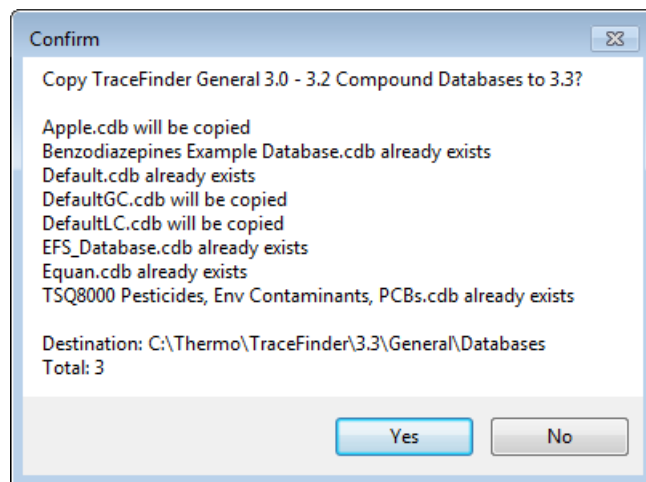
❖ To convert compound databases

1. Click **Convert CDBs** (in the upper right corner of the window).



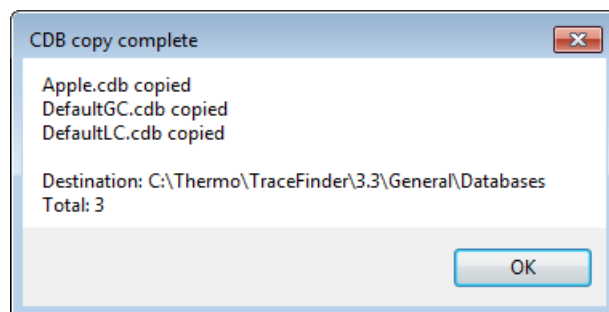
Note If your window is too narrow, you might not see the Convert CDBs button. Widen the window to expose the button in the upper right corner.

The Confirm dialog lists all databases that will be converted to TraceFinder 3.3.



2. Click **Yes**.

The Confirm dialog lists all databases that are converted to TraceFinder 3.3.



3. Click **OK**.

The converted compound databases are now available in the TraceFinder 3.3 application.

Choosing a Mode or Console

When user security is activated, the navigation pane displays the modes and consoles available to the current user's assigned roles and permissions. The following table shows the available modes and consoles for each user role.

Table 4. User roles and default access

User role	Method Development	Acquisition	Analysis	Configuration Console	Administrator Console
Security					Security only
LabDirector	✓	✓	✓	✓	✓
ITAdmin					✓
Supervisor	✓	✓	✓	✓	✓
Technician		✓	✓		
QAQC			✓		

Note When user security is not activated, all modes and consoles are available to all users.

Follow these procedures:

- [To choose a mode](#)
- [To open the Configuration console](#)
- [To open the Administrator Console](#)
- [To display a log of instrument errors](#)
- [To monitor instrument status](#)
- [To watch acquisition and processing in real time](#)

❖ **To choose a mode**


In the navigation pane, click the mode where you want to work.

The navigation pane shows only the modes that you have permission to use.



Mode	Description
Acquisition	Opens the Acquisition mode where you can create and review batches, batch data, reports, and local methods. See Chapter 8, “Using the Acquisition Mode.”
Analysis	Opens the Analysis mode where you can review batches, batch data, reports, and local methods. See Chapter 9, “Using the Analysis Mode for Quantitation Batches.” See Chapter 10, “Using the Analysis Mode for Target Screening Batches.” See Chapter 11, “Using the Analysis Mode for Unknown Screening Batches.”
Method Development	Opens the Method Development mode where you can create a master method or an instrument method. See Chapter 4, “Using the Common Features of the Method Development Mode.” See Chapter 5, “Using the Method Development Mode for Quantitation Methods.” See Chapter 6, “Using the Method Development Mode for Target Screening Methods.” See Chapter 7, “Using the Method Development Mode for Unknown Screening Methods.”

❖ **To open the Configuration console**

Click the **Application Configuration** icon, , in the upper right corner of the TraceFinder window.

When user security is activated, you must have Configuration permissions to access the Configuration Console. See [Chapter 3, “Using the Configuration Console.”](#)

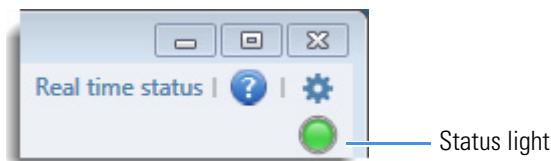
❖ **To open the Administrator Console**

Choose **Tools > Administrator Console** from the TraceFinder main menu.

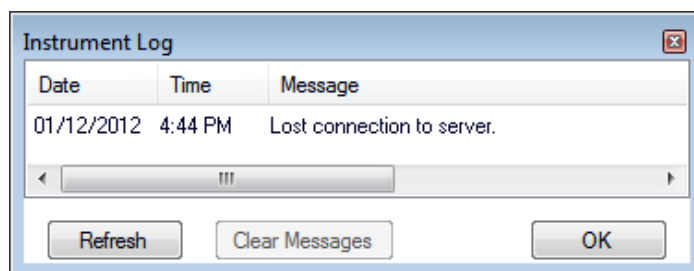
When user security is activated, you must have Administrator permissions to access the Administrator Console. Refer to the *TraceFinder Administrator Console User Guide*.

❖ **To display a log of instrument errors**

1. Click the status light in the upper right corner of the TraceFinder window.



The Instrument Log dialog box opens.



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

2. 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\3.3\General\Logs\TraceFinder.log

- Click **OK** to dismiss the Instrument Log dialog box.

❖ **To monitor instrument status**

Look at the status light in the upper right corner of the TraceFinder window.



Green indicates that the instrument is ready.





Yellow indicates that the instrument is in standby mode, waiting for contact closure, or warming up the lamp.



Red indicates that the instrument is not ready because it is turned off, not configured or connected, currently initializing, or otherwise busy.

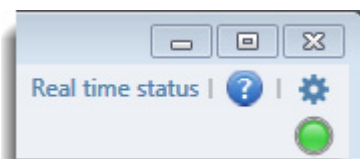
The status light (in any color) might include an exclamation mark.

- An exclamation mark on a green status light, , might indicate that the instrument method contains the wrong source (for example, APCI instead of HESI).
- An exclamation mark on a red status light, , might indicate that a vial is missing and the batch was forced to stop.

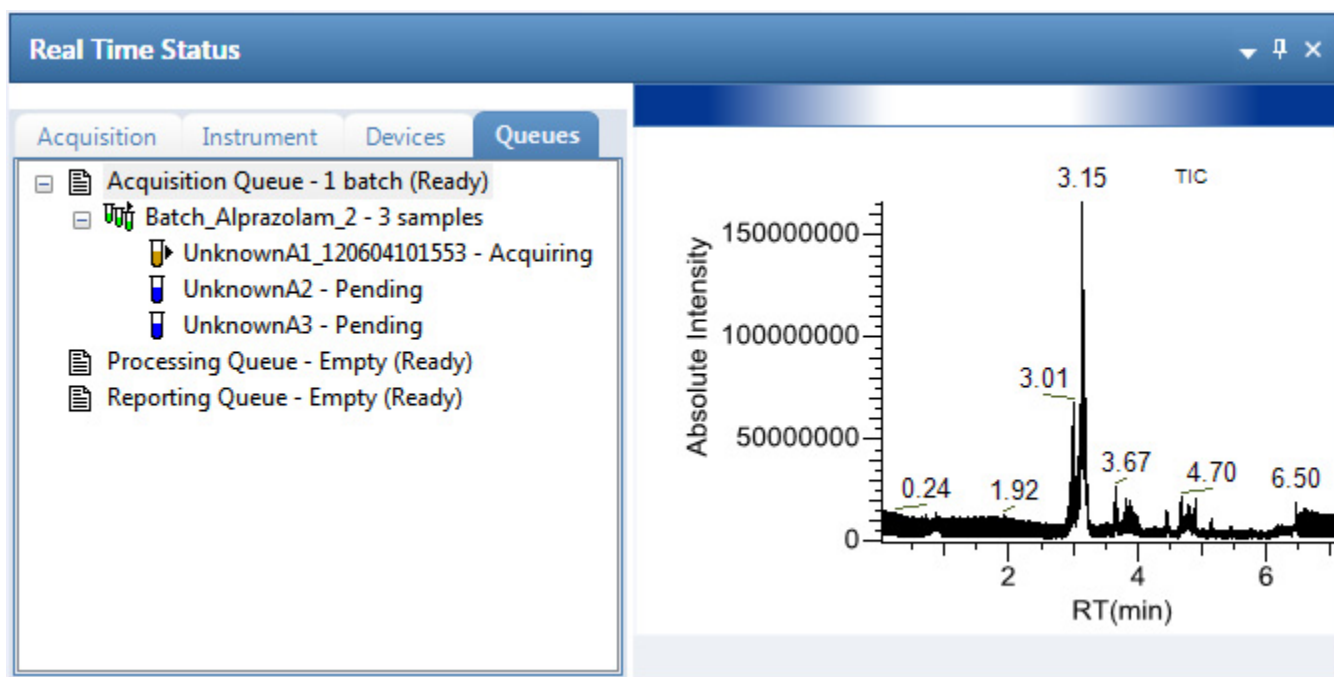
Click the status light to display details of the error.

❖ **To watch acquisition and processing in real time**

Click **Real Time Status** in the upper right corner of the TraceFinder window.



The application displays the Real Time Status pane at the bottom of the window.



For descriptions of all the features of the Real Time Status pane, see “[Real Time Status Pane](#)” on [page 388](#).

Using the Configuration Console

This chapter discusses the features of the Configuration console. When user security is activated, you must have Configuration permissions to access the features in the Configuration console.

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If you are a member of the local administrator's group and are launching the TraceFinder application for the first time, by default, you have LabDirector permissions. For information about groups and permissions, refer to the *TraceFinder Administrator Console User Guide*.

Using the features in the Configuration console, you can do any of the following:

- Activate features, such as multiplexing, intelligent sequencing, qualitative browsers, and screening libraries.
- Select the reports that are available to users, the detector types, and the algorithms used for peak detection.
- Customize adduct definitions, additional sample grid columns, and flags.

❖ **To access the Configuration console**

Click the **Application Configuration** icon, , in the upper right corner of any window.

The TraceFinder Configuration console opens.

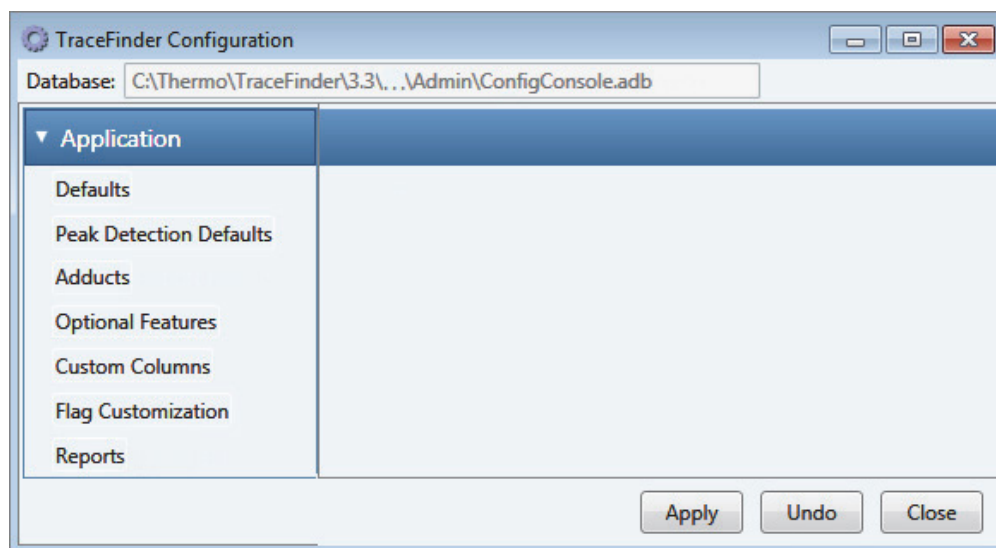


Table 5. Navigation pane functions in the Configuration console

Function	Description
Defaults	Use the Defaults view to specify the default laboratory and instrument names, the displayed mass precision, and the intensity scale to use for reporting. See “Specifying Application Defaults” on page 37.
Peak Detection Defaults	Use the Peak Detection Defaults view to specify a peak detection algorithm and its options and to determine the area under a curve. See “Specifying Default Peak Detection Parameters” on page 39.
Adducts	Use the Adducts view to specify the adducts that will be available for use in method development. See “Specifying Adducts” on page 53.
Optional Features	Use the Optional Features view to enable features, such as quick acquisition, multiplexing, intelligent sequencing, and screening libraries. See “Activating Optional Features” on page 56.
Custom Columns	Use the Custom Columns view to add six additional columns to the samples list in batches. See “Creating Custom Columns” on page 63.
Flag Customization	Use the Flag Customization view to customize error flags and conditions to indicate compound errors in Data Review for quantitation batches. See “Creating Custom Flags” on page 65.
Reports	Use the Reports view to configure which reports are available to users. See “Specifying the Reports” on page 71.

Specifying Application Defaults

Use the Application – Defaults view of the Configuration console to specify the default laboratory and instrument names, the displayed mass precision, and the chromatogram intensity scale to use for reporting. When user security is activated, you must have Configuration – Defaults permission to access these features.

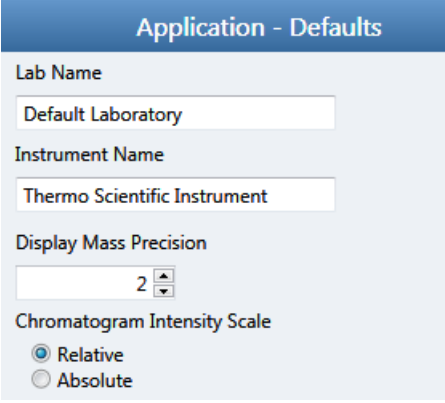
Follow these procedures:

- [To open the Defaults view](#)
- [To specify a default laboratory name and instrument name](#)
- [To specify default mass precision and the intensity scale](#)

❖ To open the Defaults view

In the navigation pane for the Configuration console, click **Defaults**.

The Application – Defaults view opens.



The screenshot shows the 'Application - Defaults' configuration window. It contains four sections: 'Lab Name' with a text box containing 'Default Laboratory'; 'Instrument Name' with a text box containing 'Thermo Scientific Instrument'; 'Display Mass Precision' with a spinner box set to '2'; and 'Chromatogram Intensity Scale' with two radio buttons, 'Relative' (selected) and 'Absolute'.

❖ 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 Processing page of the Method View. The application uses this laboratory name in the report headings.

The application does not apply this default laboratory name 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. To save your changes, click **Apply**.

The application does not apply this default instrument name to previously created batches. By default, the instrument name is Thermo Scientific Instrument.

❖ **To specify default mass precision and the intensity scale**

1. In the Display Mass Precision box, set the decimal value for the mass precision to an integer from **2** to **6**, inclusive.

The default number of digits to display is 2. The application uses this mass precision value to display mass values in the following locations:

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

IMPORTANT When you create a method using a raw data file, the application reads the filter precision value from the raw data file to create scan filters; however, the application uses the Display Mass Precision value when showing masses that are not embedded within filter strings and masses that are displayed on spectral plots.

2. Select either the **Relative** or **Absolute** option for the Chromatogram Intensity Scale.
This sets the default display type for both quantitation and qualitative chromatograms displayed in data review and reports.
3. To save your changes, click **Apply**.

Specifying Default Peak Detection Parameters

When user security is activated, you must have Configuration – Peak Detection Defaults permission to access default peak detection parameters for the Genesis, ICIS, or Avalon detection algorithms.

Use the Peak Detection Defaults view to specify a peak detection algorithm and its options and to determine the area under a curve. These parameters are available for quantitation methods only.

The following topics include procedures for specifying common peak detection parameters and the parameters used for each of the following detection algorithms:

- [Genesis Detection Method](#)
- [ICIS Detection Method](#)
- [Avalon Detection Method](#)

❖ To open the Peak Detection Defaults view

In the navigation pane for the Configuration console, click **Peak Detection Defaults**.

The Application – Peak Detection Defaults view opens.

- For parameter information about all detection algorithms, see “[Common Peak Detection Parameters](#)” on page 41.
- For parameter information about the Genesis detection algorithm, see “[Genesis Detection Method](#)” on page 43.
- For parameter information about the ICIS detection algorithm, see “[ICIS Detection Method](#)” on page 46.
- For parameter information about the Avalon detection algorithm, see “[Avalon Detection Method](#)” on page 49.

❖ To specify common detection parameters

1. In the Detector Type list, select a detector type.

For detailed descriptions of the available detector types, see “[Common Peak Detection Parameters](#)” on page 41.

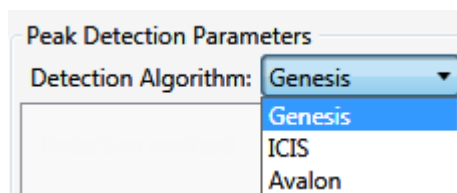
2. In the Mass Tolerance area, do the following:
 - a. Select the unit of measure that you want to use (**MMU** or **PPM**).
 - b. In the Value box, specify the number of millimass units or parts per million to use as the upper limit.

The application applies this mass tolerance to the extracted chromatograms. The default is 500 MMU.

3 Using the Configuration Console

Specifying Default Peak Detection Parameters

3. 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.
4. In the Ion Ratio Parameters area, do the following:
 - a. In the Window Type list, 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.
5. In the Peak Detection Parameters area, select one of the detection algorithms: **Genesis**, **ICIS**, or **Avalon**.



6. Specify the parameters for the selected detection algorithm.

For detailed parameter descriptions, see one of the following:

- [Genesis Detection Method](#)
- [ICIS Detection Method](#)
- [Avalon Detection Method](#)

Common Peak Detection Parameters

All of the detection algorithms use the Detector Type, Mass Tolerance, Retention Time, and Ion Ratio detection parameters.

Figure 11. Common peak detection areas

The screenshot shows a configuration window with the following sections and values:

- Detector Type:** MS
- Mass Tolerance:** Units: MMU PPM; Value: 500.00
- Retention Time:** Window (sec): 30.00; View Width (min): 0.50
- Ion Ratio Parameters:** Window type: Relative; Window (+/-%): 20.00; Ion coelution (min): 0.10

Table 6. Common peak detection parameters (Sheet 1 of 2)

Parameter	Description
Detector Type	<p>MS: Mass spectrometer that ionizes sample molecules and then separates the ions according to their mass-to-charge ratio (m/z).</p> <p>PDA: Photodiode array detector providing a linear array of discrete photodiodes on an integrated circuit chip. It is placed at the image plane of a spectrometer so that a range of wavelengths can be simultaneously detected.</p> <p>Analog: Supplemental detectors (for example, FID, ECD). When you select this detector, any reports that display a QIon value show the value as Analog and any reports that display spectra show the spectra as Not Available.</p> <p>A/D card: If your detector is 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.</p> <p>UV: A UV spectrophotometer (for variable-wavelength detection) or photometer (for single-wavelength detection) equipped with a low-volume flow cell. This detector detects analytes that readily absorb light at a selected wavelength.</p>

Table 6. Common peak detection parameters (Sheet 2 of 2)

Parameter	Description
Mass Tolerance	
Units	<ul style="list-style-type: none"> (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. Valid range: 0.1 through 50 000 Default: 500
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 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 application provides the Genesis peak detection algorithm for backward compatibility with Xcalibur 1.0 studies.

Figure 12. Genesis peak detection

The image shows a 'Peak Detection Parameters' dialog box. At the top, 'Detection Algorithm:' is set to 'Genesis'. Below this, 'Detection method:' is set to 'Nearest RT'. The 'Smoothing:' parameter is a numeric input set to '1'. 'S/N threshold:' is a numeric input set to '2.00'. There is a checkbox for 'Enable valley detection' which is unchecked. Below it, 'Expected width (sec):' is a numeric input set to '0.00'. Another checkbox, 'Constrain peak width', is also unchecked. 'Peak height (%)' is a numeric input set to '5.00'. 'Tailing factor:' is a numeric input set to '1.00'. 'Peak S/N cutoff:' is a numeric input set to '200.00'. 'Valley rise (%)' is a numeric input set to '2.00'. 'Valley S/N:' is a numeric input set to '1.10'. '# background scans:' is a numeric input set to '5'. Finally, 'Report noise as:' is set to 'Peak To Peak'.

Table 7. Genesis peak detection parameters (Sheet 1 of 3)

Parameter	Description
Detection Algorithm	Specifies the Genesis peak detection algorithm.
Detection Method	Specifies the detection method used for component identification. 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 7. Genesis peak detection parameters (Sheet 2 of 3)

Parameter	Description
Smoothing	<p>Specifies 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.</p> <p>Valid values: Any odd integer from 1 through 15 points Default: 1</p>
S/N threshold	<p>Specifies the 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.</p> <p>Valid range: 0.0 through 999.0</p>
Enable Valley Detection	<p>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.</p>
Expected Width (sec)	<p>Specifies 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.</p> <p>With valley detection enabled, any valley points nearer than the <i>expected width</i>/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width.</p> <p>Valid range: 0.0 through 999.0</p>
Constrain Peak Width	<p>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 threshold and a tailing factor. Selecting the Constrain Peak Width check box activates the Peak Height (%) and Tailing Factor options.</p>
Peak Height (%)	<p>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.</p> <p>Valid range: 0.0 through 100.0%</p>

Table 7. Genesis peak detection parameters (Sheet 3 of 3)

Parameter	Description
Tailing Factor	<p>Specifies the tailing factor that controls how the 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.</p> <p>Valid range: 0.5 through 9.0</p>
Peak S/N Cutoff	<p>Sets the peak edge to values below this signal-to-noise ratio.</p> <p>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.</p> <p>When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the application defines the right and left edges of the peak when the S/N reaches a value less than 200.</p> <p>Valid range: 50.0 through 10000.0</p>
Valley Rise (%)	<p>Specifies that 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.</p> <p>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.</p> <p>When the trace exceeds rise percentage, the application applies valley detection peak integration criteria. This test is applied to both the left and right edges of the peak.</p> <p>Valid range: 0.1 through 500.0</p>
Valley S/N	<p>Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher.</p> <p>Valid range: 1.0 through 100.0 Default: 2.0</p>
# Background Scans	<p>Specifies the number of background scans performed by the application.</p>
Report Noise As	<p>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.</p>

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 13. ICIS peak detection

The screenshot shows a configuration window titled "Peak Detection Parameters" for the "ICIS" detection algorithm. The parameters are as follows:

- Detection Algorithm: ICIS
- Detection method: Nearest RT
- Smoothing: 1
- Area noise factor: 5
- Peak noise factor: 10
- Baseline window: 40
- Constrain peak width
- Peak height (%): 5.00
- Tailing factor: 1.00
- Noise method: Incos
- Min peak width: 3
- Multiplet resolution: 10
- Area tail extension: 5
- Area scan window: 0
- RMS

Table 8. ICIS peak detection parameters (Sheet 1 of 3)

Parameter	Description
Detection Algorithm	Specifies the ICIS peak detection algorithm.
Detection Method	Specifies the detection method used for component identification. 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 8. ICIS peak detection parameters (Sheet 2 of 3)

Parameter	Description
Smoothing	<p>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.</p> <p>Valid values: Any odd integer from 1 through 15 points Default: 1</p>
Area Noise Factor	<p>Specifies 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.</p> <p>Valid range: 1 through 500 Default: 5</p>
Peak Noise Factor	<p>Specifies the noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 1 through 1000 Default: 10</p>
Baseline Window	<p>Specifies that the application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 1 through 500 Default: 40</p>
Constrain Peak Width	<p>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 activates the Peak Height (%) and Tailing Factor options.</p>
Peak Height (%)	<p>Specifies that the 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.</p> <p>Valid range: 0.0 through 100.0%</p>
Tailing Factor	<p>Specifies the tailing factor that controls how the 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.</p> <p>Valid range: 0.5 through 9.0</p>

Table 8. ICIS peak detection parameters (Sheet 3 of 3)

Parameter	Description
Noise Method	<p>Specifies the noise method as INCOS or Repetitive.</p> <p>INCOS: Uses a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value.</p> <p>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.</p>
Min Peak Width	<p>Specifies the minimum number of scans required in a peak. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 0 through 100 scans Default: 3</p>
Multiplet Resolution	<p>Specifies 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.</p> <p>Valid range: 1 through 500 scans Default: 10</p>
Area Tail Extension	<p>Specifies the number of scans past the peak endpoint to use in averaging the intensity. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 0 through 100 scans Default: 5</p>
Area Scan Window	<p>Specifies 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.</p> <p>Valid range: 0 through 100 scans Default: 0</p>
RMS	<p>Specifies that the 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.</p>

Avalon Detection Method

The Avalon peak detection algorithm is designed for UV data. The Avalon peak detection algorithm also supports negative peaks. You can edit the Event values from the [Avalon Event List](#).

Figure 14. Avalon peak detection

Peak Detection Parameters

Detection Algorithm: Avalon

Detection method: Nearest RT

Smoothing: 1

Time	Event	Value
Initial	Start Threshold	10000.000
Initial	End Threshold	10000.000
Initial	Area Threshold	10000.000
Initial	P-P Threshold	1.000
Initial	Bunch Factor	1.000
Initial	Negative Peaks	Off

Autocalc initial events Edit

Table 9. Avalon peak detection parameters

Parameter	Description
Detection Algorithm	Specifies the Avalon peak detection algorithm.
Detection Method	Specifies the detection method used for component identification. 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. Valid values: 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.
Autocalc Initial Events	Automatically calculates the events in the Event list.
Edit	Opens the Avalon Event List dialog box where you can edit the Time/Event/Value parameters. See Avalon Event List .

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](#).

Figure 15. Avalon Event List dialog box

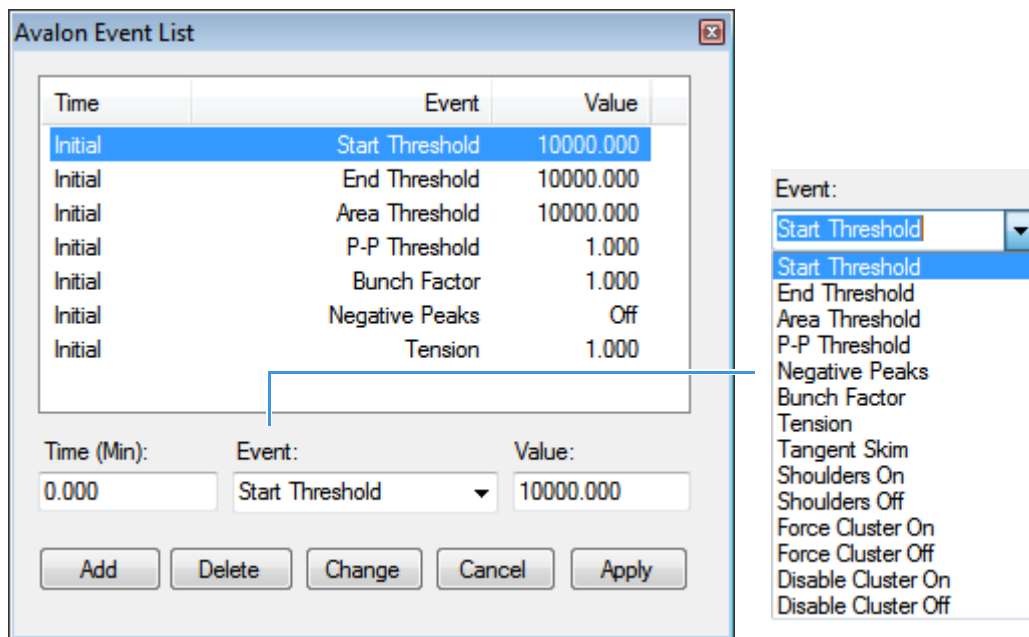


Table 10. Avalon Event List dialog box parameters

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.”
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 16. Event types

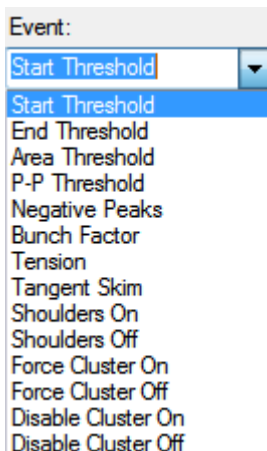


Table 11. Event type descriptions (Sheet 1 of 2)

Event type	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. Valid range: 0 through 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. Valid range: 0 through 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. Valid range: 0 through 999 999 999
P-P Threshold	Specifies 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. Valid range: 0.1 through 99.99
Negative Peaks	Permits detection of a negative going peak. Automatically resets after finding a negative peak. Valid values: On or Off

Table 11. Event type descriptions (Sheet 2 of 2)

Event type	Description
Bunch Factor	<p>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.</p> <p>Valid range: 0 through 999</p>
Tension	<p>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.</p> <p>Valid range: 0 through 999.99 minutes</p>
Tangent Skim	<p>Specifies that 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.</p> <p>Valid range: 0 through 1</p>
Shoulders On	<p>Allows peak shoulders to be detected (peaks which are separated by an inflection rather than a valley) Sets a threshold for the derivative.</p>
Shoulders Off	<p>Disables peak shoulder detection.</p> <p>Valid range: 0 through 50</p>
Force Cluster On	<p>Forces the following peaks to be treated as a cluster (single peak).</p>
Force Cluster Off	<p>Ends the forced clustering of peaks.</p>
Disable Cluster On	<p>Prevents any peaks from being clustered.</p>
Disable Cluster Off	<p>Permits clusters to occur again.</p>

Specifying Adducts

An adduct ion is formed from a precursor ion and contains all of the constituent atoms of that ion and additional atoms or molecules. Adduct ions are often formed in the mass spectrometer ion source. Adducts can be either positive or negative.

Use the Application – Adducts view to specify the adducts that will be available for you to use in method development. When user security is activated, you must have Configuration – Adducts permission to access these features.





Follow these procedures:

- [To open the Adducts view](#)
- [To add an adduct](#)
- [To remove an adduct](#)

❖ To open the Adducts view

In the navigation pane for the Configuration console, click **Adducts**.



The Application – Adducts view opens, displaying the default positive and negative adducts.

Application - Adducts							
Positive Adducts  				Negative Adducts  			
Name	Formula	Type	Neutral Mass	Name	Formula	Type	Neutral Mass
▶ Ammonium	M+NH4	Gain	18.03	▶ Hydrogen-Loss	M-H	Loss	-1.01
▶ Hydrogen	M+H	Gain	1.01	▶ Acetate	M+H3C2O2	Gain	59.01
▶ Sodium	M+Na	Gain	22.99	▶ Formate	M+HCO2	Gain	45.00
▶ Potassium	M+K	Gain	38.96				

❖ To add an adduct

1. In the Positive Adducts or Negative Adducts pane, click the **Add New Adduct** icon, .

The application adds a new, editable row at the bottom of the Adducts list.

Positive Adducts  				
Name	Formula	Type	Neutral Mass	
▶ Ammonium	M+NH4	Gain	18.03	
▶ Hydrogen	M+H	Gain	1.01	
▶ Sodium	M+Na	Gain	22.99	
▶ Potassium	M+K	Gain	38.96	
▶ New Adduct	M+H	Gain	1.01	

2. Type the formula for the new adduct ion.

The formula syntax is alphanumeric and case sensitive. It can include parentheses and brackets.

The formula specifies the difference between the neutral molecule and the charged ion that you expect to see in the results.

For example, a sodium adduct has $[M+Na]^+$ as the expected charged ion (where M is the neutral molecule), so you would type “Na” for the formula. A water adduct has $[M+H+H_2O]^+$ as the expected charged ion, so you would type “H3O” for the formula.

IMPORTANT When you create an adduct formula, you can type both uppercase and lowercase letters; however, the application interprets all uppercase input as single-letter elements and all lowercase input as two-letter elements.

For example, it interprets the string “inau” as In Au and “COSI” as C O S I.

The application displays a type and neutral mass for the adduct formula you entered.



3. Select the default name (New Adduct) and type a name for the adduct.

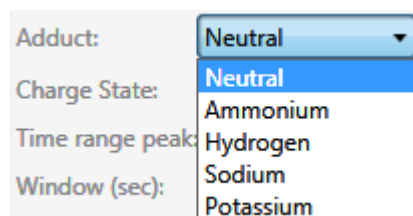
You cannot change the type or neutral mass, but the application will correctly calculate these values later.

4. Press ENTER.

The application adds the adduct to the adducts list and calculates the correct type (Gain or Loss) and the neutral mass.

Positive Adducts				
	Name	Formula	Type	Neutral Mass
>	Ammonium	M+NH4	Gain	18.03
>	Hydrogen	M+H	Gain	1.01
>	Sodium	M+Na	Gain	22.99
>	Potassium	M+K	Gain	38.96
>	Neutral	M+NH3	Gain	17.03

These adducts are available for you to select in the Compound Database view of the Method Development mode when you specify parameter values for target peaks.



❖ **To remove an adduct**

1. In the Positive Adducts or Negative Adducts pane, select the adduct that you want to remove.
2. Press DELETE and confirm that you want to delete the selected adduct.

You can delete only adducts that you added to the adducts list. You cannot delete default adducts defined by the TraceFinder installation.

Activating Optional Features

When user security is activated, you must have Configuration – Optional Features permission to access these features.

Use the Application – Optional Features view to activate the following features:

- [Quick Acquisition](#)
- [Delay Calibration](#)
- [User Peak Detection Settings](#)
- [Autosampler Tray Configuration](#)
- [Acquisition Submission Options](#)
- [Qualitative Explorer](#)
- [Screening Libraries](#)
- [Multiplexing](#)
- [Intelligent Sequencing](#)
- [Processing Options](#)

❖ To open the Optional Features page

In the navigation pane for the Configuration console, click **Optional Features**.

The Application – Optional Features page opens.

The screenshot shows the 'Application - Optional Features' configuration window. It is divided into several sections:

- General Settings:** Four checked checkboxes: 'Quick acquisition allowed', 'Delay calibration', 'User peak detection settings allowed', and 'Allow auto sampler to automatically determine tray configuration (disable for Waters Acquity)'.
- Acquisition submission options:** Two radio buttons: 'Single Sample Submission' (unselected) and 'Full Sequence Submission (Not permitted with Intelligent Sequencing)' (selected).
- Qualitative explorer to use:** Two radio buttons: 'Thermo FreeStyle' (unselected) and 'Thermo Xcalibur Qual Browser' (selected).
- Screening Libraries:** Two text input fields. The first is labeled 'Library Manager:' and has a 'Browse...' button to its right. The second is labeled 'NIST Libraries:' and has a 'Select...' button to its right.
- Multiplexing:** A checked checkbox. Below it, 'Available Channels:' is followed by four checked checkboxes: 'Channel 1', 'Channel 2', 'Channel 3', and 'Channel 4'.
- Intelligent Sequencing:** An unchecked checkbox.
- Processing Options:** Two checkboxes: 'Auto Reprocess (This option can be performance intensive)' (unchecked) and 'Allow Unknown Screening (Hides Unknown Screening options when not checked)' (checked).

Quick Acquisition

The quick acquisition option activates the Quick Acquisition feature in the Acquisition, Analysis, or Method Development mode.

❖ To activate quick acquisition

1. Select the **Quick Acquisition Allowed** check box.
2. To save your changes, click **Apply**.

The application immediately applies this feature change.

For a description of the Quick Acquisition features, see [Appendix A, “Using Quick Acquisition.”](#)

Delay Calibration

You can determine when the application calculates the calibration curve, using the Delay Calibration option. Delaying the recalibration until the application processes the last calibration sample in a batch is faster but less responsive than recalibration after each calibration sample.

❖ To delay calculation of a calibration curve

1. Select the **Delay Calibration** check box.
2. To save your changes, click **Apply**.

The application immediately applies this feature change.

User Peak Detection Settings

Use the User Peak Detection Settings Allowed option to let users modify the method integration settings for specific compounds in Data Review.

❖ To allow users to modify peak detection settings

1. Select the **User Peak Detection Settings Allowed** check box.
2. To save your changes, click **Apply**.

The application immediately applies this feature change.

Autosampler Tray Configuration

By default, the TraceFinder application lets the autosampler automatically determine the tray configuration. When you are using a Waters™ Acquity™ system, you must make this feature unavailable and explicitly specify the tray configuration when you create a batch.

❖ **To disallow automatic tray configuration**

1. Select the **Allow Auto Sampler to Automatically Determine ...** check box.
2. To save your changes, click **Apply**.

The application immediately applies this feature change.

Acquisition Submission Options

To control acquisitions, you can activate either submission option: full-sequence or single-sample. When you submit batches from the Acquisition mode or Quick Acquisition batches from any mode, they run in first-in-last-out order. The last batch submitted is the first batch to run, unless you submit a batch as a priority batch in Acquisition mode.

- When you use Full Sequence Submission, priority batches always run immediately after the currently acquiring batch is completed.
- When you use Single Sample Submission, priority batches always run immediately after the currently acquiring sample is completed.

❖ **To specify acquisition submission features**

1. Select either the **Full Sequence Submission** or the **Single Sample Submission** option:
 - **Full Sequence Submission:** Supports look-ahead features of the autosampler. When the instrument method specifies the look-ahead feature, the application functions like a multiplex driver and feeds the autosampler the next vial position.

When you submit a batch, the autosampler begins preparing for all sample injections when the pre-run condition begins. All samples in the batch must be completed before other batches (even higher priority batches) can begin.

Note The Full Sequence Submission feature is not available when you activate Intelligent Sequencing.

- **Single Sample Submission:** Supports intelligent-sequencing features. When you submit a batch, the autosampler begins preparing for one sample injection at a time. Higher priority batches can interrupt the sample sequence in the currently acquiring batch.

Note The Single Sample Submission feature is not available when you activate Multiplexing. See “Multiplexing” on page 61.

2. To save your changes, click **Apply**.

You must restart the application to apply this feature change.

Qualitative Explorer

You can use either the FreeStyle application or Qual Browser to display chromatograms and spectra, detect chromatogram peaks, search libraries, simulate spectra, subtract background spectra, apply filters, add text and graphics, create and save layouts, and view instrument parameters as they changed during the acquisition.

❖ To specify a qualitative explorer

Select either the **Thermo FreeStyle** or the **Thermo Xcalibur Qual Browser** option.

Note You can access the explorer by choosing Tools > Launch Qual Explorer in the main TraceFinder menu. See “[Launching a Qualitative Explorer](#)” on page 18.

Screening Libraries

Use the specified screening libraries for both quantitation methods and target screening methods. For more information about how you can use screening libraries in a quantitation method, see “[Screening Libraries in a Quantitation Method](#)” on page 60. For more information about how you can use screening libraries in a target screening method, see “[Screening Libraries in a Target Screening Method](#)” on page 61.

When you specify the Library Search Type on the Processing page for a target screening method, you choose either the Library Manager search type or the NIST search type. See “[Editing the Acquisition Page](#)” on page 261.

- When you choose Library Manager as the Library Search Type for a quantitation or target screening method, the application uses the Library Manager library file (.db) specified in the Configuration console. You can search only one spectral library when you process a sample.
- When you choose NIST as the Library Search Type for the method, the application uses the NIST libraries specified in the Configuration console. You can choose to search multiple NIST libraries when you process a sample.

❖ To specify a Library Manager screening library

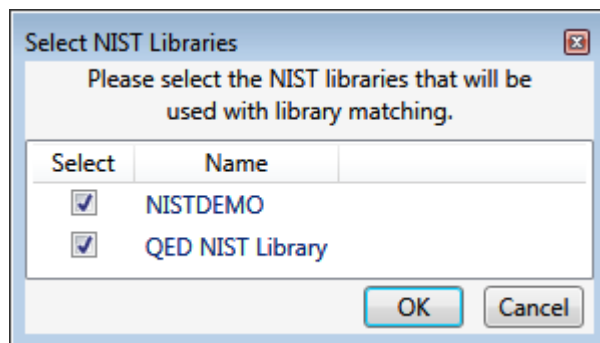
Click **Browse** and locate the library that you want to use for screening.

Note You can use only one search type when you process a sample. When you select NIST as the Library Search Type in your method, the application does not use the screening library that you specify here.

❖ **To specify a NIST screening library**

1. Click **Select**.

The Select NIST Libraries dialog box opens, listing the libraries you installed for the application.



2. Select the check box for each NIST library that you want to use for screening and click **OK**.

Note You can use only one search type when you process a sample. When you select Library Manager as the Library Search Type in your method, the application does not use the NIST libraries that you specify here.

3. To save your changes, click **Apply**.

The application immediately applies this feature change.

The application searches the specified screening library to identify or confirm a sample compound, matches the fragment ion spectrum in the library to the compound's ion spectrum, and returns the highest score (best match).

The application performs either a forward library search or a reverse library search. A forward search compares the mass spectrum of an unknown compound to a mass spectral library entry, whereas a reverse search compares a library entry to an unknown compound.

Screening Libraries in a Quantitation Method

In a quantitation master method, you can enable library matching and set a score threshold to minimize poor matches. See “Library” on page 196. To match a compound, the resulting score from a library search must be higher than the specified threshold value.

Screening Libraries in a Target Screening Method

In a target screening master method, you can specify the library search to either identify or confirm library matches and set a score threshold to minimize poor matches. See “[Editing the Processing Page](#)” on page 264.

- **Identify or Confirm:** The application identifies or confirms the sample compound by searching the specified search library and returning the highest score (as a percentage value) for the fragment ion spectrum in that library that matches the compound’s ion spectrum.
- **Score Threshold:** To identify or confirm the presence of a compound, the resulting score from a library search must be higher than the specified threshold value.

IMPORTANT To use a library search for identification or confirmation, the application requires meeting these conditions:

- The raw data file must contain higher energy collision-induced dissociation (HCD), source collision-induced dissociation (CID), or all ions fragmentation (AIF) ion spectra.
- The spectra must exist at a time point within the compound’s elution time range.

Screening Libraries in an Unknown Screening Method

Unknown screening methods do not use screening libraries.

Multiplexing

The application uses multiplexing features in the Acquisition mode when you specify channels for a sample in a batch (see “[Defining a Sample List](#)” on page 360) or monitor an acquisition (see “[Devices Page](#)” on page 391).

❖ To specify multiplexing features

1. Select the **Multiplexing** check box.

Note Multiplexing is not available when you activate Intelligent Sequencing. See [Intelligent Sequencing](#).

2. Select the check box for each channel that you want to use for acquisition.
3. To save your changes, click **Apply**.

The application immediately applies this feature change.

Note When you activate multiplexing, the Single Sample Submission option is not available.

Intelligent Sequencing

Use Intelligent Sequencing for single-sample submission. When you submit a batch, the autosampler begins preparing for one sample injection at a time. Higher priority batches can interrupt the sample sequence in the currently acquiring batch.

❖ To activate the intelligent sequencing feature

1. Select the **Intelligent Sequencing** check box.

Note Intelligent Sequencing is not available when you activate Multiplexing. See “Multiplexing” on page 61.

The Acquisition Submission Options default to Single Sample Submission. The Full Sequence Submission option is not available when you select the Intelligent Sequencing option.

2. To save your changes, click **Apply**.

The application immediately applies this feature change.

Processing Options

Use these options to enable auto-batch processing or to allow unknown screening.

❖ To allow auto-reprocessing

1. Select the **Auto Reprocess** check box.

- When you select this option, the Auto Reprocess option is selected by default in the banner of all application views.
- When you clear this option, the Auto Reprocess option is cleared by default in the banner of all application views.

2. To save your changes, click **Apply**.

The application immediately applies this feature change.

Note When you use auto-reprocessing, it can slow batch processing.

❖ To allow unknown screening

1. Select the **Allow Unknown Screening** check box.

- When this option is selected, Unknown Screening features are displayed in the application.
- When this option is cleared, Unknown Screening features are not displayed in the application.

2. To save your changes, click **Apply**.

The application immediately applies this feature change.

Creating Custom Columns

Use the Custom Columns page to add six additional columns to the samples list in batches. The application treats these custom columns the same as other columns when you export data to a Microsoft Excel™ spreadsheet or to a CSV file.

When user security is activated, you must have Configuration – Custom Columns permission to access these features.

You can use the Modify Columns dialog box to display and change the order of these columns in the sample list (see the Column Display topic in the appropriate Analysis chapter for your quantitation, target screening, or unknown screening batch).

You can use the Field Chooser to display and change the order of these columns in the Data Review Samples pane (see the Samples Pane topic in the appropriate Analysis chapter for your quantitation, target screening, or unknown screening batch).

You can use the information in these columns (for example) for temperature control when you use Aria™ MX for multiplexing or for injector and multiple column module ports when you use the TurboFlow™ method with the Prelude™ or TLX data systems.

Follow these procedures:

- [To open the Custom Columns page](#)
- [To add custom columns to new batches](#)
- [To create new batches without custom columns](#)
- [To control the display of custom columns](#)

❖ To open the Custom Columns page

Click **Custom Columns** in the navigation pane.

The Application – Custom Columns page opens.

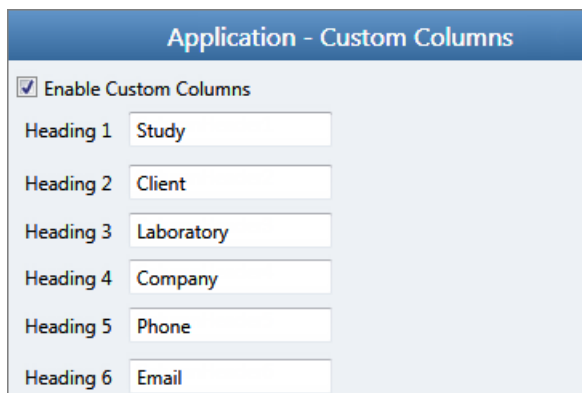
❖ To add custom columns to new batches

1. Select the **Enable Custom Columns** check box.

The application adds six additional columns to the samples list in all new batches that you create.

The Enable Custom Columns check box controls both the creation of custom columns on new batches and the display of custom columns in the Modify Columns dialog box in the Batch View and the Field Chooser in the Data Review Samples pane.

2. For each custom column, select the default column name and type your custom name, as in this example:



3. Click **Apply**.

The application adds the six custom columns to all new batches that you create.

Note Only new batches include these custom columns. The application does not add custom columns to previously created batches.

Note If you return to this page and change the custom column names, the application uses the new names only for future batches.

❖ **To create new batches without custom columns**

Clear the **Enable Custom Columns** check box and click **Apply**.

When you create new batches, they will not include custom columns, and the application hides the display of the custom columns for any previous batches that you created with custom columns enabled.

❖ **To control the display of custom columns**

Do one of the following:

- To make custom columns available for all batches, select the **Enable Custom Columns** check box and click **Apply**.
- To make custom columns not available for batches, clear the **Enable Custom Columns** check box and click **Apply**.

Creating Custom Flags

Use the Flag Customization view to customize error flags and conditions that indicate compound errors in Data Review for quantitation batches. You can edit the priority assigned to an error condition (flag rule) and the shape and color of the icon used to indicate the error. You can also delete an error condition or create a new one. When user security is activated, you must have Configuration – Custom Flags permission to access these features.

❖ To open the Flag Customization view

Click **Flag Customization** in the navigation pane.

The Application – Flag Customization view opens.

Application - Flag Customization

Priority Groups

Priority	Name	Shape	Color	
1000	Green Flag	Flag		
10	Orange Flag	Flag		
1	Red Flag	Flag		
100	Yellow Flag	Flag		

Create New Priority Group

Priority	Name	Shape	Color	
0	<input style="width: 50px;" type="text"/>	Circle		<input type="button" value="Create"/>

Flag Rules

Name	Description	Flags	PriorityGroup	
Confirming Ion Coelution	Flag is shown when RT diffe	Confirming Ion Coelution	Red Flag	
Ion Ratio Failure	Flag is shown when ion ratic	Ion Ratio Failure	Red Flag	
QC Amount Out Of Range	Flag is shown when calculat	QC Amount out of range	Red Flag	
QC RF Diff Out Of Range	Flag is shown when respons	QC RF Diff out of range	Red Flag	
QC RF Out of Range	Flag is shown when respons	QC RF out of range	Red Flag	
QC Out of Range	Flag is shown when respons	Out of range	Red Flag	
Library Search	Flag is shown when library n	Library result not found	Red Flag	
LOD	Flag is shown when calculat	Limit Of Detection	Orange Flag	

Create New Flag Rule









Name	Description	Flags	PriorityGroup	
<input style="width: 100px;" type="text"/>		<div style="border: 1px solid #ccc; padding: 5px;"> Area out of range Auto sample ran out Breakdown Cal Amount out of r Cal Out of range Cal R2 out of range Cal RF Diff out of rar Cal RF out of range </div>	<input type="button" value="Create"/>	

Follow these procedures:

- [To edit priority groups](#)
- [To create a new priority group](#)
- [To edit flag rules](#)
- [To create a new flag rule](#)
- [To remove all customization](#)

In the Priority Groups area, you can edit the priority, shape, or color of a flag. You can also delete a flag or create a new one. You cannot change the name of a flag.

❖ **To edit priority groups**

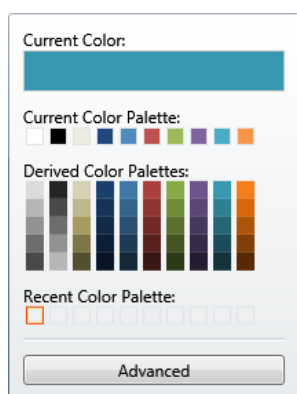
Priority	Name	Shape	Color	
1000	Green Flag	Flag	 ▾ 	
10	Orange Flag	Flag	 ▾ 	
1	Red Flag	Flag	 ▾ 	
100	Yellow Flag	Flag	 ▾ 	

1. Do any of the following:

- Select the default Priority value and type a new value.

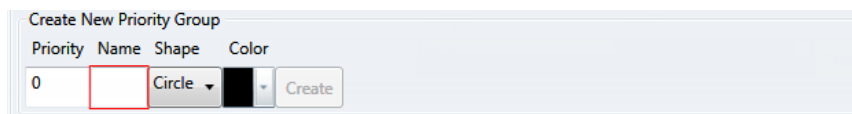
A priority of 1 is the highest priority. The higher the Priority number, the lower the priority.

- Double-click the Shape value and select a new shape from the list.
- Click the Color arrow and select a new color from the color palette.



2. When you have completed all your changes, click **Apply** to save your changes.

❖ To create a new priority group



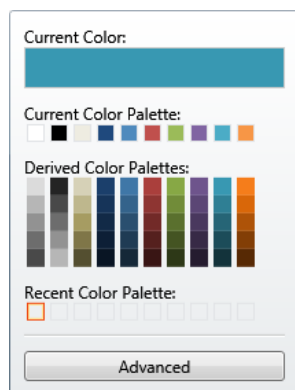
1. In the Priority box, type a value.

You can enter positive or negative numbers. The lower the number, the higher the priority.

2. In the Name box, type a name for the new priority group.

3. Select a flag shape from the Shape list: **Circle**, **Square**, or **Flag**.

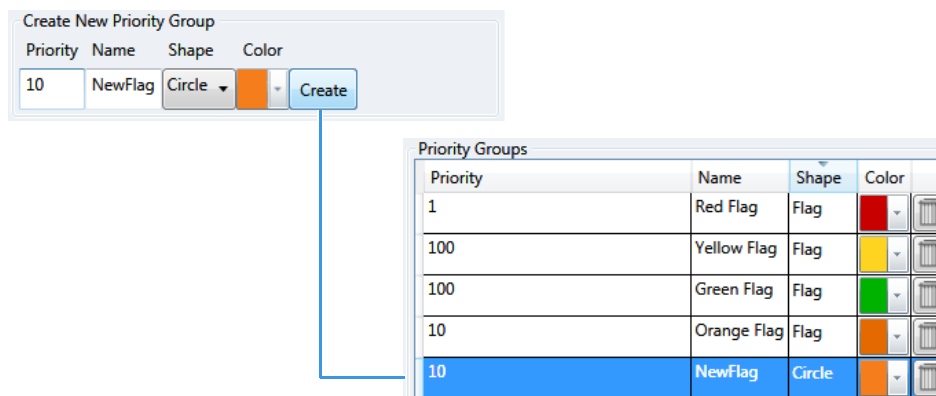
4. Click the Color list and select a color from the color palette.



5. (Optional) Click **Advanced** and select a color based on RGB, HSL, or CMYK color palettes. See [“Advanced Dialog Box”](#) on page 69.

6. Click **Create**.

The application adds the new flag to the Priority Groups list, as in this example:



❖ **To edit flag rules**

Note You can edit the description and priority group for a flag rule, and you can delete a rule. You cannot edit the name or flag type for a rule.

1. Do any of the following:

- In the Description column, select the current text and type a new description.
- Double-click the PriorityGroup value and select a new group from the list.
- Click **Delete**.

The application immediately removes the flag rule. To restore the deleted rule, click **Undo**.

2. When you have completed all your changes, click **Apply** to save your changes.

❖ **To create a new flag rule**

Name	Description	Flags	PriorityGroup
<input type="text"/>		Area out of range Auto sample ran out Breakdown Cal Amount out of range Cal Out of range Cal RF out of range	<input type="text"/>

1. In the Name box, type a name for the new rule.

Keep the name short and make it intuitive.

2. In the Description box, type a description for the new flag rule.

This description can be anything that you want and use as many characters as you want.

3. From the Flags list, select an error condition.

4. From the PriorityGroup list, select a priority group.

This list includes both the default priority groups and any priority groups that you created. See [“To create a new priority group”](#) on page 67.

5. Click **Create**.

The application adds your new flag rule to the end of the Flag Rules list.

❖ **To remove all customization**

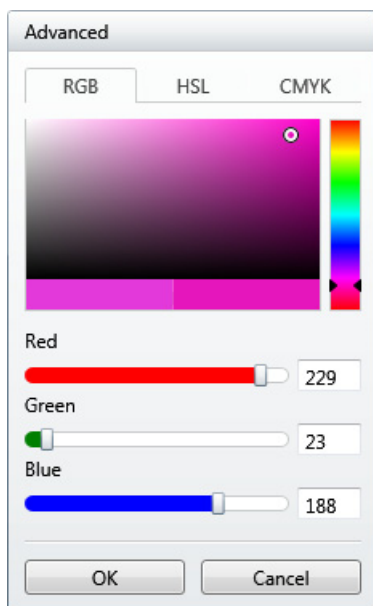
Click **Reset to Factory Defaults**.

The application removes all new priority groups, new flag rules, and any edits to the groups or rules.

Advanced Dialog Box

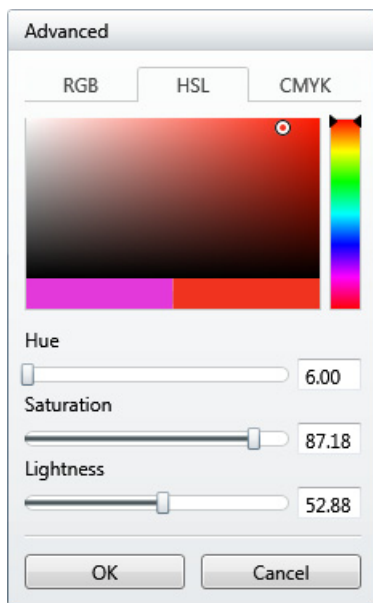
Use the features in the Advanced dialog box to select custom colors for your flags, using RGB, HSL, or CMYK color standards.

Figure 17. Advanced RGB colors



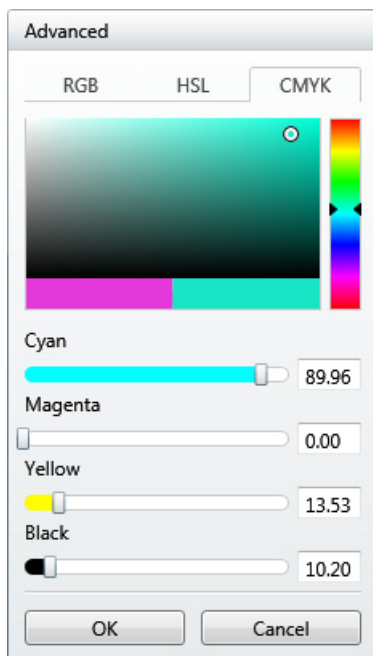
With the Red/Green/Blue (RGB) color palette, you can select a color with a specific RGB value, as displayed on a computer monitor.

Figure 18. Advanced HSL colors



With the Hue/Saturation/Lightness (HSL) color palette, you can select a color with a specific HSL value, as is commonly used in computer graphics.

Figure 19. Advanced CMYK Colors



With the Cyan/Magenta/Yellow/Key (CMYK) color palette, you can select a color with a specific CMYK value, as you might specify in a color printer. The key (K) color used on printers is always black.

Specifying the Reports

When user security is activated, you must have Configuration – Reports permission to configure a list of reports that are available to all users when they generate reports from the Method Development, Analysis, or Acquisition modes.

❖ To open the Application – Reporting view

In the Configuration console navigation pane, click **Reports**.

The Application – Reporting view opens.

The application displays the Excel template files in the following folder:

```
...\TraceFinderData\3.3\Templates\ReportTemplates
```

Each template has an XLS file and a metadata file to support report generation.

❖ To specify which reports are available

Select the check box for each report that you want to make available.

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

Your report settings are immediately available in the application.

Reports

The application can generate any of the following reports.

Figure 20. Reports

Application - Reporting

- Ad Hoc Tune Report
- Batch Report
- Blank Report
- Breakdown Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report - Alternate
- Compound Calibration Report
- Confirmation Report 2
- Confirmation Report
- High Density Calibration Report
- High Density Internal Standard Report Long
- High Density Report
- High Density Sample Report 1 Long
- Intelligent Sequencing
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report - 2
- Quantitation Report
- Screening Batch Report
- SGS Report
- Solvent Blank Report
- Standard Addition Report
- Surrogate Recovery Report
- Target Screening High Density Sample Report 2
- Target Screening High Density Sample Report
- Target Screening Summary Report
- TIC Report
- TIC Summary Report
- Tune Report
- Unknown Screening Summary Report

Using the Common Features of the Method Development Mode

This chapter includes method development tasks common to quantitation, target screening, and unknown screening methods.

Contents

- [Working with the Compound Database](#)
- [Working with Instrument Methods](#)

For information about creating either a quantitation method, a target screening method, or an unknown screening method, see the appropriate chapter:

- [Chapter 5, “Using the Method Development Mode for Quantitation Methods.”](#)
- [Chapter 6, “Using the Method Development Mode for Target Screening Methods.”](#)
- [Chapter 7, “Using the Method Development Mode for Unknown Screening Methods.”](#)

❖ To access the Method Development mode

Click **Method Development** in the navigation pane.

The Method Development navigation pane opens.



See descriptions of all the features in the Method Development navigation pane by method:

For a quantitation method, see [“Opening a Master Method” on page 115](#) (Chapter 5).

For a target screening method, see [“Opening a Master Method” on page 257](#) (Chapter 6).

For an unknown screening method, see [“Opening a Master Method” on page 303](#) (Chapter 7).

Working with the Compound Database

When user security is activated, you must have Method Development permission to manage compound definitions in the current database from either the [Compound Detail Page](#) or the [Grid Page](#) in the Compound Database view. From either of these pages, you can export compounds to a CSV file or mass list, or you can import compounds from an XML, a CSV, or a CDB file.

Follow these procedures:

- [To export compounds to a CSV file](#)
- [To export compounds to a mass list](#)
- [To import compounds](#)

In addition to procedures for importing and exporting compound data, see the following topics:

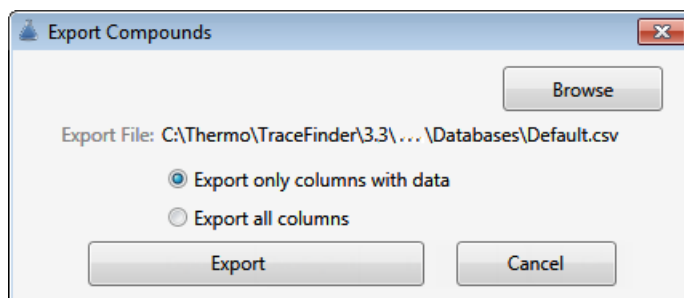
- [Compound Database Names Mapped to CSV Column Names](#)
- [Data Columns with Default Values](#)

❖ To export compounds to a CSV file

1. Choose **Compound Database > Export All Compounds to CSV File** from the main menu.

Note If you have unsaved changes in your current compound database, a message prompts you to save the changes. Click **Yes** and continue with the export procedure.

The Export Compounds dialog box opens.



2. (Optional) Click **Browse** and locate a different folder or file name where you want to write the exported compound database.

Each parameter in the compound database editor is represented by a column of data in the spreadsheet. When you export compound data to a CSV file, each parameter is assigned to a column and each compound is assigned to a row.

3. Select one of these options:

- **Export Only Columns with Data:** Writes only columns that contain nondefault data for at least one compound. This option does not export columns that contain only default data. See “Data Columns with Default Values” on page 107.
- **Export All Columns:** Writes all columns to the CSV file, including columns that contain no data for any compound.

4. Click **Export**.

The application stores the database as

...\\Thermo\\TraceFinder\\3.3\\General\\Databases*databaseName.csv*

An Excel window opens with the compound data in spreadsheet format.

Figure 21. Compound data in an Excel spreadsheet

	A	B	C
1	TraceFinder Compound Database Export	Schema Version 1	
2			PEAK 1
3	CompoundName	ExperimentType	Precursor
4	15-acetyldeoxynivalenol	SRM	339.1
5	15-acetyldeoxynivalenol+NH4	SRM	356.1
6	17beta-estradiol_neg	SRM	271
7	1-Naphthylacetic_acid_neg	SRM	185.04
8	2,3,5-Trimethacarb	SRM	194
9	2,4-DB_neg	SRM	247

Column names in an exported Excel spreadsheet do not always match the parameter names in the compound database editor. See “Compound Database Names Mapped to CSV Column Names” on page 104.

You can use the tools in the spreadsheet to edit the data in the compound database and then import the data in the CSV file back into the TraceFinder application. If you delete a column from the spreadsheet and then import the CSV file, the application replaces the data in that column with default values. For a list of default values, see “Data Columns with Default Values” on page 107.

❖ To export compounds to a mass list

1. Select the compounds that you want to export.

You can export any experiment type to any instrument format. The application writes the data to the XML file in a format that is compatible with the specified instrument, regardless of the original experiment type.

2. Choose **Compound Database > Export Selected Compounds to Mass List** from the main menu.

Note If you have unsaved changes in your current compound database, a message prompts you to save the changes. Click **Yes** and continue with the export procedure.

The application writes the mass data for the selected compounds to the following folder, using a format compatible with your configured instrument:

```
...\TraceFinderData\3.3\Methods\Methodname\*.xml
```

Note If your configured is other than a TSQ, an ISQ, a Q Exactive, a TSQ Endura™, or a TSQ Quantiva™ mass spectrometer, a message asks which format you want to export: Triple Quadrupole, Q Exactive, TSQ Quantiva/Endura SIM, or TSQ Quantiva/Endura SRM.

For examples of exported mass lists, “[Mass Data Formats](#)” on [page 79](#).

❖ To import compounds

1. Choose **Compound Database > Import Compounds** from the main menu.

Note If you have unsaved changes in your current compound database, a message prompts you to save the changes. Click **Yes** and continue with the import procedure.

The Select File to Import into the Current Compound Database dialog box opens.

You can import compounds from the following file types:

- ToxID™ Exactive CSV
- ToxID MS2 CSV
- TraceFinder CSV
- TraceFinder Mass List XML
- TraceFinder 3.2 Legacy CDB
- ExactFinder™ 2.0 CDB
- .include-masses

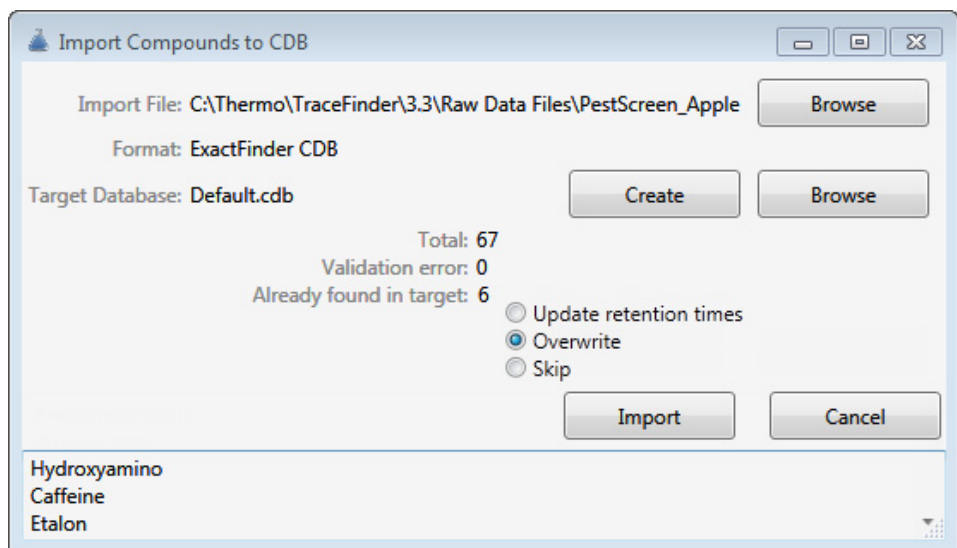
IMPORTANT Before you import data from a CSV file, verify that the following required columns have data for each compound. These columns have no default values and must have a value before you can import CSV data into the TraceFinder compound database:

- CompoundName
- ExperimentType
- ProductMass (target peak)
- Confirm Product (confirming peak)
- Fragment

If you delete any of these columns from the spreadsheet and attempt to import the CSV data into the TraceFinder application, the application warns that it is unable to parse the file and identifies the missing column.

2. Locate the CDB, CSV, or XML compound database file that you want to import and click **Open**.

The Import Compounds to CDB dialog box opens.



Note If the import file is missing required compound information, the application warns that it is unable to parse the file and identifies the missing columns. For a list of required columns, see “[Compound Detail Page](#)” on [page 80](#).

3. To select a different compound database, click **Browse**, locate an XML, a CSV, or a CDB compounds file, and click **Open**.
4. To select a different target database, do one of the following:
 - a. Click **Browse**.
 - b. Locate an XML, a CSV, or a CDB compounds file.
 - c. Click **Open**.

4 Using the Common Features of the Method Development Mode

Working with the Compound Database

–or–

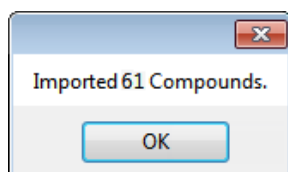
- a. Click **Create**.
 - b. Type a name for a new compound database.
 - c. Click **OK**.
5. Confirm that the import file and the target database are correct.

The dialog box reports the total number of compounds in the import file, the number of compounds with validation errors, and the number of compounds that already exist in the target database.

6. (Optional) Select one of these options:
- **Skip**: Imports only those compounds that do not already exist in the target database.
 - **Overwrite**: Replaces compounds that already exist in the target database with the imported compounds.
7. Click **Import**.

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

The application reports the number of imported compounds.



8. Click **OK**.

Mass Data Formats

In the TraceFinder application, you can export the mass data list from the Compound Database to an XML file that can be read by the TSQ, ISQ, Q Exactive, TSQ Endura, or TSQ Quantiva applications.

Triple Quadrupole Format

IMPORTANT You can export only SRM or SIM data types to the Triple Quadrupole format.

The application writes the mass data to the following file:

```
...\TraceFinderData\3.3\Methods\Methodname\*.xml
```

The data in this file matches the TSQ XML data, which you can use in the instrument method editor of a TSQ application.

Q Exactive Format

IMPORTANT You can export only XIC data types to the Q Exactive format.

The application writes the mass data to the following file:

```
...\TraceFinderData\3.3\Methods\Methodname\Methodname.xml.include-masses
```

The data in this file matches the Exactive XML data, which you can use in the instrument method editor of a Q Exactive application.

TSQ Quantiva/Endura SIM Format

IMPORTANT You can export only SIM data types to the TSQ Quantiva/Endura SIM format.

The application writes the mass data to the following file:

```
...\TraceFinderData\3.3\Methods\Methodname\Methodname.xml
```

The data in this file matches the TSQ Endura, TSQ Quantiva, and Xcalibur XML data, which you can use in the instrument method editors of the associated applications. The application exports only the following compound parameters to the XML file:

- Compound (as Name in the XML file)
- Product Mass (as Mass in the XML file)
- RT range (as StartTime and StopTime in the XML file)
- Polarity
- Lens (as TubeLens or S-Lens in the XML file)

TSQ Quantiva/Endura SRM Format

Note You can export only SRM data types to the TSQ Quantiva/Endura SRM format.

The application writes the mass data to the following file:

```
...\\TraceFinderData\\3.3\\Methods\\Methodname\\Methodname.xml
```

The data in this file matches the TSQ Endura, TSQ Quantiva, and Xcalibur XML data, which you can use in the instrument method editors of the associated applications. The application exports only the following compound parameters to the XML file:

- Compound (as Name in the XML file)
- Precursor Mass
- Product Mass
- RT range (as StartTime and StopTime in the XML file)
- Polarity
- Lens (as TubeLens or S-Lens in the XML file)
- Collision Energy

Compound Detail Page

When you open the Compound Database view, the Compound Detail page is the default.

The screenshot shows the 'Compound Database - Default' window. On the left is a list of compounds with columns for 'Compound' and 'Formula'. The selected compound is '2,3,5,6-tetrachloroaniline' with formula 'SRM'. The main area displays 'Compound Detail' for '2,3,5,6-tetrachloroaniline'. It shows 'Experiment: SRM', 'Category: CAS: 3481-20-7', and 'Formula:'. Below that, 'Ionization: EI' and 'Neutral Mass: 0' are listed. A 'Target Peaks' section shows 'Peak 1' with 'Precursor Mass: 231.000' and 'Product Mass: 158.000'. A 'Confirming Peaks (Quan Only)' table follows:

Precursor	Product Mass	Collision Energy:
231.000	160.000	22.00

The compound details are different depending on which experiment type the selected compound uses.

- [Compound Detail page for SRM experiments](#)
- [Compound Detail page for SIM experiments](#)
- [Compound Detail page for XIC experiments](#)

See the following topics:

- [Sorting Compounds in the Database](#)
- [Editing Compounds in the Database](#)

Figure 22. Compound Detail page for SRM experiments

Compound Database - Default

Search (all) ▾

Bentazone	SRM
Bentazone_neg	SRM
Benzobicyclon	SRM
Benzofenap	SRM
Benzophenone	SRM
Benzoyl_peroxide+NH4	SRM
Bifenox	SRM
Bifenthrin+NH4	SRM
Bioresmethrin	SRM
Bispheno_A_neg	SRM
Bispyribac	SRM
bitertanol	SRM
Bromochloroacetonitrile_neg	SRM
Bromoxynil_neg	SRM
Buprofezin	SRM
Buspirone	SRM
Butachlor	SRM
Butafenacil+NH4	SRM
Butamifos	SRM
butocarboxim	SRM
Butocarboxim_sulfoxide	SRM
Butocarboxim+NH4	SRM
Cafenstrole	SRM
Caffeine	SRM

Compound Detail

Compound: Caffeine

Experiment: SRM Category: CAS: 58082 Formula: C8H10N4O2

Ionization: None Neutral Mass: 194.0803755

Target Peaks

Peak 1

Precursor Mass: 194.08038

Product Mass: 194.07983

Adduct: Neutral

Polarity: Positive

Charge State: 1

Window (sec): 60

RT (min): 5

Collision Energy: 19

Lens: 0

Energy Ramp: 0

Confirming Peaks (Quan Only)

Precursor	Product Mass	Collision Energy:
194.08038	193	30

Figure 23. Compound Detail page for SIM experiments

Compound Database - Default

Search (all) ▾

Compound	Formula
Caffeine	SIM
captafol+NH4	SIM
captafol+NH4	SIM
Captan_MeOH-a	SIM
Captan_MeOH-b	SIM
Captan_neg-a	SIM
Captan_neg-b	SIM
Captan+NH4-a	SIM
Captan+NH4-b	SIM
Carbamazepine	SIM
Carbaryl	SIM
Carbaryl_fragment	SIM
CARBENDAZIM	SIM
Carbofuran	SIM
Carbofuran-3-hydroxy	SIM
Carbosulfan	SIM
Carpropamid	SIM
Carpropamid+HCOOH_neg	SIM
Dicamba	SIM
Diethofencarb	SIM
Diflufenican	SIM
Dioxacarb	SIM

Compound Detail

Compound: Caffeine

Experiment: SIM Category: CAS: 58082 Formula: C8H10N4O2

Ionization: None Neutral Mass: 194.0803755

Target Peaks

Peak 1

Mass: 194.07983

Adduct: Neutral

Polarity: Positive

Charge State: 1

Window (sec): 60

RT (min): 5

Lens: 0

Energy Ramp: 0

Confirming Peaks (Quan Only)

Mass
193

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Figure 24. Compound Detail page for XIC experiments

Compound Database - Default

Search (all)

Compound	Formula
17a-Estradiol	XIC C18H24O2
17a-Ethinylestradiol	XIC C20H24O2
1-Naphthyl_acetic_aci	XIC C12H10O2
245-T	XIC C8H5Cl3O3
24D	XIC C8H6Cl2O3
24-Diaminotoluene	XIC C7H10N2
24-Dimethylaniline	XIC C8H11N
26-dichlorobenzamide	XIC C7H5Cl2NO
26-Difluorobenzoic_ac	XIC C7H4F2O2
33'-Dimethoxybenzidi	XIC C14H16N2O2
34-Dichloroaniline	XIC C6H5Cl2N
3-Amino-2-oxazolidin	XIC C3H6N2O2
4-Aminobiphenyl	XIC C12H11N
4-Aminophenol	XIC C6H7NO
4-Bromo-35-dimethyl	XIC C10H12BrNO2
4-Chlorophenoxyaceti	XIC C8H7ClO3
6a_Methylprednisolon	XIC C22H30O5
Acemetacin	XIC C21H18ClNO6
Acephate	XIC C4H10NO3PS
Aceprometazine	XIC C19H22N2OS
Acetaminophen	XIC C8H9NO2
Acetamidrid	XIC C10H11ClN4
Acetochlor	XIC C14H20ClNO2
Acetylsalicylic_acid	XIC C9H8O4
Acibenzolar-S-methyl	XIC C8H6N2OS2
Acifluorfen	XIC C14H7ClF3NO5
Aclonifen	XIC C12H9ClN2O3
Acrinathrin	XIC C26H21F6NO5

Compound Detail

Compound: **Acetaminophen**

Experiment: XIC Category: CAS: Formula: C8H9NO2

Ionization: None Response Threshold: 5000 Neutral Mass: 151.06332

Target Peaks

Peak 1

Extracted Mass: 152.0706

MS Order: ms1

Adduct: H-Gain

Polarity: Positive

Charge State: 1

Window (sec): 10

RT (min): 0

Lens: 0

Energy Ramp: 0

Confirming Peaks (Quan Only)

Precursor	Extracted Mass	MS Order
	152	ms1

Fragments (Screening Only)

Extracted Mass

111

Sorting Compounds in the Database

On the Compound Detail page, you can sort the list of compounds that you want to display.

Compound Database - database1

Search (all)

Compound	Formula
Aldicarb	XIC C7H14N2O2S
Azinphos-methyl	XIC C10H12N3O3PS2
Bendiocarb	XIC C11H13NO4
Carbaryl	XIC C12H11NO2
Dioxacarb	XIC C11H13NO4
Ethiofencarb	XIC C11H15NO2S
Fenpyroximate	XIC C24H27N3O4
Flusilazole	XIC C16H15F2N3Si
Linuron	XIC C9H10Cl2N2O2
Methiocarb	XIC C11H15NO2S
Monocrotophos	XIC C7H14NO5P
Napropamide	XIC C17H21NO2
Omethoate	XIC C5H12NO4PS
Phosalone	XIC C12H15ClNO4PS2
Pyriproxyfen	XIC C20H19NO3
Tolyfluanid	XIC C10H13Cl2FN2O2S2

Follow these procedures:

- [To search for compounds by name](#)
- [To display compounds by experiment type](#)
- [To display truncated compound names](#)

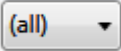
❖ **To search for compounds by name**

In the Search box, begin typing any part of a compound name.

As you type, the list of displayed compounds narrows to match the typed text.

For example, you can use this feature in combination with the experiment type list to display only SIM compounds that begin with the letter “a”.

❖ **To display compounds by experiment type**

Select an experiment type from the  list.

The list displays experiment types that each use a different structure for the mass filter.

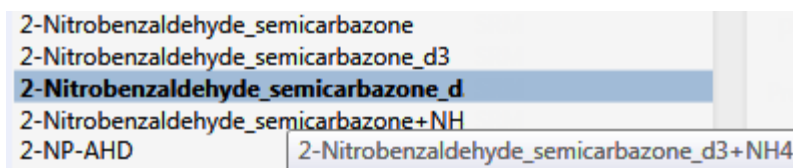
- SRM: Selected Reaction Monitoring
- XIC: Extracted Ion Chromatogram
- SIM: Single Ion Monitoring

For detailed descriptions of each experiment type, see [“Experiment Types”](#) on [page 101](#).

For example, you can use this feature in combination with the text search to display only SRM compounds that begin with the letter “f”.

❖ **To display truncated compound names**

Hold your cursor over long, truncated names to display a ToolTip with the entire name.



Editing Compounds in the Database

On the Compound Detail page of the Compound Database view, you can import compounds into the database, add or remove compounds from the database, add target or confirming peaks to a compound, or remove target or confirming peaks from a compound.

Follow these procedures:

- [To add a compound to the database](#)
- [To remove compounds](#)
- [To make a compound editable](#)
- [To add a target peak to a compound](#)
- [To add a confirming peak to a target peak](#)
- [To copy target peaks from one compound to another](#)
- [To copy window values from one peak to another](#)
- [To add a fragment to a target peak](#)


❖ To add a compound to the database



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

The application adds a new, empty compound page and highlights the required parameters in red.

2. Click the Compound box, and type the required Compound name.
3. Select the Experiment type: **SRM**, **SIM**, or **XIC**.

The required parameters are different for each experiment type. See [“Experiment Types”](#) on [page 101](#).

4. In the Target Peaks area, do the following:
 - For SRM experiments, enter values for Precursor Mass and Product Mass.
 - For SIM or XIC experiments, enter a value for Extracted Mass.
5. In the Confirming Peaks area, do the following:
 - For SRM experiments, enter values for Precursor and Product Mass.
 - For SIM or XIC experiments, enter a value for Precursor and Extracted Mass.
6. Enter or edit any of the other optional parameters described in the [“Compound Parameters”](#) on [page 95](#).
7. When you have finished your changes, click the **Complete Edit** icon, .

Tip You cannot add another new compound or access the menu commands until you complete the edit, , or cancel the edit, .

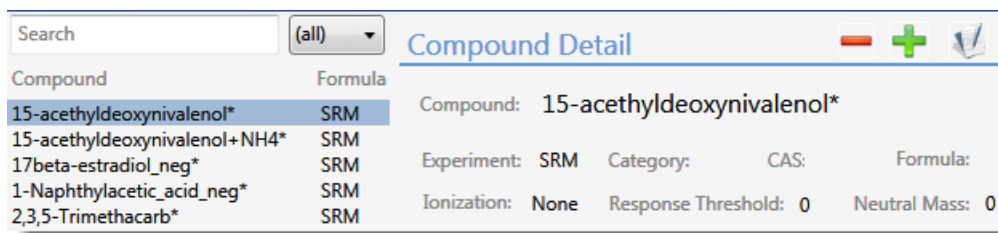
IMPORTANT After you complete the edits for the compounds, the header in the Compound Database page marks the database name with an asterisk, indicating that the database is not saved. To save the database with your compound changes, choose **File > Save Compound Database** from the main menu.


❖ To remove compounds

1. In the Compound list, select the compounds that you want to delete.

The application supports the following methods to delete multiple compounds:

- CTRL+A to select all compounds
- CTRL+click to select noncontiguous compounds
- SHIFT+click to select contiguous compounds

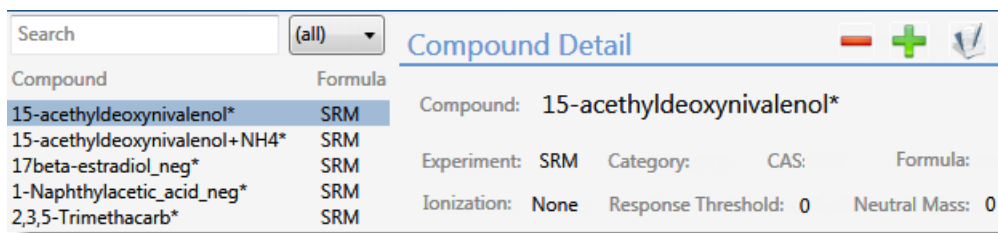


2. Click the **Delete Selected Compounds** icon, .
3. To confirm that you want to delete the selected compounds, at the prompt click **OK**.

The application removes the selected compounds and all their peak information.

❖ To make a compound editable

1. In the Compound list, select the compound that you want to edit.




4 Using the Common Features of the Method Development Mode

Working with the Compound Database

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

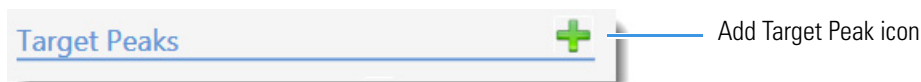
The application makes the compound parameters editable and displays the

Add icon, , so that you can add target peaks, confirming peaks, and fragments to the compound details.

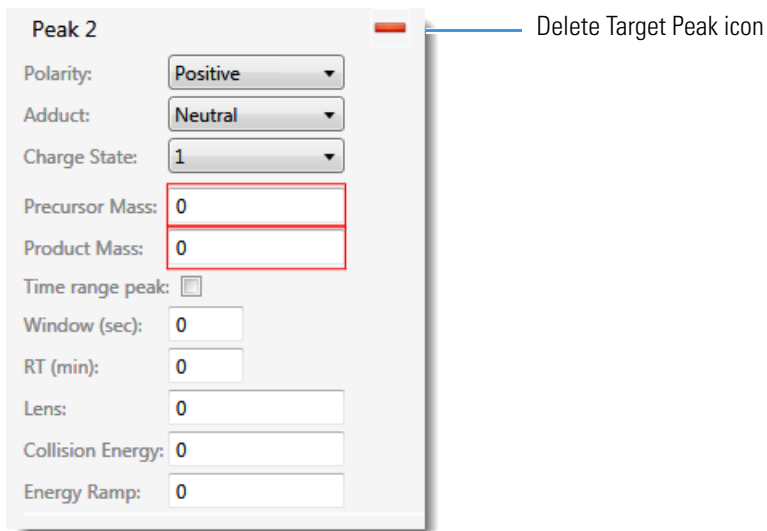
Note If you are adding a new compound, it is editable by default.

❖ To add a target peak to a compound

1. In the Target Peaks header, click the **Add Target Peak** icon.




The application adds a new target peak to the compound. A target peak includes quantitative values for the compound.



2. Enter all required parameters.

The required target peak values differ for each experiment type. See [“Experiment Types”](#) on [page 101](#).

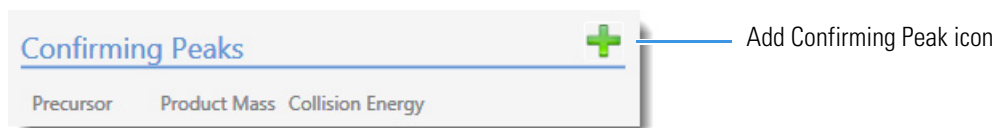
For a list of required and optional parameters, see the list of [“Compound Parameters”](#) on [page 95](#).

Tip You cannot add another new target peak or save the compound until you enter all required peak parameters or delete  the new target peak.

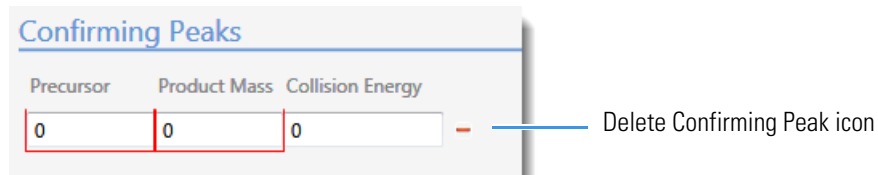
3. Repeat these steps to add as many as six target peaks to the compound.

❖ **To add a confirming peak to a target peak**

1. In the Confirming Peaks header, click the **Add Confirming Peak** icon.



The application adds a new confirming peak to the target peak.



2. Type the required values for the confirming peak.

The required confirming peak values differ for each experiment type. See “[Experiment Types](#)” on page 101.

For a list of required and optional parameters, see “[Compound Parameters](#)” on page 95.

3. Repeat these steps to add as many as 10 confirming peaks to the target peak.

Tip You cannot add another new confirming peak or save the compound until you enter all required peak parameters or delete  the new confirming peak.

❖ **To copy target peaks from one compound to another**

1. In the compounds list, select the compound whose target peak you want to copy.

Compound	Formula
Acrinathrin+NH4	SRM
AflatoxinB1	SRM
AflatoxinB2	SRM
AflatoxinG1	SRM
AflatoxinG2	SRM
Alachlor	SRM

Source compound

2. When the target peak includes more than one peak, in the Target Peaks area for the selected compound, scroll to the peak that you want to copy.

Target Peaks			
Peak 1	Confirming Peaks (Quan Only)		
Precursor Mass: 313	Precursor	Product Mass	Collision Energy:
Product Mass: 285	313	241	40

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Working with the Compound Database

3. In the compounds list, keep the source compound selected and use the SHIFT or CTRL keys to select the compounds that you want to copy the target peak to.

Compound	Formula
Acrinathrin+NH4	SRM
AflatoxinB1	SRM
AflatoxinB2	SRM
AflatoxinG1	SRM
AflatoxinG2	SRM
Alachlor	SRM

Source compound

IMPORTANT Be careful to keep the source compound selected.

4. In the Target Peaks area for the selected compound, right-click the target peak area and choose **Add Peak 1 to N Selected Compounds** from the shortcut menu.

Target Peaks	
Peak 1	
Preursor	Add Peak 1 to 2 selected compounds
Product	Set the Window for all peaks of 2 selected compounds to 54.00

Right-click the target peak area.

The application reports that the peak was copied to the specified number of compounds.

The application copies the peak information to the selected compounds, adding this peak to the peaks already defined for the compounds.

5. Click **OK**.

❖ To copy window values from one peak to another

1. In the compounds list, select the compound with the window value that you want to copy.

Compound	Formula
Acrinathrin+NH4	SRM
AflatoxinB1	SRM
AflatoxinB2	SRM
AflatoxinG1	SRM
AflatoxinG2	SRM
Alachlor	SRM

Source compound

- In the Target Peaks area for the selected compound, identify the peak whose window you want to copy.

Target Peaks		Confirming Peaks (Quan Only)		
Peak 1				
Precursor Mass:	231	Precursor	Product Mass	Collision Energy:
Product Mass:	158	231	160	22
Adduct:	Neutral			
Polarity:	Positive			
Charge State:	1			
Window (sec):	54			
RT (min):	10.76			
Collision Energy:	20			
Lens:	0			
Energy Ramp:	0			

- In the compounds list, keep the source compound selected and use the CTRL key to select the compounds that you want to copy the window to.

Compound	Formula
Acrinathrin+NH4	SRM
AflatoxinB1	SRM
AflatoxinB2	SRM
AflatoxinG1	SRM
AflatoxinG2	SRM
Alachlor	SRM

Source compound

IMPORTANT Be careful to keep the source compound selected.

- In the Target Peaks area for the selected compound, right-click the target peak area and choose **Set the Window for All Peaks of selected Compounds to window Value** from the shortcut menu.

Target Peaks	
Peak 1	
Precursor	Add Peak 1 to 2 selected compounds
Product	Set the Window for all peaks of 2 selected compounds to 54.00

Right-click the target peak area.

The application reports that the retention time and window were copied to the specified number of compounds, including the source compound when it has multiple peaks.

The application copies the retention time and window information to all peaks in the selected compounds and all additional peaks in the source compound, overwriting the values for these parameters.

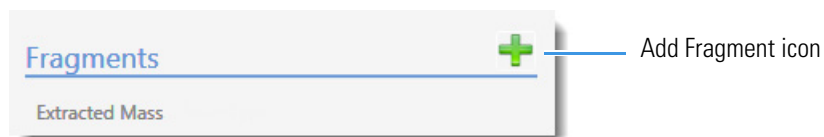
- Click **OK**.

4 Using the Common Features of the Method Development Mode

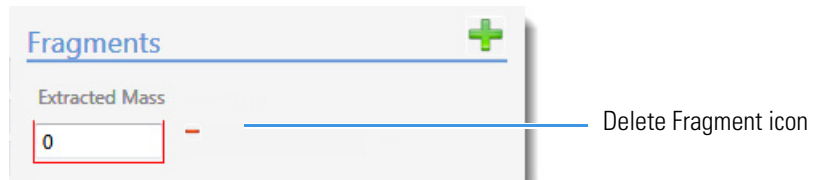
Working with the Compound Database

❖ To add a fragment to a target peak


1. In the Fragments header, click the **Add Fragment** icon.



The application adds a new fragment to the target peak.



2. Click the Extracted Mass box, and type a value between **10** and **2999,999**.
3. Repeat these steps to add as many fragments as you want.

Tip You cannot save the compound until you enter all required fragment parameters or delete  the new fragment.

Grid Page

The Grid page of the Compound Database view displays the data in the compound database as a grid similar to a spreadsheet. The data on the Grid page reflects all populated values on the Compound Detail page.

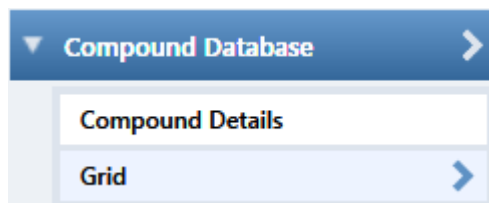
- There must be at least one compound in the compound database to view the Grid page.
- There are no empty columns on the Grid page. There must be at least one value for a parameter in the compound database or that parameter column is not displayed.

Note If a column of interest is not displayed on the Grid page, return to the Compound Detail page, edit at least one compound to have a value for that parameter, and then return to the Grid page.

On the Grid page, you can import compounds into the database, add compounds to or remove compounds from the database, add target or confirming peaks to a compound, or remove target or confirming peaks from a compound.

❖ To display the compound database on the Grid page

Click **Grid** in the Compound Database navigation pane.



The current database opens on the Grid page.

Compound Database - Default									
	Compound Name	Experiment Type	Ionization	CAS	Neutral Mass	Peak 1	Peak 1 Precursor Mass	Peak 1 Polarity	Peak 1
	▲	▲	▲	▲	▲	▲	▲	▲	▲
1	2,3,5,6-tetrachloroan	SRM	EI	3481-20-7	0	158.000	231.000	Positive	1
2	2,4-D-1-butyl ester	SRM	EI	94-80-4	0	240.000	285.000	Positive	1
3	2,4'-DDD	SRM	EI	53-19-0	0	91.000	238.000	Positive	1
4	2,4'-DDE	SRM	EI	3424-82-6	0	302.000	359.000	Positive	1
5	2,4'-DDT	SRM	EI	789-02-6	0	299.840	406.780	Positive	1

The parameters displayed in the compound database depend on which experiment type the selected compound uses. For detailed descriptions of all parameters used in the compound database, see “[Compound Parameters](#)” on [page 95](#).

Follow these procedures:

- [To add a compound](#)
- [To remove a compound](#)
- [To edit values in the compound database grid](#)
- [To edit Experiment Type values in the compound database](#)
- [To sort the grid on column data](#)
- [To organize compounds by column data](#)

❖ To add a compound

1. Scroll to the bottom of the compound database grid.

There is always one blank row in the grid.

2. In the blank row, type or paste values into the columns.

Note Some columns have dropdown lists from which you can select values.

3. Press ENTER to add another blank row to the grid.

❖ To remove a compound

1. Click anywhere in a row to select the compound.

18	Alachlor	SRM	EI	15972-60-8	0	93.000	286.000
19	Aldrin	SRM	EI	309-00-2	0	193.000	263.000

2. Press the DELETE key.

Note Do not use CTRL+X to delete a compound. CTRL+X deletes only the parameter values in the selected cells.

3. At the prompt to confirm that you want to delete the compound, click **Yes**.

The application removes the compound from the database grid.

❖ To edit values in the compound database grid

Do either of the following:

- Select the current column value and type a new value.

–or–

- Select single cells or entire columns whose values you want to copy, using a copy-and-paste operation.

You can use this method to replicate entire columns. Click the column header to select the entire column, and then use CTRL+C and CTRL+V to replicate the column values.

When you edit a value in the Formula column, the application calculates the m/z for the precursor and product masses.

When you change the charge state, adduct, or polarity for a compound, the application recalculates the m/z for the precursor and product masses.

Note Do not use CTRL+X to delete a compound. CTRL+X deletes only the parameter values in the selected cells.

❖ To edit Experiment Type values in the compound database

1. Select a new experiment type for one compound from the Experiment Type list.

Compound Name	Experiment Type
Δ ⁿ	Δ ⁿ
2,3,5,6-tetrachloroan	SRM
2,4-D-1-butyl ester	SRM
2,4'-DDD	SIM
	XIC

2. Double-click the new type in the cell, and press CTRL+C.
3. Select all Experiment Type cells in all the compounds in the database.
4. Press CTRL+V.

The application pastes the copied experiment to all compounds in the database.

IMPORTANT If you change one experiment type, you must change the experiment type for all compounds. The Grid page cannot display a database unless all compounds use the same experiment type.

❖ To sort the grid on column data

1. Click the header of a column.

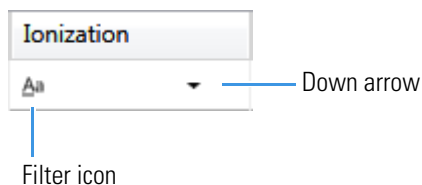
The application sorts the grid by ascending column values (alphabetically or numerically).

Note Columns with alphanumeric values sort from 1 to n and then A to Z.

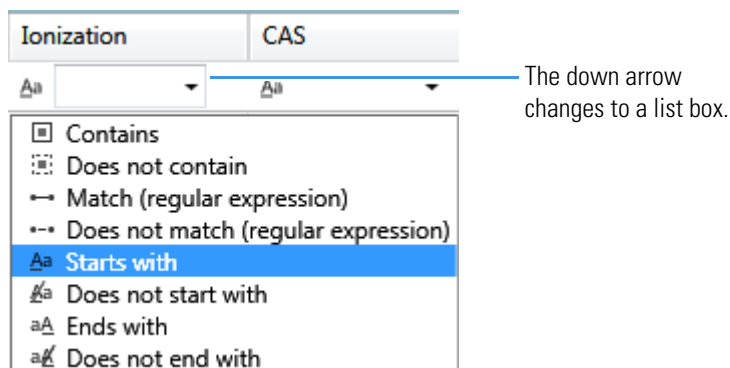
2. Click the header a second time to sort by descending column values.

❖ To organize compounds by column data

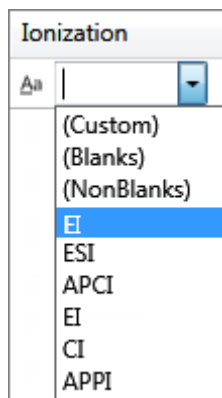
1. In the banner at the top of the column, click the filter icon.



2. Select one of the filtering options, for example, **Starts With**.



3. Click the down arrow and choose one of the column values in the list, for example, **EI**.



The grid displays only compounds that match the selected filter and data.

Ionization	
Aa EI	▼
EI	▼
EI	▼
EI	▼
EI	▼
EI	▼

Compound Parameters

The Compound Detail page and the Grid page occasionally use different names for the same parameter. The Parameter column in [Table 12](#) indicates if the parameter name is different, for example, “Compound” for the Compound Detail page and “Compound Name” for the Grid page.

The parameters that are displayed in a compound database on either the Compound Detail page or the Grid page depend on which experiment type the selected compound uses. The Description column in the table includes the applicable experiment types.

Table 12. Compound parameters (Sheet 1 of 6)

Parameter	Description
(Compound Detail page) Compound	Alphanumeric name assigned to the compound.
(Grid page) Compound Name	
(Compound Detail page) Formula	Chemical formula for the compound. Used to calculate the neutral mass for the compound.
(Grid page) Chemical Formula	
(Compound Detail page) Experiment	Experiment type: SRM, XIC, or SIM. For details about the differences, see “ Experiment Types ” on page 101 .
(Grid page) Experiment Type	
Compound Type	Specifies the compound type as Analyte or Internal Standard.
(Compound Detail page) ISTD Concentration	Specifies the concentration for the internal standard. Available only when the Compound Type is Internal Standard. Used when you enable semi-quant features in the method.
(Grid page) Internal Standard Concentration	Valid range: 0 through 10 000 000 (1e7)
Concentration Units	Specifies the user-defined units of measure that you entered in the database.
Ionization	Alphanumeric identifier. Valid values: None, ESI, APCI, EI, CI, or APPI Default: None
Category	(Optional) Alphanumeric identifier, such as Class 1, Class 2, Opiates, and so forth.
CAS	The Chemical Abstract Service (CAS) number that the application matched with the compound. The Grid display shows the CAS column only when at least one compound has a CAS value.

Table 12. Compound parameters (Sheet 2 of 6)

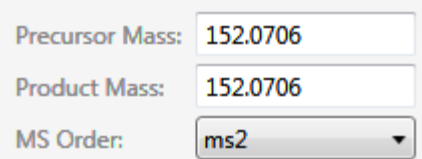
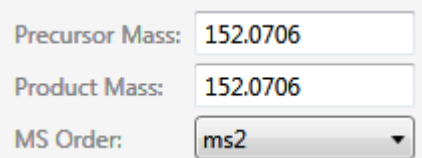
Parameter	Description
Response Threshold	The threshold used to integrate only peaks with a response greater than this value. The response threshold is a minimum response that must be met to allow peak confirmation. Used only for target screening methods and XIC experiments. Valid range: 1000 or greater Default: 5000
Neutral Mass	Mass calculated from the chemical formula. The neutral mass is the sum of all AMU elements in the compound. This parameter is informational only; it is not used for peak detection.
Target Peaks	
(Compound Detail page) Precursor Mass	The mass-to-charge ratio (m/z) of a target peak. The location of the center of a target precursor ion peak in mass-to-charge ratio units. In confirming peaks, the precursor mass is the same as the target peak precursor mass.
(Grid page) Peak n Precursor Mass	Valid range: 10.000 through 6000.000 Default: 0.0 Available for all SRM experiments and for XIC experiments with the MS Order set to MS2.
	
	For mass values in XIC experiments when the MS Order is set to MS1, see Extracted Mass .
(Compound Detail page) Product Mass	The mass-to-charge ratio of the confirming peak. The location of the center of a target quan ion peak in mass-to-charge ratio (m/z) units.
(Grid page) Peak n	Valid range: 10.000 through 6000.000 Default: 0.0 Available for all SRM experiments and for XIC experiments with the MS Order set to MS2.
	
	For mass values in XIC experiments when the MS Order is set to MS1, see Extracted Mass .

Table 12. Compound parameters (Sheet 3 of 6)

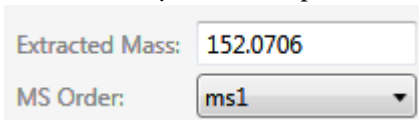
Parameter	Description
(Compound Detail page) Mass	The mass-to-charge ratio of the confirming peak. The location of the center of a target quan ion peak in mass-to-charge ratio (m/z) units. Available only for SIM experiments.
(Grid page) Peak n Mass	
(Compound Detail page) Extracted Mass	The mass-to-charge ratio of the target peak. The location of the center of a target quan ion peak in mass-to-charge ratio (m/z) units. You can enter a value for the Extracted Mass, but when you change the values for Formula, Adduct, Polarity, or Charge State, the application recalculates the Extracted Mass value, overwriting the value you entered.
(Grid page) Peak n Extracted Mass	Valid range: 10.000 through 2999.999 Default: 0.0 Available only for XIC experiments with the MS Order set to MS1.
	
	For mass values in XIC experiments when the MS Order is set to MS2, see Precursor Mass or Product Mass .
(Compound Detail page) Polarity	Positive or Negative
(Grid page) Peak n Polarity	
(Compound Detail page) Adduct	The adducts specified in the configuration file. To add or remove adducts from the default lists, see “ Specifying Adducts ” on page 53 .
(Grid page) Peak n Adduct	Adducts affect the calculated amount of the extracted mass by adding to or subtracting from the neutral mass. Adducts are polarity sensitive. Select the Polarity parameter before selecting the Adduct value. Default Positive valid values: Neutral, NH ₄ , H, Na, K Default Negative valid values: Neutral, H, H ₃ C ₂ O ₂ , HCO ₂ Default: Neutral
(Compound Detail page) Charge State	The charge state of the ion (the z value in m/z). For example, a charge state of 2 with a negative polarity means that the compound has 2 more electrons than protons.
(Grid page) Peak n Charge State	Valid range: 1 through 10 Default: 1

Table 12. Compound parameters (Sheet 4 of 6)

Parameter	Description
MS Order	The confirming peaks come from the same scan (MS) or are fragments from an adjacent scan (MS2). Available only for XIC experiments.
Time Range Peak	The acquisition time specified as either a window around a specified RT value or as a retention time range in minutes. This parameter is visible only when you are editing a compound.
Window (sec)	The Window value used to determine the start and stop time for the acquisition. Available only when the Time Range Peak option is not selected. Valid range: 0.00 through 499.50 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 through 999.00
(Compound Detail page) RT (min)	Retention time. The application uses RT and Window values to determine the start and stop time for the acquisition. When the Time Range Peak option is selected, the RT value is specified as a range.
(Grid page) Peak <i>n</i> RT	Valid range: 0.00 through 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 through 999.00
(Compound Detail page) Lens	Valid range: –400 through 400
(Grid page) Peak <i>n</i> Lens	
(Compound Detail page) Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments.
(Grid page) Peak <i>n</i> Collision Energy	Valid range: –250.00 through 250.00
(Compound Detail page) Energy Ramp	Valid range: 0.00 through 200.00
(Grid page) Peak <i>n</i> Energy Ramp	

Table 12. Compound parameters (Sheet 5 of 6)

Parameter	Description
Confirming Peaks	Use confirming peak parameters in quantitation methods only.
(Compound Detail page) Precursor	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 or XIC experiments with the MS Order set to MS2.
(Grid page) Peak n Confirming n Precursor	Valid range: 10.000 through 2999.999 Default: 0.0
(Compound Detail page) Product Mass	The mass-to-charge ratio of the quantitation 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.
(Grid page) Peak n Confirming n	Valid range: 10.000 through 2999.999 Default: 0.0
(Compound Detail page) Mass	The mass-to-charge ratio of the confirming peak. The location of the center of a target quan ion peak in mass-to-charge ratio (m/z) units. Available only for SIM experiments.
(Grid page) Peak n Confirming n Extracted Mass	
(Compound Detail page) Extracted Mass	The mass-to-charge ratio of the target peak. The location of the center of a target quan ion peak in mass-to-charge ratio (m/z) units. Available only for XIC experiments.
(Grid page) Peak n Confirming n Extracted Mass	Valid range: 10.000 through 2999.999 Default: 0.0
(Compound Detail page) Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments.
(Grid page) Peak n Confirming n Collision Energy	Valid range: -250.00 through 250.00
Target Ratio (%)	Specifies the theoretical ratio of the confirming ion's response to the quantification ion's response. Valid range: 1 through 100
Window Type	Specifies an Absolute or a Relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	Specifies the acceptable ion ratio range. Valid range: 1 through 100

Table 12. Compound parameters (Sheet 6 of 6)

Parameter	Description
Ion Coelution (min)	Specifies the maximum difference in retention time between a confirming ion peak and the quantification ion peak. Valid range: 0.025 through 0.1
(Compound Detail page) MS Order	Specifies whether the confirming peaks or fragments come from the same scan (MS) or an adjacent scan (MS2). Available only for XIC experiments.
(Grid page) Peak <i>n</i> Confirming <i>n</i> MS Order	
Fragments	Fragment parameters are used for XIC experiment types in target screening methods. The application uses fragments to define masses that are present in an adjacent scan (MS2).
(Compound Detail page) Extracted Mass	The mass-to-charge ratio of the target peak. The location of the center of a target quan ion peak in mass-to-charge ratio (<i>m/z</i>) units. Available only for XIC experiments. Valid range: 10.000 through 2999.999 Default: 0.0

Experiment Types

The TraceFinder application uses three experiment types: [SRM](#), [SIM](#), and [XIC](#).

Each of these experiment types uses a different structure for the mass filter. The target peak and confirming peak parameters for each experiment type are defined in the “[Compound Parameters](#)” on [page 95](#).

A compound database 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 peaks include values for precursor mass, product mass, and collision energy.

Compound Detail

Compound:
Experiment: SRM
Category:
CAS:
Formula:

Ionization: None
Neutral Mass: 0

Target Peaks +

Peak 1 -
+

Precursor Mass:

Product Mass:

Adduct: Neutral

Polarity: Positive

Charge State: 1

Time range peak:

Window (sec):

RT (min):

Collision Energy:

Lens:

Energy Ramp:

Confirming Peaks + (Quan Only)

Precursor	Product Mass	Collision Energy:
0		

4 Using the Common Features of the Method Development Mode

Working with the Compound Database

SIM: Single Ion Monitoring

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

Confirming peaks include an extracted mass value.

Compound Detail

Compound:

Experiment: **SIM** Category: CAS: Formula:

Ionization: **None** Neutral Mass: 0

Target Peaks

Peak 1

Confirming Peaks (Quan Only)

Mass: <input type="text"/>	Mass: <input type="text"/>
Adduct: Neutral	<input type="text"/>
Polarity: Positive	<input type="text"/>
Charge State: 1	<input type="text"/>
Time range peak: <input type="checkbox"/>	
Window (sec): 30	
RT (min): 0	
Lens: 0	
Energy Ramp: 0	

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 peaks include an extracted mass value and a choice of mass order: **MS1** or **MS2**.

Compound Detail

Compound:

Experiment: **XIC** Category: CAS: Formula:

Ionization: **None** Response Threshold: **5000** Neutral Mass: **0**

Target Peaks

Peak 1

Confirming Peaks (Quan Only)

Extracted Mass:	Precursor	Extracted Mass	MS Order
<input type="text"/>	<input type="text"/>	<input type="text"/>	ms1

Fragments (Screening Only)

Extracted Mass
<input type="text"/>

Extracted Mass:

MS Order: **ms1**

Adduct: **Neutral**

Polarity: **Positive**

Charge State: **1**

Time range peak:

Window (sec): **30**

RT (min): **0**

Lens: **0**

Energy Ramp: **0**

Compound Database Names Mapped to CSV Column Names

Column names in an Excel spreadsheet do not always match the parameter names in the compound database editor. The following table maps the parameter names for both the Compound Detail page and the Grid page to the column headings in a CSV spreadsheet.

Table 13. CSV column names for compound parameters (Sheet 1 of 3)

Compound database parameter	CSV column heading
(Compound Detail page) Compound	CompoundName
(Grid page) Compound Name	
(Compound Detail page) Experiment	ExperimentType
(Grid page) Experiment Type	
Category	Category
CAS	CAS
Formula	ChemicalFormula
Ionization	Ionization
Response Threshold	ResponseThreshold (XIC only)
Target Peaks	
(Compound Detail page) Precursor Mass	PrecursorMass (SRM only)
(Grid page) Peak <i>n</i> Precursor Mass	
(Compound Detail page) Product Mass	ProductMass (SRM only)
(Grid page) Peak <i>n</i>	
(Compound Detail page) Mass	ProductMass (SIM only)
(Grid page) Peak <i>n</i> Mass	
(Compound Detail page) Extracted Mass	Extracted Mass (XIC only)
(Grid page) Peak <i>n</i> Extracted Mass	

Table 13. CSV column names for compound parameters (Sheet 2 of 3)

Compound database parameter	CSV column heading
(Compound Detail page) Product Mass Mass Extracted Mass	Extracted Mass (when the Compound Detail page of a compound database contains any combination of SRM, XIC, and SIM experiments)
(Compound Detail page) Adduct	Adduct
(Grid page) Peak <i>n</i> Adduct	
Polarity	Polarity
(Compound Detail page) Charge State	ChargeState
(Grid page) Peak <i>n</i> Charge State	
Window	Window
(Compound Detail page) RT (min)	RT
(Grid page) Peak <i>n</i> RT	
(Compound Detail page) Collision Energy	CollisionEnergy (SRM only)
(Grid page) Peak <i>n</i> Collision Energy	
(Compound Detail page) Lens	Lens
(Grid page) Peak <i>n</i> Lens	
Energy Ramp	EnergyRamp
Confirming Peaks	
(Compound Detail page) Precursor	Confirm Precursor (SRM and XIC only)
(Grid page) Peak <i>n</i> Confirming <i>n</i> Precursor	

Table 13. CSV column names for compound parameters (Sheet 3 of 3)

Compound database parameter	CSV column heading
(Compound Detail page) Product Mass	Confirm Product (SRM only)
(Grid page) Peak <i>n</i> Confirming <i>n</i>	
(Compound Detail page) Mass	Confirm Product (SIM only)
(Grid page) Peak <i>n</i> Confirming <i>n</i> Extracted Mass	
(Compound Detail page) Extracted Mass	Confirm Extracted (XIC only)
(Grid page) Peak <i>n</i> Confirming <i>n</i> Extracted Mass	
(Compound Detail page) Product Mass Mass Extracted Mass	Confirm Extracted (when the Compound Detail page of a compound database contains any combination of SRM, XIC, and SIM experiments)
(Compound Detail page) Collision Energy	Confirm Energy (SRM only)
(Grid page) Peak <i>n</i> Confirming <i>n</i> Collision Energy	
Fragments	
Extracted Mass	Fragment (XIC only)

Data Columns with Default Values

When you export compounds to a CSV file with the Export Only Columns with Data option, the application writes only columns that contain nondefault data for at least one compound. This option does not export columns that contain only default data.

When you import compounds from a CSV data file that has missing columns, the application replaces the missing columns and uses default values for all compounds.

Table 14. Default values for compound parameters

CDB parameter	Default value
Compound Detail	
Formula	Blank
CAS	Blank
Category	Blank
Ionization	None
Response Threshold (XIC only)	5000
Target Peaks	
Precursor Mass	Blank
Collision Energy	0
Adduct	Neutral
Lens	0
Energy Ramp	0
Confirming Peaks	
Precursor	0
Collision Energy	Blank

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.

Follow these 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 open the Instrument View

1. Click **Method Development** in the navigation pane.

The Method Development navigation pane opens.

2. Click **Instrument View**.



The Instrument View opens.

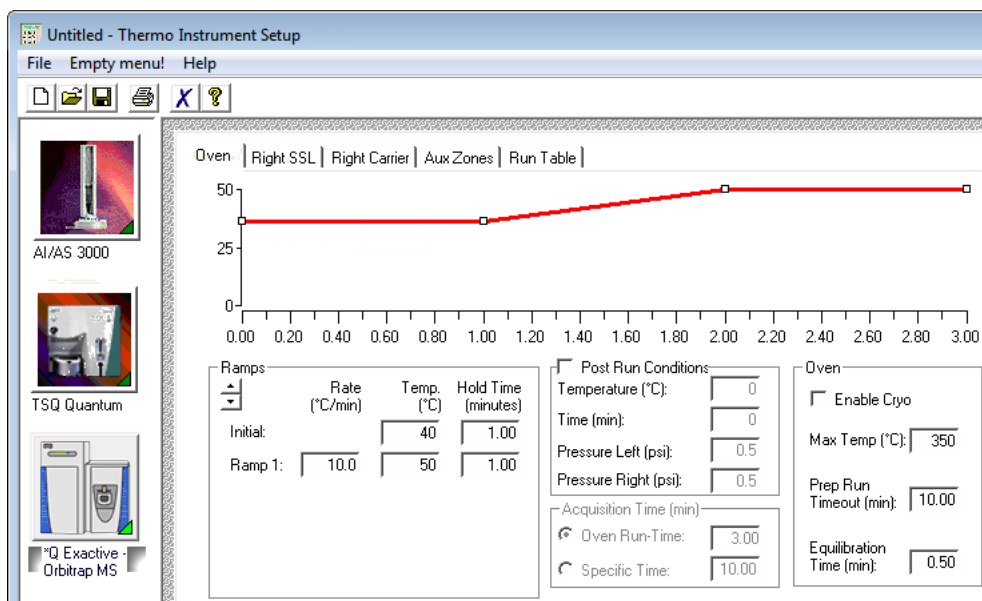


❖ To create a new instrument method

1. Choose **File > New Instrument Method** from the main menu.

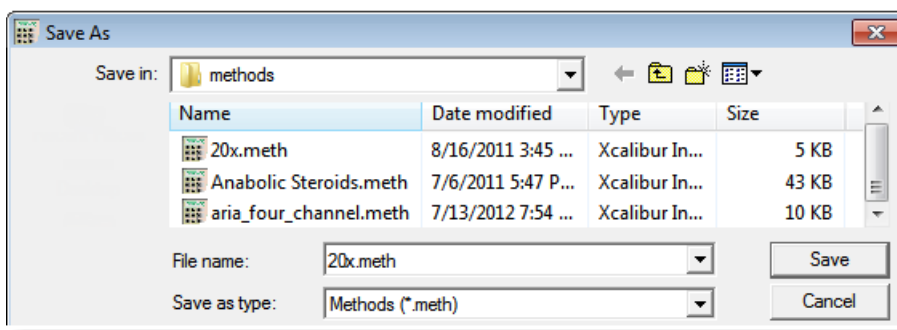
The Thermo Xcalibur Instrument Setup window opens.

Figure 25. Example instrument setup showing multiple configured instruments



2. Click the icon for the instrument that you want to use for the method.
3. Edit the values on the instrument page.
4. From the main menu in the Thermo Xcalibur Instrument Setup window, choose **File > Save As**.

The Save As dialog box opens.

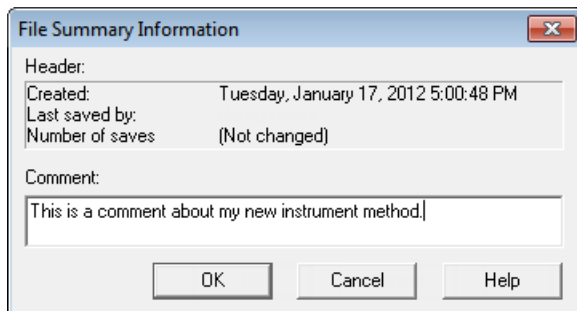


4 Using the Common Features of the Method Development Mode

Working with Instrument Methods

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 application saves the new instrument method in the following folder:

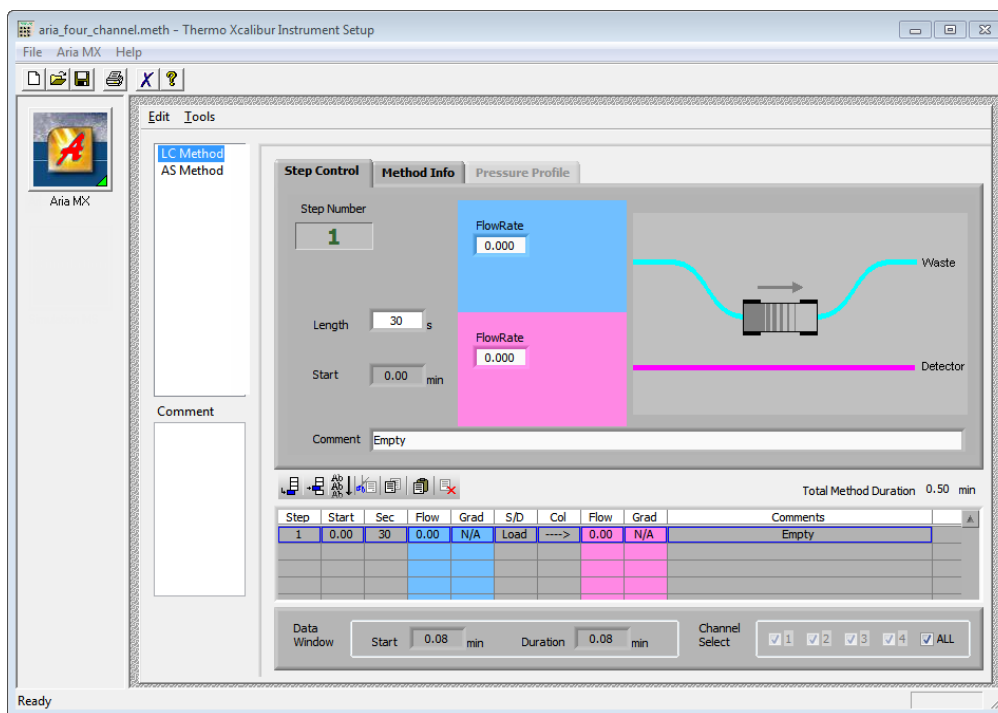
...\Xcalibur\methods

❖ To create a new multiplexing instrument method

1. Choose **File > New Instrument Method** from the main menu.

The Thermo Xcalibur Instrument Setup window opens.

Figure 26. Example instrument setup showing a configured multiplexed instrument

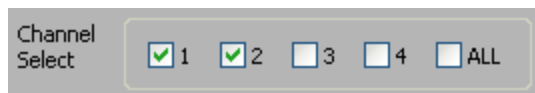


2. Click the icon for the instrument that you want to use for the method.

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 that you want to use for acquisition, as in this example:

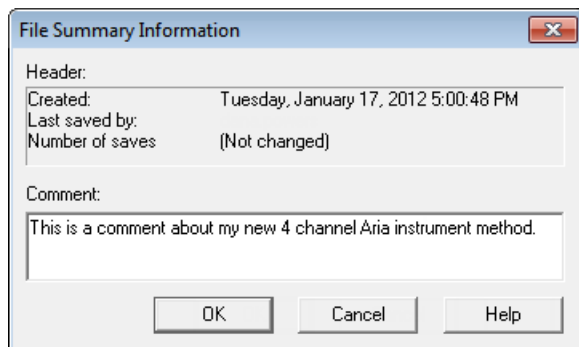


5. From the main menu in the Thermo Xcalibur Instrument Setup window, choose **File > Save As**.

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 application saves the new instrument method in the following folder:

... \Xcalibur\methods

❖ To open an instrument method

1. From the File menu, choose **Open Instrument Method**.

An instrument method browser opens.

2. Select an instrument method from the list and click **Open**.

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 with another name.

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

Using the Method Development Mode for Quantitation Methods

This chapter includes method development tasks for creating and editing a quantitation method. (See [Method Development navigation pane](#).) When user security is activated, you must have Method Development Access permission to use these features.

Contents

- [Opening a Master Method](#)
- [Starting a New Quantitation Master Method](#)
- [Editing a Master Method](#)
- [Saving a Master Method to a New Name](#)
- [Creating a Method Template](#)
- [Exporting Mass Data](#)

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 your application. A quantitation master method contains a list of compounds and the settings for detecting, processing, and reporting those compounds.

When you create a master method, the application uses the method to determine how the application 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 displays the results, and how the reporting functionality defines the output for your data and results.

The 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 application saves all of your commonly used method settings in a template, such as the number of confirming ions or the use of data-dependent scans.

Figure 27. Method Development navigation pane

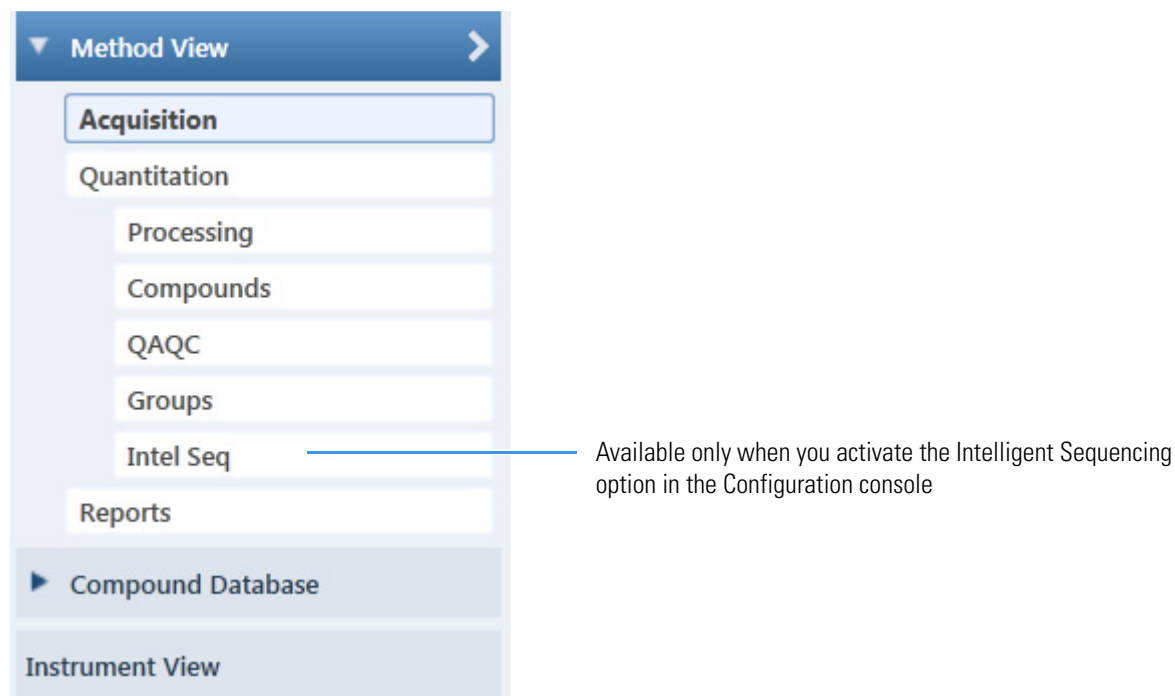


Table 15. Method Development navigation pane commands

Command	Description
Method View	Displays the Method View for the master method.
Acquisition	Displays the Acquisition page of the Method View. See “Editing the Acquisition Page” on page 137.
Quantitation	
Processing	Displays the Processing page of the Method View. See “Editing the Processing Page” on page 141.
Compounds	Displays the Compounds page of the Method View. See “Editing the Compounds Page” on page 150.
QAQC	Displays the QAQC page of the Method View. See “Editing the QAQC Page” on page 217.
Groups	Displays the Groups page of the Method View. See “Editing the Groups Page” on page 226.
Intel Seq	Displays the Intelligent Sequencing page of the Method View. See “Editing the Intelligent Sequencing Page” on page 228. Available only when you activate the Intelligent Sequencing option in the Configuration console.
Reports	Displays the Reports page of the Method View. See “Editing the Reports Page” on page 236.
Compound Database	See “Working with the Compound Database” on page 74.
Instrument View	See “Working with Instrument Methods” on page 108.

Opening a Master Method

Use the TraceFinder application to open a master method that was created and saved in the current application or converted from previous versions of TraceFinder. To convert legacy methods, see [“Converting Legacy Data”](#) on page 20.

❖ To open a quantitation method in the Method Development mode

1. Click **Method Development** in the navigation pane.

The Method Development navigation pane opens.



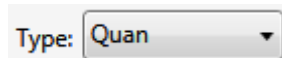
For descriptions of all the features in the Method Development navigation pane, see [“Starting a New Quantitation Master Method”](#) on page 117.

2. Choose **File > Open > Master Method** from the main menu.

Tip You can also open one of your most recently used master method files. Choose **Files > Recent Files > Method**.

The Open Master Method dialog box opens, displaying all available methods. See [Open Master Method dialog box](#).

3. Select **Quan** in the Type list.



The method list displays all quantitation methods.

4. Select a quantitation master method and click **Open**.

The Acquisition page for the selected method opens. For detailed descriptions of all the features on the Acquisition page, see [“Acquisition Page for a Quantitation Method”](#) on page 140.

5 Using the Method Development Mode for Quantitation Methods

Opening a Master Method

Figure 28. Open Master Method dialog box

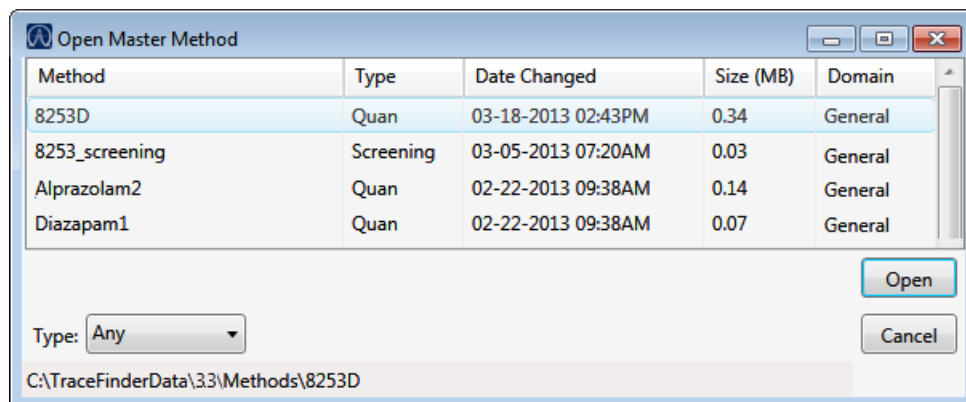


Table 16. Open Master Method dialog box parameters

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan, Screening, or Unknown Only.
Date Changed	Date the method was last updated.
Size	Size of the method in megabytes.
Domain	TraceFinder domain for which the method was created.
Type	Type of method to display: Quan, Screening, Unknown Only, or Any.
<i>Path</i>	Path to the selected method in the TraceFinderData\3.3\Methods folder.

Starting a New Quantitation Master Method

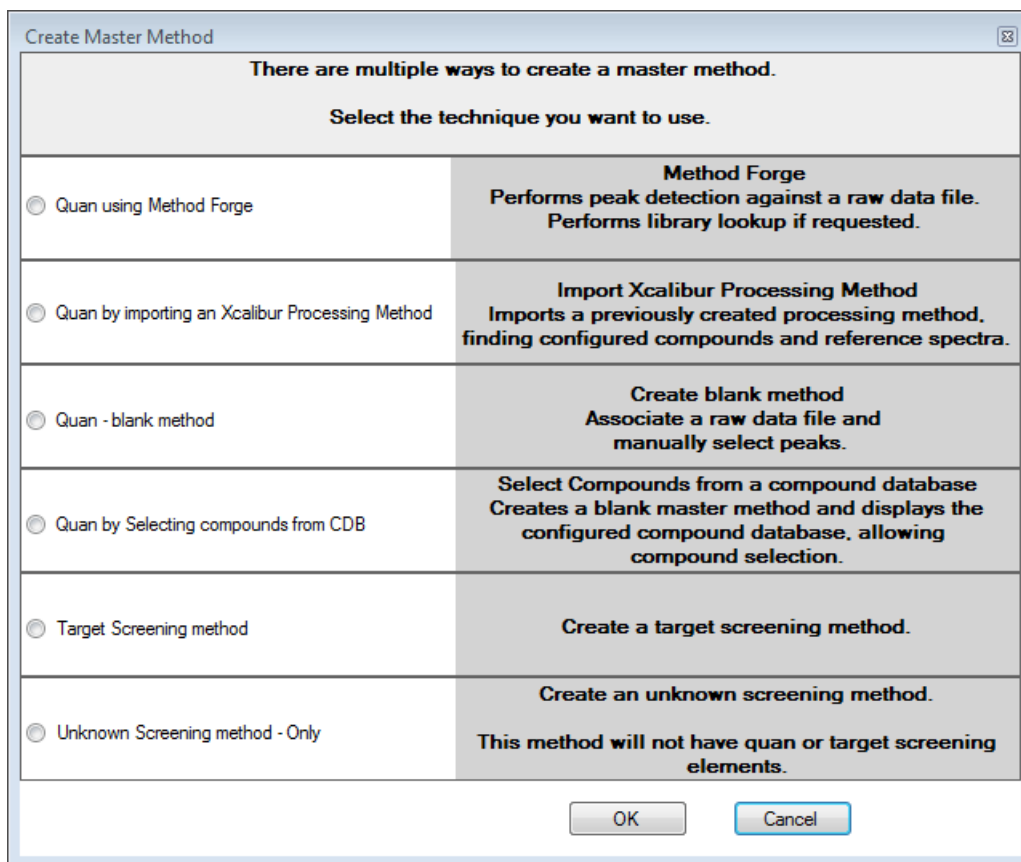
To create or start a specific method, select as applicable from one of the four different quantitation method procedures (or techniques) in the Create Master Method dialog box:

- [Creating a New Method with Method Forge](#)
- [Importing an Xcalibur Master Method](#)
- [Creating a Blank Method](#)
- [Selecting Compounds from the Compound Database](#)

Then, use the features of the Method View to complete and save the master method.

To open the Create Master Method dialog box, choose **File > New > Master Method** from the main menu.

Figure 29. Create Master Method dialog box



IMPORTANT The Unknown Screening Method - Only technique is displayed only when you select the Allow Unknown Screening option in the application configuration console.

Creating a New Method with Method Forge

With Method Forge, you can create a new quantitation 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 application automatically create a master method for you. For detailed descriptions of all the Method Forge parameters, see “[Method Forge Dialog Box](#)” on [page 125](#).

When the 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.

Note When the identified peak is from an analog trace, the application does not perform a library search and does not identify any confirming ions.

Follow these procedures:

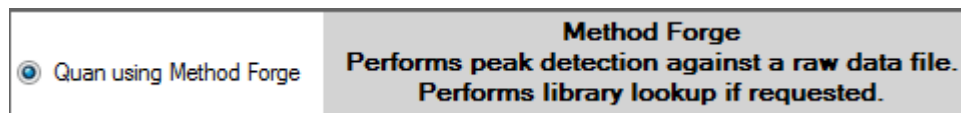
- [To automatically select compounds to create a new method](#)
- [To manually select compounds to create a new method](#)

❖ To automatically select compounds to create a new method

1. From the File menu, choose **New > Master Method**.

The Create Master Method dialog box opens. To view all available ways to create a master method, see “[Create Master Method dialog box](#)” on [page 117](#).

2. Select the **Quan Using Method Forge** option and click **OK**.



The Method Forge dialog box opens. For detailed descriptions of all the features in the Method Forge dialog box, see “[Method Forge Dialog Box](#)” on [page 125](#).

Use 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.

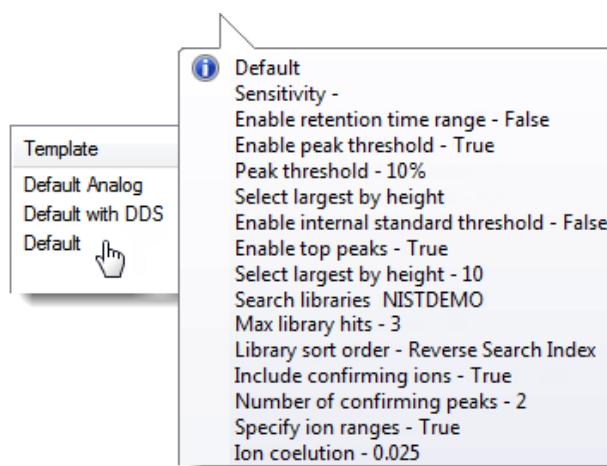
Each method requires a processing method template. The application displays all saved method templates in the template list.

Template	Libraries
Default Analog	1
Default	1

3. To select a processing method template, do one of the following:

- Click **Open Method Template Editor** to create and save a new method template.
See “Creating a Method Template” on page 243.
- Select a method template from the template list, and click **Open Method Template Editor** to edit and save the method template.
- Select a method template from the template list.

The selected template is now selected by default each time you open the Method Forge dialog box until you restart the application. To view the parameters for each available method template, hold your cursor over the template name, as in this example:



4. Select the **Name the Master Method** check box and type a name for your master method.

You can enter a new method name, or you can enter an existing method name to overwrite when you create the method. If you do not select this option, the method is named for the raw data file used to create the method.

Note When the Name the Master Method check box is selected, you must enter a method name. To let the application name the method with the raw data file name, clear the Name the Master Method check box.

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

6. Specify a raw data file by doing one of the following:

- a. In the Raw File Selection area, select the **Use an Existing Raw Data File** option.
- 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, select the **Acquire a New Raw Data File** option.
- b. From the Instrument method list, select a method (.meth) file to use for acquiring the data.

5 Using the Method Development Mode for Quantitation Methods

Starting a New Quantitation Master Method

- c. In the Raw Filename box, type the name of the file where the 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. To acquire a new raw data file, do one of the following:

Select the **Manual Injection** option.

–or–

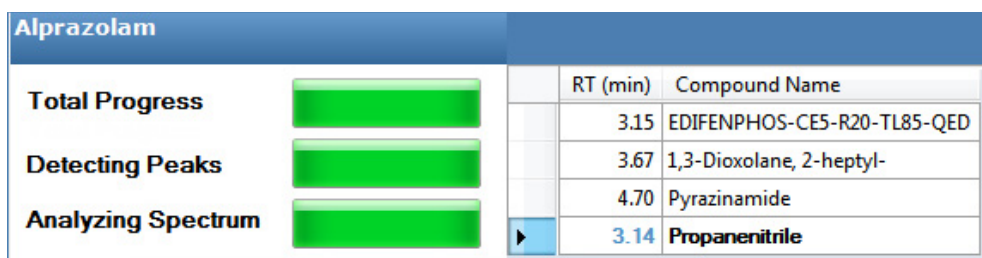

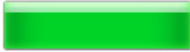
Specify the autosampler settings:

- a. Select the **Use Autosampler** option.
- b. In the Vial Position box, type a vial position.
- c. In the Injection Volume box, type an injection volume.

Valid range: 0.1 through 2000 µL

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

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

Alprazolam		RT (min)	Compound Name
Total Progress		3.15	EDIFENPHOS-CE5-R20-TL85-QED
Detecting Peaks		3.67	1,3-Dioxolane, 2-heptyl-
Analyzing Spectrum		4.70	Pyrazinamide
		3.14	Propanenitrile

- For analog peaks, the Method Forge displays the detected peak as *Peak@(RT)Analog*. The Method Forge does not perform a library search for peaks found in analog traces.
 - For mass spectral peaks, the Method Forge process searches the associated libraries and displays the identified compound names instead of the peak times.
- When the acquisition is completed, Method Forge performs peak detection, library searching (except for analog peaks), and identification of characteristic ion and reference spectra. Method Forge then loads this information into a new master method. This process occurs immediately if you selected a previously acquired raw data file.
9. From the Instrument Method list, select an instrument method.
 10. From the Qualitative Peak Processing Template list, select a method template for performing peak detection on quantitation samples following target compound analysis.
 11. (Optional) 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.

When you create a reference spectrum with background subtraction, the application uses the selected method to conduct background subtraction of peak spectra during quantitative processing and reports the background-subtracted reference spectrum (indicated with BS in the scan heading) as the last scan for each compound in the Quantitation Report - 2 report. The application does not use background subtraction with qualitative processing.

12. In the Steppoff Value box, enter a number.

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

Background subtraction range option:

Number of scans to subtract:

Steppoff value:

If you entered 3 in the Number of Scans To Subtract box and the steppoff value is 5, the 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.

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

For a detailed description of how to modify all the parameters in a master method, see “[Editing a Master Method](#)” on [page 135](#).

❖ To manually select compounds to create a new method

1. From the File menu, choose **New > Master Method**.

The Create Master Method dialog box opens. See “[Create Master Method dialog box](#)” on [page 117](#).

2. Select the **Quan Using Method Forge** option and click **OK**.

<input checked="" type="radio"/> Quan using Method Forge	Method Forge Performs peak detection against a raw data file. Performs library lookup if requested.
--	--

The Method Forge dialog box opens. For detailed descriptions of all the features in the Method Forge dialog box, see “[Importing an Xcalibur Master Method](#)” on [page 127](#).

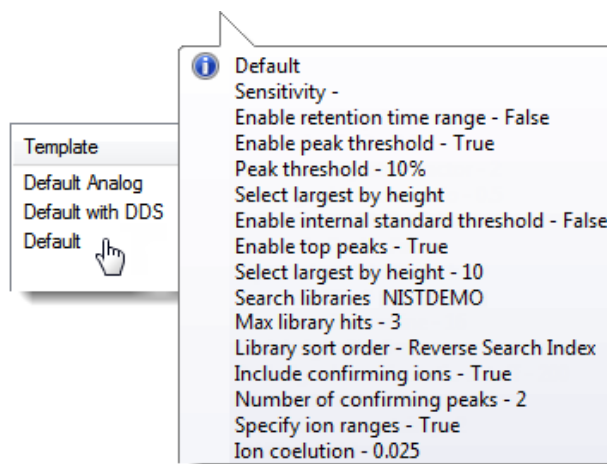
Each method requires a qualitative peak processing template. The application displays all saved method templates in the template list.

Template	Libraries
Default Analog	1
Default	1

- To select a qualitative peak processing template, do one of the following:
 - Click **Open Method Template Editor** to create and save a new method template. See “[Creating a Method Template](#)” on page 243.
 - Select a method template from the template list, and click **Open Method Template Editor** to edit and save the method template. The application saves the methods to the following folder:
...\\TraceFinderData\\3.3\\Templates\\Methods\\General
 - Select a method template from the template list.

The selected template is now selected by default each time you open the Method Forge dialog box until you restart the application.

To view the parameters for each available method template, hold your cursor over the template name, as in this example:



- Select the **Name the Master Method** check box and type a name for your master method.

You can enter a new method name, or you can enter an existing method name and overwrite it when you create the method. If you do not select this option, the method is named for the raw data file used to create the method.

IMPORTANT When the Name the Master Method check box is selected, you must enter a method name. To let the application name the method with the raw data file name, clear the Name the Master Method check box.

- Ensure that the **Automatically Create the Master Method** check box is cleared.
- To select a raw data file, browse to the file location.

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

The method forge results view opens, listing all peaks found in the raw data file.

For each peak listed in the RT column, the application displays a list of possible matches in the Libraries pane. The application selects the best match, displays the name in the Compound Name list, and displays the peak spectrum for that compound in the first Libraries pane.

Figure 30. Method forge results view

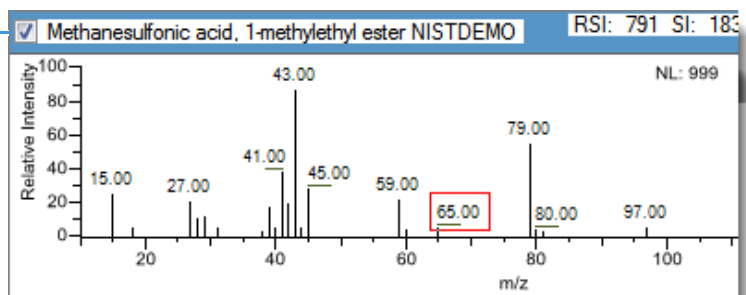


5 Using the Method Development Mode for Quantitation Methods

Starting a New Quantitation Master Method

8. (Optional) To use a library compound other than the compound chosen by the application, do the following:
 - a. Select the peak in the RT column.
 - b. In the Libraries pane, scroll to the spectrum for the compound that you want to use.
 - c. Select the check box in the header of the spectrum pane.

Selected
compound



- d. Repeat these steps for each peak that you want to replace.
9. In the Compound Name list, use the CTRL or SHIFT keys to select each compound that you want to include in the method compound.

Note When you select multiple compounds, the method forge results view does not display any spectrum panes.

10. (Optional) To exit the method forge results view without creating a method, click **Cancel**.

The method forge results view closes and the application returns to the Method View without creating a method.

Note To return to the method forge results view to create a method from the same results, choose **Method View > View Method Forge Results** from the main menu.

11. Click **Create**.


The application uses all selected compounds to create the method and displays the Acquisition page of the Method View. For detailed descriptions of all the features on the Acquisition page, see [“Acquisition Page for a Quantitation Method”](#) on page 140.

12. From the Instrument Method list, select an instrument method.

13. 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 135.



This animation shows how to create a new quantitation method using Method Forge. To view the animation, click , and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.

Method Forge Dialog Box

Use the Method Forge dialog box to create a new master method.

Figure 31. Method Forge dialog box

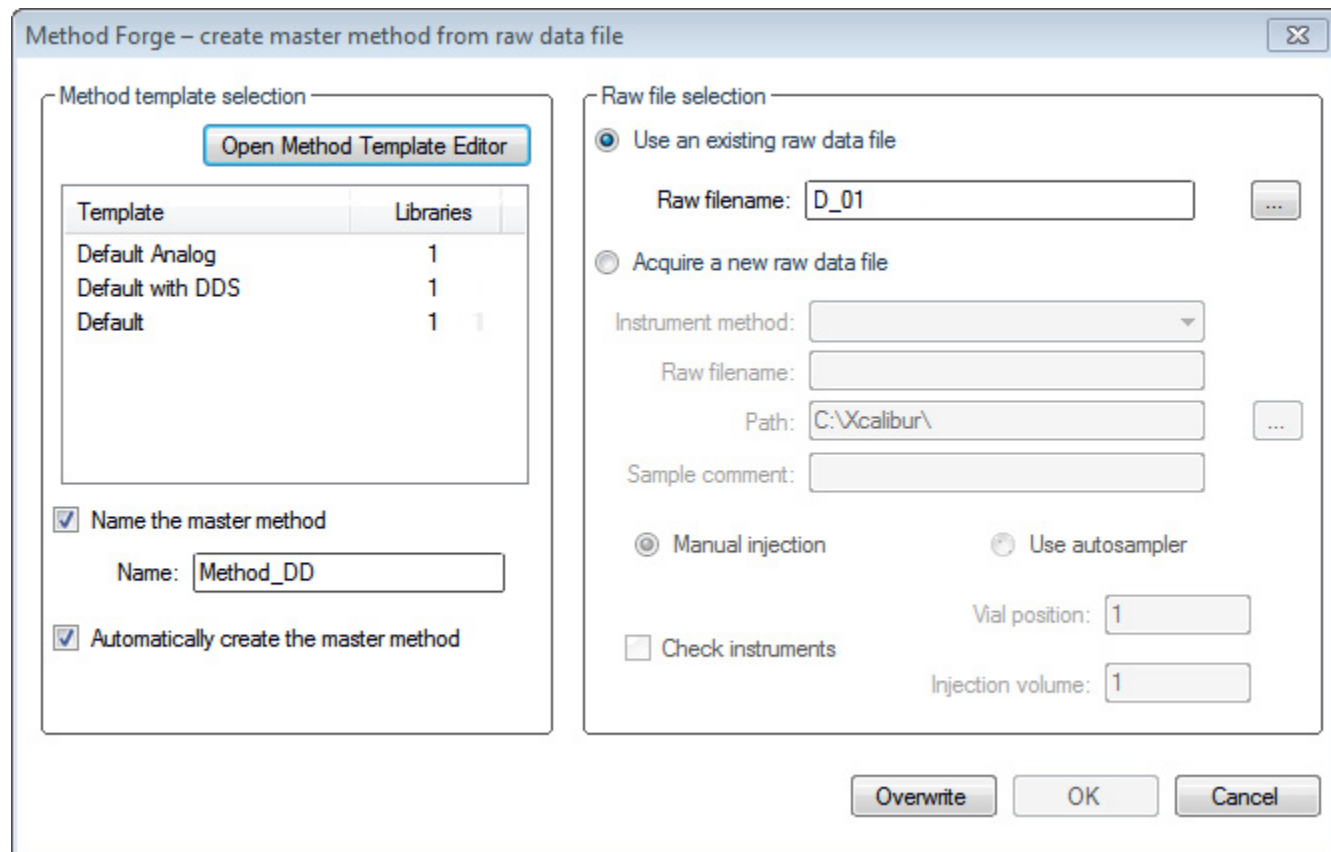


Table 17. Method Forge dialog box parameters (Sheet 1 of 2)

Parameter	Description
Method template selection	
Open Method Template Editor	Opens the Method Template Editor, where you can edit the currently selected method template. See “Creating a Method Template” on page 243.
Template	Specifies the method template to use to create this master method. All methods require a method template. To view the parameters of each template, hold your cursor over the method name. See the Method Template Parameters example in “To automatically select compounds to create a new method” on page 118.
Name the Master Method	Specifies the name for the new master method. If you do not specify a method name, the application uses the raw data file name for the method.
Automatically Create the Master Method	Specifies that when acquisition is completed, Method Forge performs peak detection, library searching, and identification of characteristic ion and reference spectra. This information is loaded into a new master method. This process occurs immediately when you specify an existing raw data file.

Table 17. Method Forge dialog box parameters (Sheet 2 of 2)

Parameter	Description
Raw file selection	
Use an Existing Raw Data File	Activates the Raw Filename box where you can select a raw data file used in creating the master method.
Acquire a New Raw Data File	Activates functions to acquire data to create a raw data file used in creating the master method.
Instrument Method	Specifies the saved method (.meth) file used for acquiring the data.
Raw Filename	Specifies the file name where the application writes the raw data.
Path	Specifies the location where the application saves the raw data file.
Sample Comment	(Optional) Specifies a comment about the acquired sample or the data file.
Manual Injection	Performs a manual acquisition.
Use Autosampler	Performs an autosampler acquisition.
Vial Position	Specifies the tray vial number used for the autosampler acquisition.
Injection Amount	Specifies the volume (in milliliters) injected by the autosampler acquisition.
Check Instruments	Opens the Submit to Acquisition dialog box that prompts you to prepare the instrument before you acquire the sample used to create a method. Available only when you select the Acquire a New Raw Data File option.
Function button	
Overwrite	Overwrites the specified master method name. This function is activated only when the specified master method name already exists.
OK	Creates a master method using the data and parameters that you specified.
Cancel	Closes 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

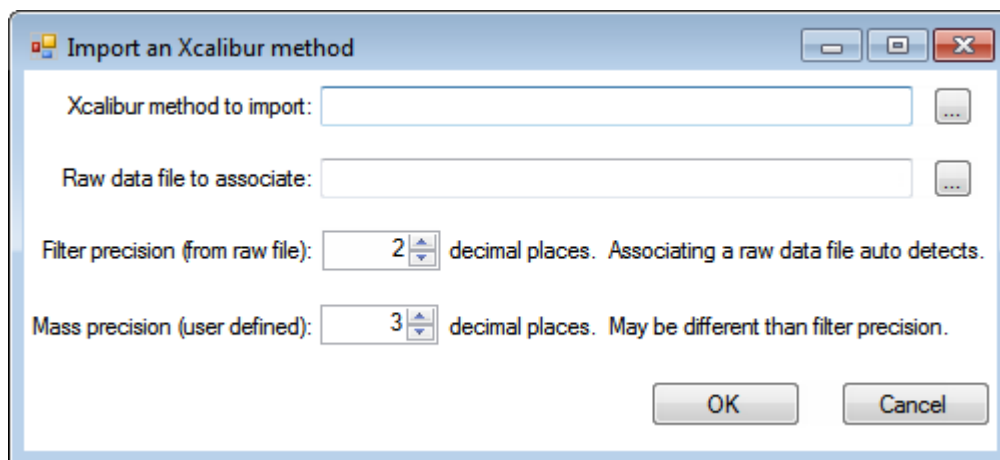
1. Choose **File > New > Master Method** from the main menu.

The Create Master Method dialog box opens. To view all available ways to create a master method, see “[Create Master Method dialog box](#)” on [page 117](#).

2. Select the **Quan by Importing an Xcalibur Processing Method** option and click **OK**.



The Import an Xcalibur Method dialog box opens.



3. For the Xcalibur Method to Import box, browse to the location of the Xcalibur processing method file, and open the file.

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

4. (Optional) For the Raw Data File to Associate box, browse to the location of a raw data file to associate with the method (or select from the list of previously associated raw data files), and open the file.

To assure that this raw data file is always available to the method (for example, if you move the method to another system), the application saves the raw data file in the Methods folder:

...\\TraceFinderData\\3.3\\Methods*Methodname*

5 Using the Method Development Mode for Quantitation Methods

Starting a New Quantitation Master Method

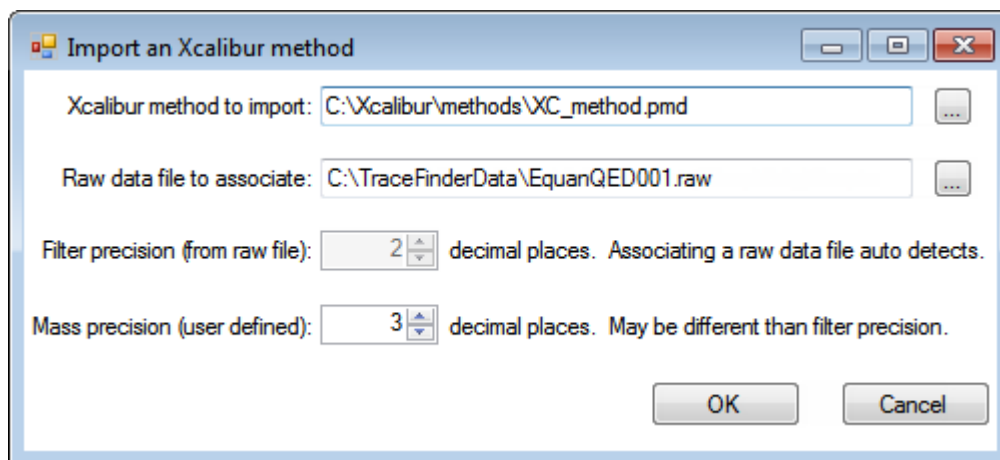
5. (Optional) Change the number of decimal places in the Filter Precision box.

You can set the number of filter precision decimal places to any integer between 2 and 5, inclusive.

Note When you select a raw data file to associate, the application reads the filter precision from the file and this feature is not available.

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

You can set the number of mass precision decimal places to any integer between 2 and 6, inclusive.



Note When you associate a raw data file, the application reads the filter precision from the associated file so that you cannot change the Filter Precision value.


7. Click **OK**.

The application adds all compounds found in the imported Xcalibur method and displays the Acquisition page of the Method View. For detailed descriptions of the features on the Acquisition page, see “[Acquisition Page for a Quantitation Method](#)” on page 140.

8. From the Instrument Method list, select an instrument method.
9. 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 135.



This animation shows how to create a new quantitation method by importing an Xcalibur processing method. To view the animation, click , and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.

Creating a Blank Method

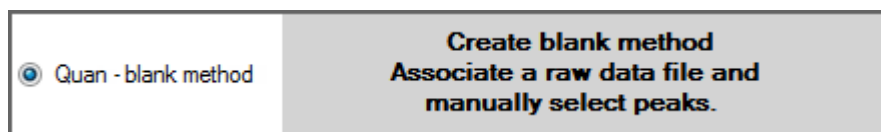
You can use the compounds in a previously acquired raw data file to create a new blank master method.

❖ To create a blank method

1. From the File menu, choose **New > Master Method**.

The Create Master Method dialog box opens. To view all available ways to create a master method, see “[Create Master Method dialog box](#)” on [page 117](#).

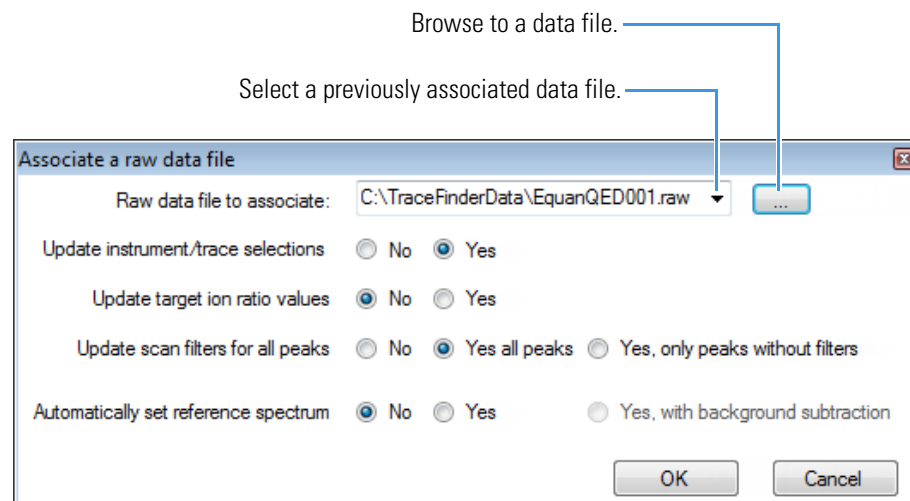
2. Select the **Quan – Blank Method** option and click **OK**.



The Method View for a new, unnamed method opens. This method has no associated data. You can use the compounds in a previously acquired raw data file to create a new master method.

3. From the Method View menu, choose **Associate a Raw Data File**.

The Associate a Raw Data File dialog box opens.



4. Browse to a raw data file to associate with the method (or select from the list of previously associated raw data files) and open the file.

To assure that this raw data file is always available to the method (for example, if you move the method to another system), the application saves the raw data file in the Methods folder:

...\\TraceFinderData\3.3\Methods\Methodname

5. Select the update options to use for creating your method:

- **Update Instrument/Trace Selections:** Reads the Detector and Trace options from the associated raw data file. On the Detection page, only detector types and traces that are defined in the raw data file are available. For detailed descriptions of the available Detector and Trace values, see “Signal” on page 168.
- **Update Target Ion Ratio Values:** Reads the ion ratio values from the associated raw data file.
- **Update Scan Filters for All Peaks:**
 - **Yes, All Peaks** updates all peaks to use the scan filters from the associated raw data file.
 - **Yes, Only Peaks Without Filters** updates only peaks without scan filters to use the scan filters from the associated raw data file; it does not override any existing scan filter.
- **Automatically Set Reference Spectrum:** Reads a reference spectrum from the associated raw data file.

When you select Yes, with Background Subtraction, the application uses the background-subtracted reference spectrum during quantitative processing and reports the background-subtracted reference spectrum (indicated with BS in the scan heading) as the last scan for each compound in the Quantitation Report - 2 report.

Note The background subtraction option is available only when you select a background subtraction method on the Acquisition page in the master method. See “Editing the Acquisition Page” on page 137.

Options that are set to No use the standard values in the method.

6. Click **OK**.

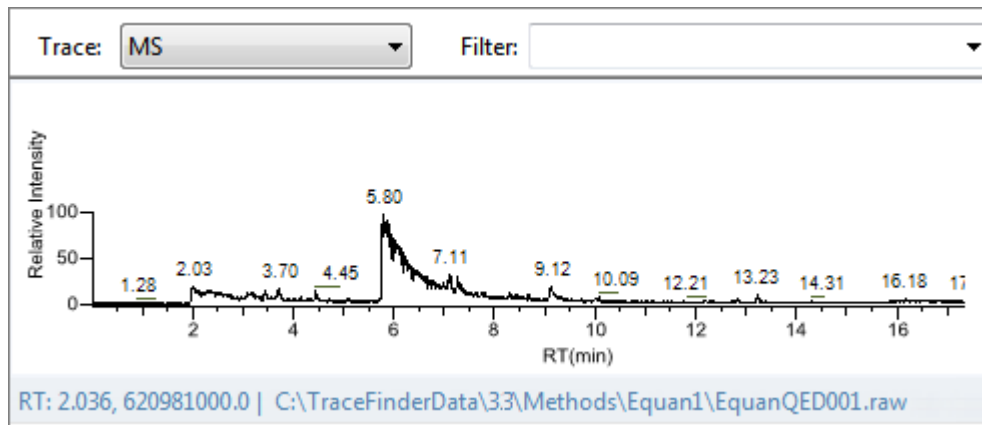
The application displays the Acquisition page of the Method View.

7. Click **Compounds** in the navigation pane.

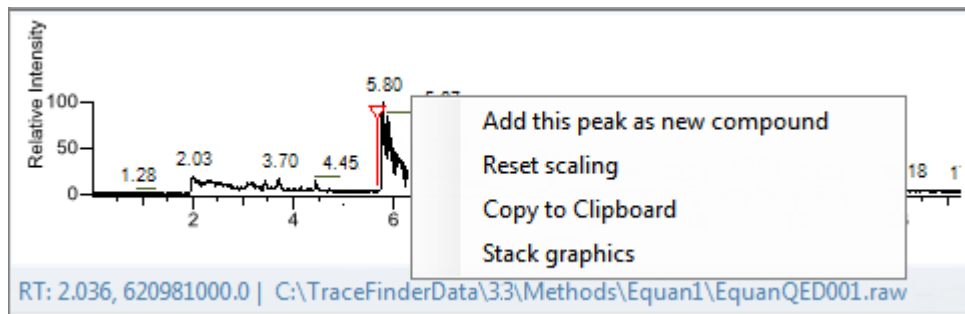
The method must include at least one compound.

- Click the **Detection** tab.

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



- Select a filter from the Filter list.
- Select the peak in the chromatogram that represents the compound that you want to add to the method.
- Right-click and choose **Add This Peak as New Compound** from the shortcut menu.



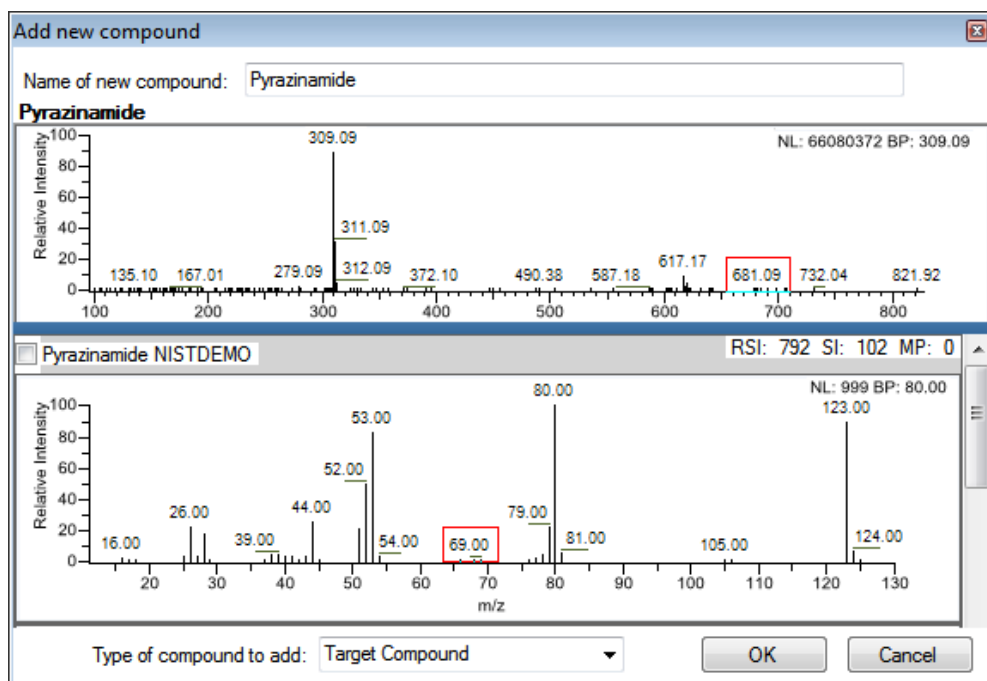
The application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quantitative peak, and the second and third largest ions as the confirming ion peaks.

Note When the peak is from an analog trace, the application does not perform a library search and does not identify any confirming ions.

5 Using the Method Development Mode for Quantitation Methods

Starting a New Quantitation Master Method

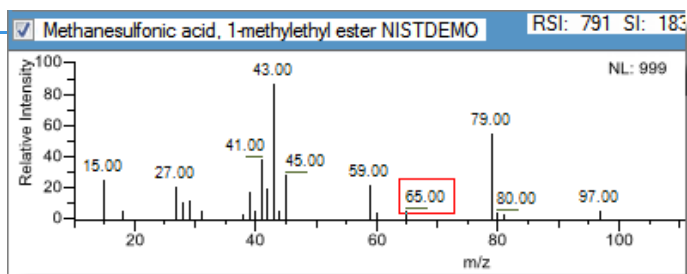
If the name of the first match is already in the library, the Add New Compound dialog box opens.



12. (Optional) Do the following:

- 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



- In the Type of Compound To Add list, select a compound type.
- Click **OK**.

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

For detailed descriptions of all the features on the Detection page, see [“Editing the Compounds Page”](#) on page 150.


14. Click **Acquisition** in the navigation pane.

The Acquisition page for the method opens. For detailed descriptions of all the features on the Acquisition page, see [“Acquisition Page for a Quantitation Method”](#) on page 140.

15. From the Instrument Method list, select an instrument method.
16. To save the new method, choose **File > Save** from the main menu and name the method.

For a detailed description of how to modify the parameters in a master method, see “[Editing a Master Method](#)” on [page 135](#).



This animation shows how to create a new quantitation method by associating a raw data file. To view the animation, click , and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.

Selecting Compounds from the Compound Database

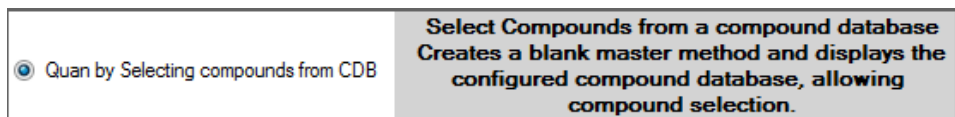
You can select compounds from the compound database to create a new master method.

❖ To select compounds from the compound database

1. Choose **File > New > Master Method** from the main menu.

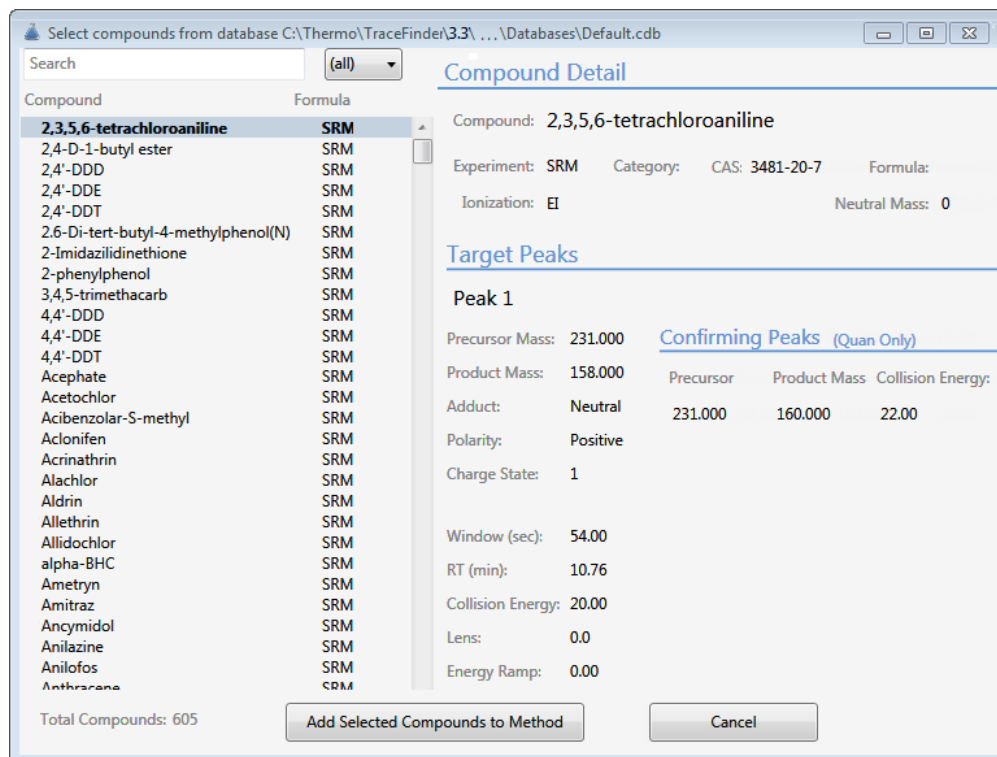
The Create Master Method dialog box opens. To view all available ways to create a master method, see “[Create Master Method dialog box](#)” on [page 117](#).

2. Select the **Quan by Selecting Compounds from CDB** option and click **OK**.



The Select Compounds from Database dialog box opens, listing all the compounds defined in the compound database. See [Select Compounds from Database dialog box](#).

Figure 32. Select Compounds from Database dialog box




3. Select the check box for each of the compounds that you want to add to the method.
4. To select all compounds in the database, select the **Compound** check box at the top of the list.
5. Click **Apply**.
6. Click **Acquisition** in the navigation pane.
7. From the Instrument Method list, select an instrument method.
8. To save the new method, choose **File > Save** from the main menu and name the method.

The application adds the selected compounds to the method.

The Acquisition page for the method opens. For detailed descriptions of all the features on the Acquisition page, see [“Acquisition Page for a Quantitation Method”](#) on page 140.

For a detailed description of how to modify a master method, see [“Editing a Master Method”](#) on page 135.



This animation shows how to create a new quantitation method by selecting compounds from the compound database. To view the animation, click , and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.

Editing a Master Method

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

See the instructions for the following tasks:

- [Modifying Retention Times](#)
- [Enabling Auto Reprocessing](#)
- [Editing the Acquisition Page](#)
- [Editing the Processing Page](#)
- [Editing the Compounds Page](#)
- [Editing the QAQC Page](#)
- [Editing the Groups Page](#)
- [Editing the Intelligent Sequencing Page](#)
- [Editing the Library Settings Page](#)
- [Editing the Reports Page](#)

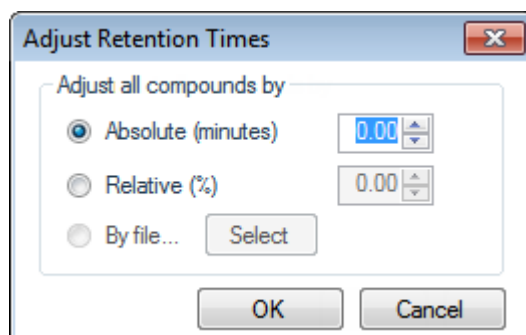
Modifying Retention Times

Use the Adjust Retention Times dialog box from any page in the Method View or Local Method view.

❖ To modify retention times in a method

1. Do one of the following:
 - Choose **Method View > Adjust Retention Times** from the main menu of the Method View in the Method Development mode.
 - Choose **Local Method > Adjust Retention Times** from the main menu of the Local Method view in the Analysis mode.

The Adjust Retention Times dialog box opens.



2. Do one of the following:

- a. Select the **Absolute** option.
- b. Specify a positive or negative value to increase or decrease the expected retention times. (Valid range: -100.00 through 100.00)
- c. Click **OK**.

The application increases or decreases the expected retention times for all compounds in the method by the specified number of minutes.

–or–

- a. Select the **Relative** option.
- b. Specify a positive or negative value to increase or decrease the expected retention times. (Valid range: -100.00 through 100.00)
- c. Click **OK**.

The application increases or decreases the expected retention times for all compounds in the method by the specified percentage.

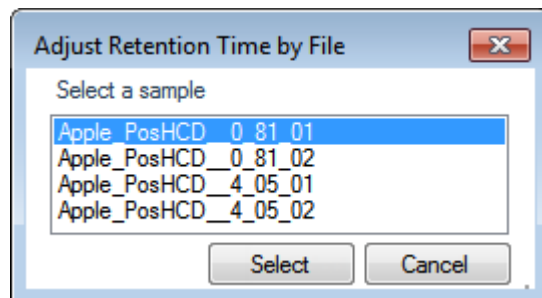
–or–

- a. Select the **By File** option.

Note This option is available only from the Local Method view after you have processed the samples in a batch.

- b. Click **Select**.

The Adjust Retention Time by File dialog box opens, displaying all processed samples.



- c. Select the sample whose retention times you want to use in the method.
- d. Click **Select**.
- e. Click **OK**.

For each detected peak in the selected, processed sample, the application overwrites the retention times for the matching compounds in the method. If the method contains compounds not detected in the selected sample, the retention times for those compounds are not affected.

Enabling Auto Reprocessing

The Auto Reprocess option is displayed in the banner of all TraceFinder application views.

Auto Reprocess (Quan Only)

- When you select this option, the application automatically reprocesses a batch and displays the updated results in Data Review when you make changes to the method or make any manual integration changes.

Note Batch processing can be slower when you use auto reprocessing.

- When you clear this option, the application does not automatically reprocess batches or update the results in Data Review when you make changes to the method or make any manual integration changes. The application simply stores the changes to the method or the manual integration. The application updates the Data Review results only when you manually reprocess the batch.

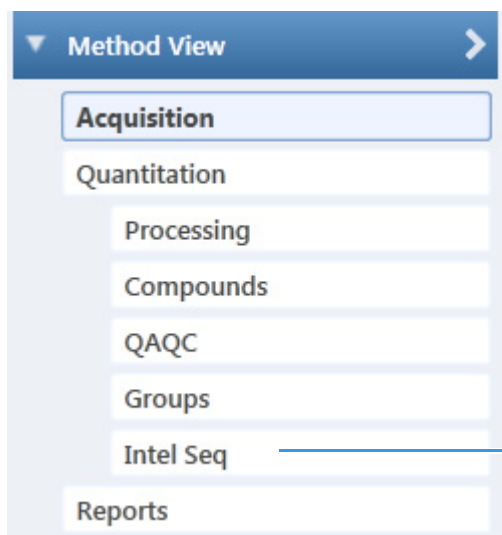
Editing the Acquisition Page

The Acquisition page defines basic information about the master method. For detailed descriptions of all the features, see “[Acquisition Page for a Quantitation Method](#)” on [page 140](#).

Follow these procedures:

- [To open the Acquisition page](#)
 - [To specify Acquisition information for a master method](#)
 - [To edit an instrument method](#)
- ❖ **To open the Acquisition page**

Click **Acquisition** in the Method View navigation pane.



Available only when you activate the Intelligent Sequencing option in the Configuration console

❖ To specify Acquisition information for a master method

1. In the Lab Name box, type the name to be displayed at 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 an injection volume (between **0.1** and **2000** μL) to be used for sample injection.

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

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

4. From the Mass Precision box, select a precision value (between **2** and **6** inclusive) as the number of decimal places to be used in reports and in peak and spectrum displays.
5. From the Ion Range Calc Method list, select a method for calculating the ion ratio range windows.

When you select Level, the application displays a Use Level list where you can choose a calibration level. To define the available calibration levels on the Compounds page, see “[Editing the Compounds Page](#)” on [page 150](#).




Ion range calc method:

Use level:

❖ To edit an instrument method

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

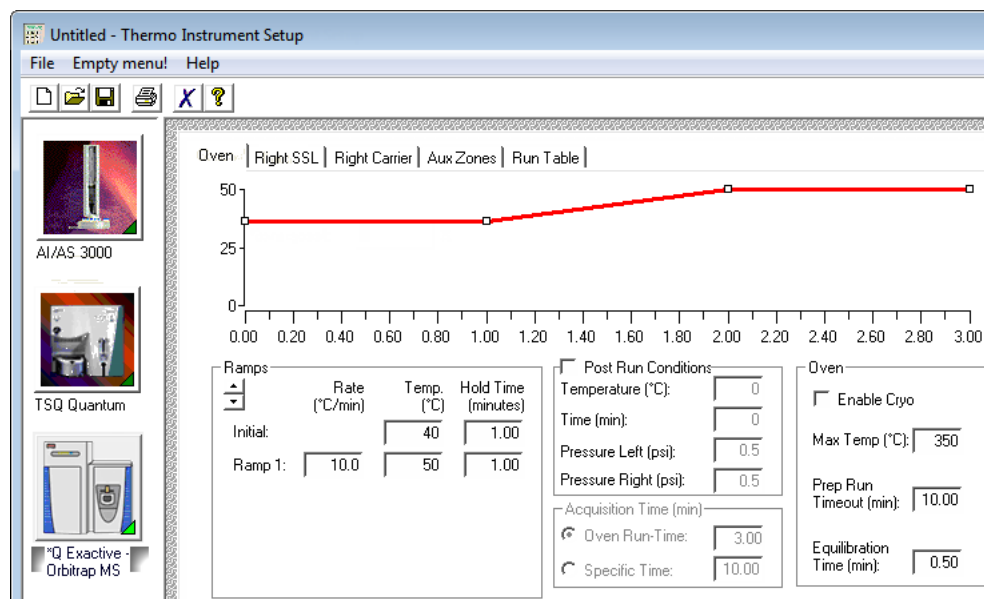


Instrument method:

2. To edit the selected instrument method, click **Edit**.

The Thermo Instrument Setup window opens. This example of an instrument setup shows multiple configured instruments. (See [Thermo Instrument Setup window](#).)

Figure 33. Thermo Instrument Setup window

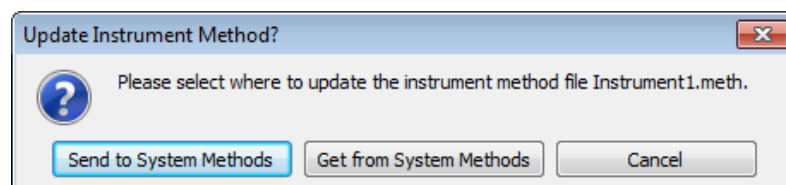


3. Edit the values on the instrument page for your instrument.
4. From the main menu in the Thermo Instrument Setup window, choose **File > Save** and then choose **File > Exit**.

The application returns you to the Acquisition page. See [Acquisition Page for a Quantitation Method](#).

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 System Methods:** Overwrites the instrument method in the C:\TraceFinderData\3.3\Methods folder with the current instrument method.
 - **Get from System Method:** Overwrites the current instrument method with the instrument method in the C:\TraceFinderData\3.3\Methods folder.
 - **Cancel:** Makes no changes to the instrument method in the current master method.

Acquisition Page for a Quantitation Method

Use the features on the Acquisition page to define basic information about the master method.

Figure 34. Acquisition page for a quantitation method

Table 18. Acquisition page parameters (Sheet 1 of 2)

Parameter	Description
Lab Name	Specifies the laboratory name to be displayed at the top of each printed, saved, or exported report. Default: Default Laboratory To specify this default laboratory name, see “Specifying Application Defaults” on page 37 .
Assay Type	Specifies 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).
Injection Volume	Specifies 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. Valid range: 0.1 through 2000 μL

Table 18. Acquisition page parameters (Sheet 2 of 2)

Parameter	Description
Mass Precision	Specifies the number of decimal places used in reports and in peak and spectrum displays. Valid range: Integers from 2 through 6, inclusive.
Ion Range Calc Method	Specifies the selected ion range calc method used 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 150.
Instrument Method	Specifies the instrument method used for acquiring samples.
Edit	Opens the Thermo Xcalibur Instrument Setup window where you can edit the instrument method.
Update	Specifies one of the following: Send to System Methods: Overwrites the system method in the C:\TraceFinderData\3.3\Methods folder with the current instrument method. Get from System Methods: Overwrites the current instrument method with the system method in the C:\TraceFinderData\3.3\Methods folder.

Editing the Processing Page

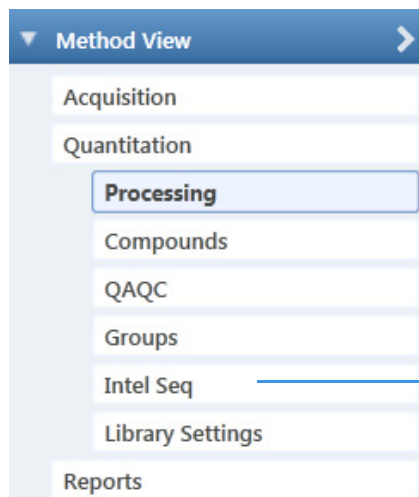
The Quantitation – Processing page defines basic information about the master method. For detailed descriptions of all the features, see [“Processing Page for a Quantitation Method”](#) on page 147.

Follow these procedures:

- [To set automated background subtraction options](#)
- [To set automated background subtraction options](#)
- [To specify mass tolerance](#)
- [To include data-dependent filters](#)
- [To specify a threshold override](#)
- [To specify qualitative peak processing parameters](#)
- [To specify library selection](#)
- [To add unknown screening to the method](#)

❖ **To open the Processing page**

Click **Processing** in the Method View navigation pane.



Available only when you activate the Intelligent Sequencing option in the Configuration console

❖ **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 after the apex of the peak.
 - **Both Sides of Peak:** Subtracts a specified number of scans from each side of the apex of the peak.

When you create a reference spectrum with background subtraction, the application uses the selected method to conduct background subtraction of peak spectra during quantitative processing. The application then reports the background-subtracted reference spectrum (indicated with BS in the scan heading) as the last scan for each compound in the Quantitation Report - 2 report. It does not use background subtraction with qualitative processing.

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

The application subtracts this number of scans from the background after averaging. When you select the Both Sides of Peak option, the application subtracts this number of scans from **each** side of the peak.

3. In the Steppoff Value box, enter a number.

The application uses this offset value to average and subtract scans that are not adjacent to the apex of the peak, as in this example:

Background subtraction range option:

Number of scans to subtract:

Steppoff value:

Before Peak example:

When the Number of Scans to Subtract equals 3 and the Steppoff Value equals 5, the 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.

After Peak example:

When the Number of Scans to Subtract equals 3 and the Steppoff Value equals 5, the application ignores the first 5 scans to the right of the peak and applies the averaging and subtraction to the 6th, 7th, and 8th scans to the right of the peak.

Both Sides of Peak example:

When the Number of Scans to Subtract equals 3 and the Steppoff Value equals 5, the application ignores the first 5 scans to the left of the peak and the first 5 scans to the right of the peak. Then it applies the averaging and subtraction to both the 6th, 7th, and 8th scans to the left of the peak and the 6th, 7th, and 8th scans to the right of the peak.

❖ To specify mass tolerance

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

The application applies this mass tolerance to the extracted chromatograms.

❖ To include data-dependent filters

Select the **Include Data Dependent Filters** option.

The application includes data-dependent filters when you specify filters in the method. See “Signal” on page 168.

Data-dependent filters are indicated with a “d”.

Filter:

— Data-dependent filter

When you process a sample using a data-dependent filter, 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 MSⁿ scan.

❖ To specify a threshold override

To set a threshold override and include only peaks with areas above this designated threshold, do the following:

- a. Select the **Threshold Override** check box.
- b. In the associated box, type the threshold as an area value.

This threshold overrides the Response Threshold value set in the compound database. The application ignores the peaks with areas below your specified threshold.

❖ To specify qualitative peak processing parameters

1. 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 application uses the Enable Peak Threshold filter to determine which peaks meet the specified percentage of the height or area of the largest peak.

2. 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.
3. 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 that you specify. For additional information about the Genesis algorithm, see [“Genesis Detection Method”](#) on page 43.

4. Select or clear the **Exclude Matching Quan Peaks** check box and specify a value for the exclusion window.

The application excludes quantitative peaks in a range plus or minus the value that you specify.

5. 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 MSⁿ scan.

This option constrains the Data Review to only data-dependent scan spectra.

In addition to the peak information, the TIC Report and TIC Summary Report display information about the data-dependent filtered data.

- To indicate whether to select peaks above a minimum percentage of the nearest internal standard peak that results in compound selection, select the **Enable ISTD Threshold** check box and specify a minimum percentage.

To consider a peak for a processing method, the application uses the Enable ISTD Threshold filter to determine which peaks meet the specified percentage of the height of the nearest internal standard peak.

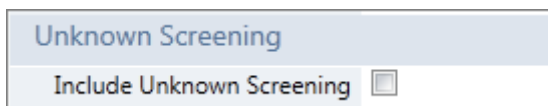
When you select the Enable ISTD Threshold parameter, the method ignores values set for the Enable Peak Threshold parameter in the method template.

Note When you create a method with the Method Forge, the application ignores the parameters in the Qualitative Peak Processing area.

❖ To specify library selection

- In the Use these Libraries box, select the libraries that you want to search.
All libraries loaded on your instrument are displayed in the Use these Libraries box.
- To limit the number of matches returned when the system searches a spectrum against the selected libraries, set a value in the Limit Library Hits box.
- To specify how to sort the library searches, select a value from the Best Match Method list.

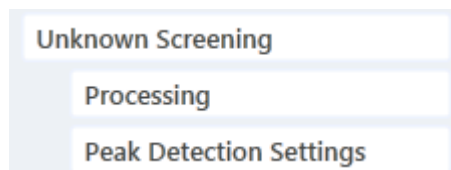
❖ To add unknown screening to the method



IMPORTANT The Include Unknown Screening check box is available only when you select the Allow Unknown Screening option in the application configuration console. See “[Processing Options](#)” on [page 62](#).

- Select the **Include Unknown Screening** check box.

The application adds the Unknown Screening features to the Method View navigation pane.



- To specify unknown screening settings for peaks, libraries, databases, elements, and ChemSpider™ searches, click **Processing**.

For further instructions, see “[Editing the Processing Pages](#)” on [page 311](#).

5 Using the Method Development Mode for Quantitation Methods


Editing a Master Method

3. To specify unknown screening peak detection settings, click **Peak Detection Settings**.

For further instructions, see [“Editing the Peak Detection Settings Page”](#) on page 334.

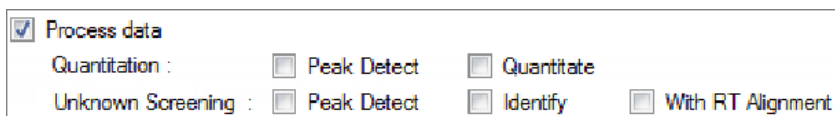
The application indicates that a quantitation method includes unknown screening features in the following locations:

- In the Batch View in the Analysis mode, when you create a batch using a quantitation method, the title bar indicates that the method includes unknown screening features.



Batch View - Batch_X [Quan with Unknown]

- In the Analysis navigation pane, the application displays access to local methods for both quantitation and unknown screening.
- In the Submit Options dialog box, when you submit a batch, the Process Data area shows all available process data for the batch.



<input checked="" type="checkbox"/> Process data				
Quantitation :	<input type="checkbox"/> Peak Detect	<input type="checkbox"/> Quantitate		
Unknown Screening :	<input type="checkbox"/> Peak Detect	<input type="checkbox"/> Identify	<input type="checkbox"/> With RT Alignment	

You can select the detection options for each processing method that you want to use when you submit the batch.

Processing Page for a Quantitation Method

Use the features on the Processing page to define basic information about the master method.

Figure 35. Processing page for a quantitation method

Table 19. Processing page parameters (Sheet 1 of 3)

Parameter	Description
Background Subtraction Range Option	Specifies the range used for background subtraction. Valid values: None, Before Peak, After Peak, Both Sides of Peak Default: None

Table 19. Processing page parameters (Sheet 2 of 3)

Parameter	Description
Number of Scans To Subtract	Valid values: Even numbered integers Default: 0
Stepoff Value	Offset from the selected peak to the first subtracted peak.
Mass Tolerance	Specifies the upper limit of MMU or PPM. Default: 500 Valid range: 0.1 through 50 000 <ul style="list-style-type: none"> • (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.
Include Data Dependent Filters	Specifies that the method includes data-dependent filters. Available only for quantitation methods.
Threshold Override	Overrides the Response Threshold value set in the compound database. The application ignores the peaks with areas below this specified threshold. Valid range: 1000 through 1 000 000 000 Default: 5000
Qualitative Peak Processing	
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.
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.
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 that you specify.
Use Data Dependent Scans	Constrains the Data Review to only data-dependent scan spectra. In addition to the peak information, the TIC Report and TIC Summary Report display information about the data-dependent filtered data.

Table 19. Processing page parameters (Sheet 3 of 3)

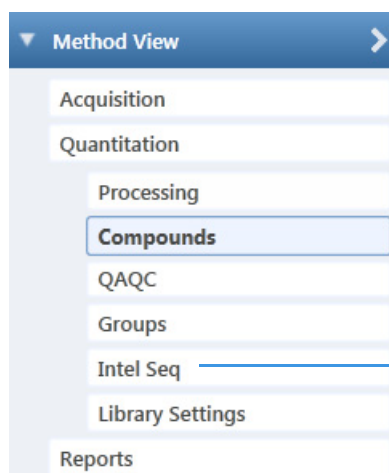
Parameter	Description
Enable ISTD Threshold	Specifies that, when identifying a peak, qualitative peak processing use the minimum threshold specified as a percentage of the nearest internal standard peak, rather than the threshold specified in the Enable Peak Threshold parameter in the method template.
% of Internal Standard	Percentage of the nearest internal standard peak to use as the minimum threshold for identifying a peak.
Library Selection	Specifies the libraries to use for qualitative peak processing.
Limit Library Hits	Specifies the number of matches 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
Unknown Screening	
Include Unknown Screening	Adds unknown screening features to the quantitation method.

Editing the Compounds Page

Use the Compounds page to set all parameters for identifying, detecting, and quantifying the target compound list.

❖ To open the Compounds page

Click **Compounds** in the Method View navigation pane.



Available only when you activate the Intelligent Sequencing option in the Configuration console

From the Compounds page of the Method View, you can access the following pages:

Acquisition List	See also Acquisition List page .
Identification	See also Identification page .
Detection	See also Detection .
Calibration	See also Calibration page .
Calibration Levels	See also Calibration Levels page .
Chk Std Levels	See also Chk Std Levels page .
Real Time Viewer	See also Real Time Viewer page parameters .


Each page on the Compounds page (except the Acquisition List and Real Time Viewer pages) uses a right-click shortcut menu. See “[Using the Shortcut Menu Commands](#)” on [page 212](#).

Acquisition List

The Acquisition List page displays all compounds defined for the current method in a display similar to the Compound Database view. From the Acquisition List page, you can add additional compounds from the Compound Database or delete compounds from the method. See [Acquisition List page](#).

For detailed descriptions of all the features in the Compound Database views, see “[Working with the Compound Database](#)” on [page 74](#).

❖ To remove a compound from the method

1. Select the compound in the Compound list.
2. Click the **Remove Compound** icon, .
3. To confirm that you want to delete the selected compound, at the prompt, click **OK**.

The application removes the selected compound and all its peak information.

4. To remove multiple compounds, use the CTRL or SHIFT keys.

The application confirms that you want to remove the selected compounds.

❖ To add a compound to the method

1. Click the **Add Compound from Compound Database** icon, .

The Select Compounds from Database dialog box opens, listing all the compounds defined in the compound database. This dialog box is identical to the Compound Database with the exception that you cannot edit the compound data from here; you can only choose which compounds you want to include in your method.

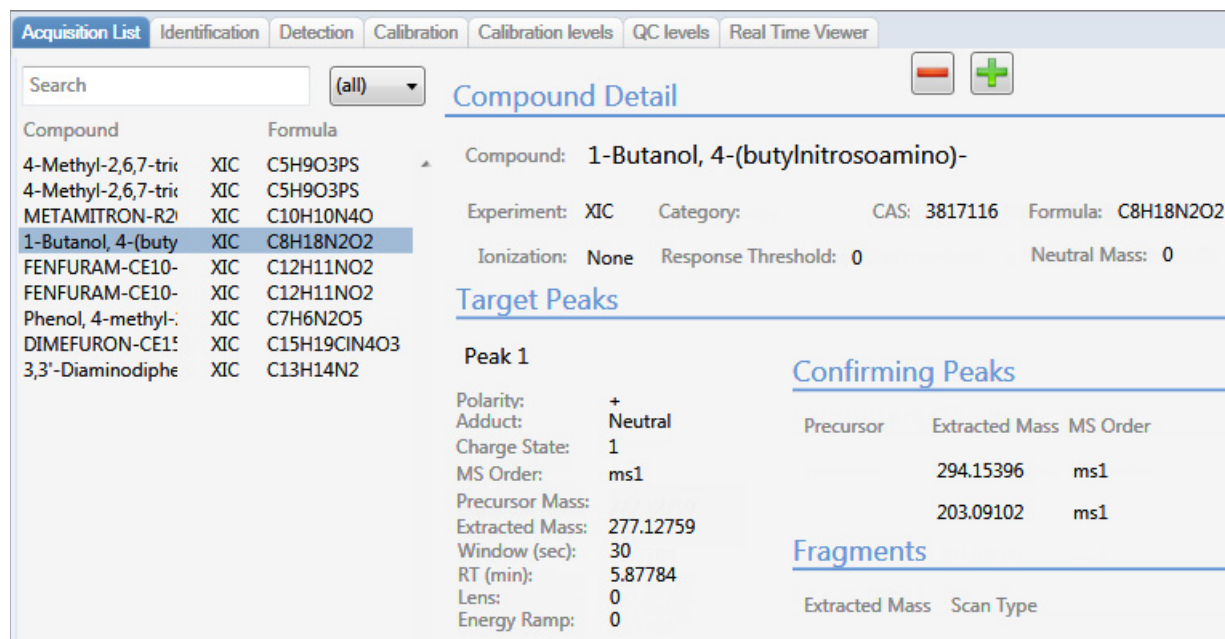
2. Select the compounds to add to the method.

You can use the SHIFT or CTRL keys to select multiple compounds.

3. Click **Add Selected Compounds to Method**.

The application adds the selected compounds to the acquisition list for the method.

Figure 36. Acquisition List page



Compound	XIC	Formula
4-Methyl-2,6,7-tric	XIC	C5H9O3PS
4-Methyl-2,6,7-tric	XIC	C5H9O3PS
METAMITRON-R2	XIC	C10H10N4O
1-Butanol, 4-(buty	XIC	C8H18N2O2
FENFURAM-CE10-	XIC	C12H11NO2
FENFURAM-CE10-	XIC	C12H11NO2
Phenol, 4-methyl-	XIC	C7H6N2O5
DIMEFURON-CE1!	XIC	C15H19CIN4O3
3,3'-Diaminodiphe	XIC	C13H14N2

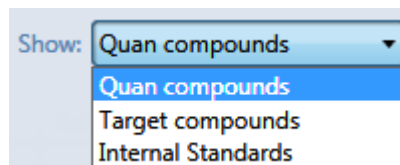
Compound Detail			
Compound: 1-Butanol, 4-(butylnitrosoamino)-			
Experiment:	XIC	Category:	CAS: 3817116
Formula:	C8H18N2O2	Ionization:	None
Response Threshold:	0	Neutral Mass:	0
Target Peaks			
Peak 1			
Polarity:	+		
Adduct:	Neutral		
Charge State:	1		
MS Order:	ms1		
Precursor Mass:			
Extracted Mass:	277.12759		
Window (sec):	30		
RT (min):	5.87784		
Lens:	0		
Energy Ramp:	0		
Confirming Peaks			
Precursor	Extracted Mass	MS Order	
	294.15396	ms1	
	203.09102	ms1	
Fragments			
Extracted Mass	Scan Type		

Identification

The Identification page lists the compounds that are targeted for analysis, reporting, and other compound-specific values. For descriptions of all values on the Identification page, see [“Identification Page.”](#)

❖ To filter the displayed compounds

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



Compound type	Description
Quan Compounds	Displays only quantitation compounds, such as target compounds and internal standards.
Target Compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.

Identification Page

Use the features on the Identification page to display all compounds targeted by the method.

Figure 37. Identification page

Acquisition List Identification Detection Calibration Calibration levels QC levels Real Time Viewer								
	RT	Compound	Compound type	Active	CAS No	LIMS ID	Use as RT Reference	Reference compound
1	3.14	Propanenitrile	Target Compound	<input checked="" type="checkbox"/>	107120		<input type="checkbox"/>	
2	3.15	Pyrazinamide	Target Compound	<input checked="" type="checkbox"/>	98964		<input type="checkbox"/>	
3	3.67	1,3-Dioxolane, 2-...	Target Compound	<input checked="" type="checkbox"/>	4359573		<input type="checkbox"/>	

Table 20. Identification 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. The application uses the RT and Window values to determine the start and stop time for the acquisition. Valid range: 0.00 through 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 through 999.00
Compound	A list of identified compounds. To customize the compound names, click the cell and type a new name. To display a filtered list of compounds, use the Show list.
Compound Type	Displays the compound types as Target Compound or Internal Standard. The application uses target compounds and internal standards 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 the Batch View and Data Review view in the Analysis mode.
CAS No	The Chemical Abstract Service (CAS) number that the application matched with each compound. To change or add a number, click the CAS No cell and enter a new number.
LIMS ID	Laboratory Information Management System identification number.
Use as RT Reference	When performing peak detection with retention time standards, the application first identifies those compounds identified as retention time standards and then uses their observed retention times to adjust any associated target compound.
Reference Compound	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.
Shortcut menu	The Identification page uses a right-click shortcut menu. See “Using the Shortcut Menu Commands” on page 212.

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	See also Times page parameters .
Signal	See also Signal page parameters .
Detect	See also Detect page parameters for Genesis . See also Detect page parameters for ICIS . See also Detect page parameters for Avalon .
Suitability	See also System Suitability dialog box parameters .
Spectrum	See also Spectrum page shortcut menu commands .
Library	See also Library page parameters .
Isotopes	See also Isotopes page parameters .
Fragments	See also Fragments page parameters .
Ratios	See also Ratios page parameters .

On the Detection page (see “[Detection page](#)” on [page 165](#)), 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 quantitative peak, mass range, or confirming ion peak. The application automatically uses the first match it finds as the compound name, the base peak of the mass spectrum as the quantitative peak, and the second and third largest ions as the confirming ion peaks.

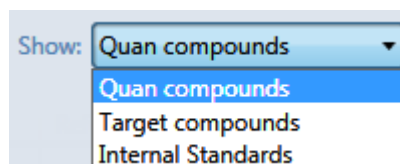
Follow these procedures:

- [To filter the displayed compounds](#)
- [To change the displayed information for detected peaks](#)
- [To add compounds to the method](#)
- [To change the compound reference spectrum](#)
- [To replace a quantitation mass](#)
- [To add a mass to the existing quantitation mass ranges](#)
- [To add a quantitative peak](#)
- [To add a spectral peak as a new compound](#)
- [To replace a quantitative peak with a confirming ion peak](#)
- [To set a confirming ion peak as an additional quantitative peak](#)
- [To add a trace to the Real Time Status pane](#)
- [To replace a confirming ion peak](#)

- To add a mass as a new confirming ion peak
- To use the cut-and-paste feature on confirming ion peaks
- To save the new method

❖ To filter the displayed compounds

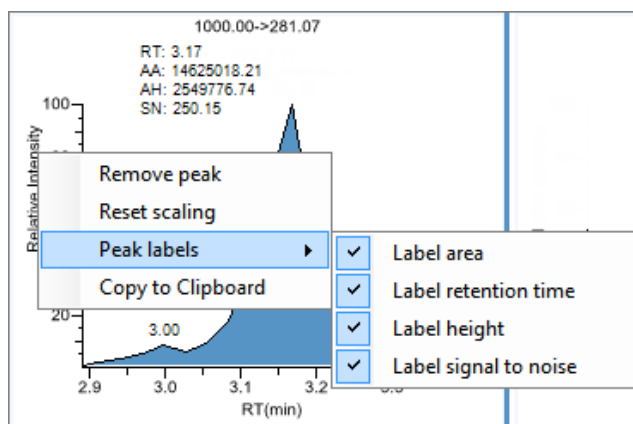
From the Show list, select the type of compounds that you want to display in the compounds list.



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

❖ To change the displayed information for detected peaks

1. Right-click the chromatogram plot for any of the quan or confirming peaks and hold the cursor over **Peak Labels**.
2. Choose to display labels for the peak area, peak retention time, peak height, or signal-to-noise.



3. To remove a label, choose the label type again and clear it.

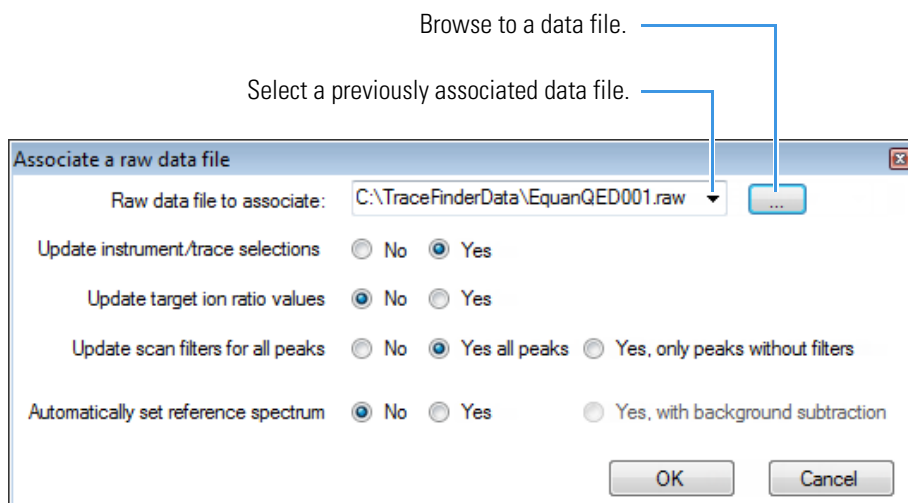
The application globally applies these label settings to all quantitative peaks, confirming peaks, and internal standard peaks in the method.

❖ **To add compounds to the method**

Tip You can add compounds from the current raw data file (begin at [step 7](#)), or you can associate another raw data file and add compounds from that file (begin at [step 1](#)).

1. From the main menu, choose **Method View > 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 (or click the arrow and select from the list of previously associated raw data files) and open the file.

To assure that this raw data file is always available to the method (for example, if you move the method to another system), the application saves the file in the Methods folder:

...\TraceFinderData\3.3\Methods*Methodname*

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–

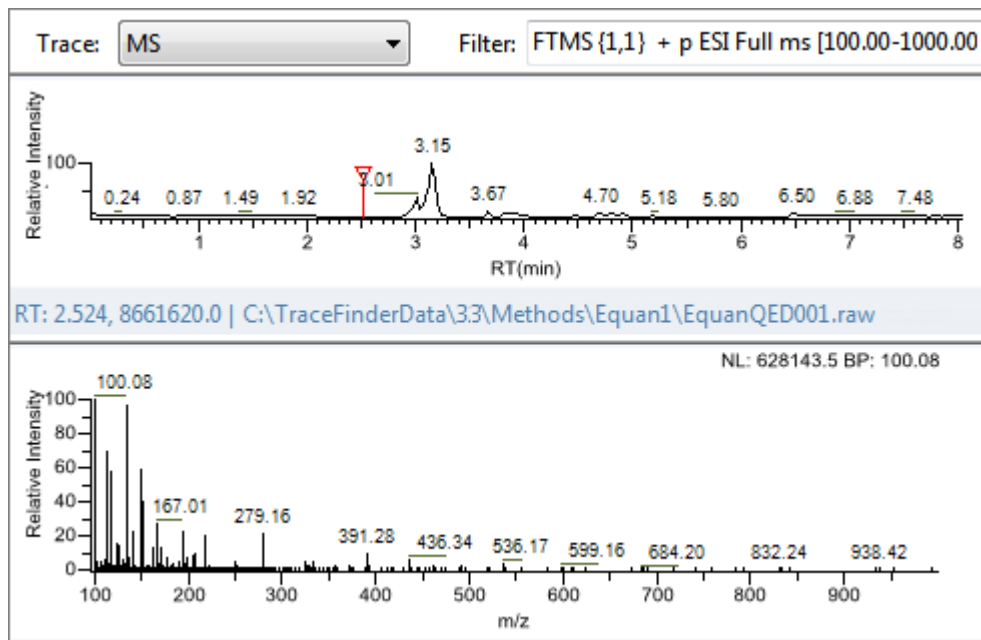
Select the **Yes, with Background Subtraction** option.

The application uses the background-subtracted reference spectrum during quantitative processing and reports the background-subtracted reference spectrum (indicated with BS in the scan heading) as the last scan for each compound in the Quantitation Report - 2 report.

Note This option is available only when you select a background subtraction method on the Acquisition page in the master method. See [“Editing the Acquisition Page”](#) on [page 137](#).

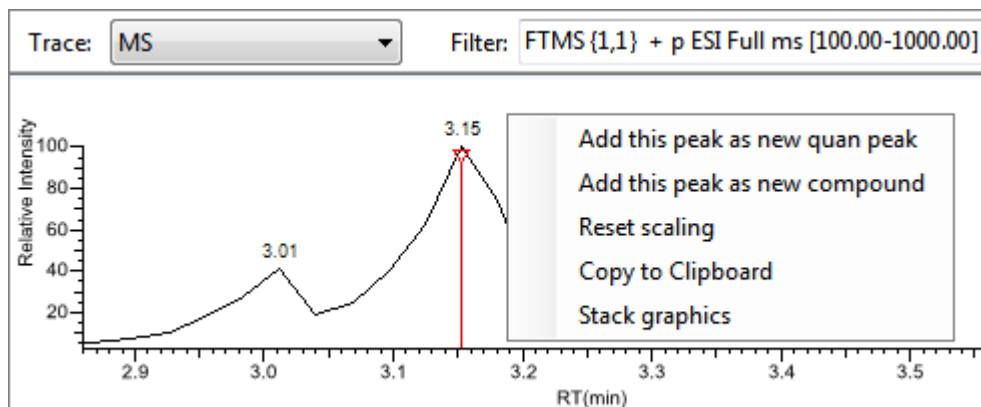
6. Click **OK**.

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



IMPORTANT While the spectra pane displays the associated raw data file, you cannot display peak information for an original compound in the Compound list. You can display peak information only for compounds in the associated raw data file. To return the display functionality for all compounds in the method, save the method.

7. Select a filter from the Filter list.
8. Click to select the peak in the chromatogram that represents the compound that you want to add to the method.
9. Right-click and choose **Add This Peak as New Compound** from the shortcut menu.



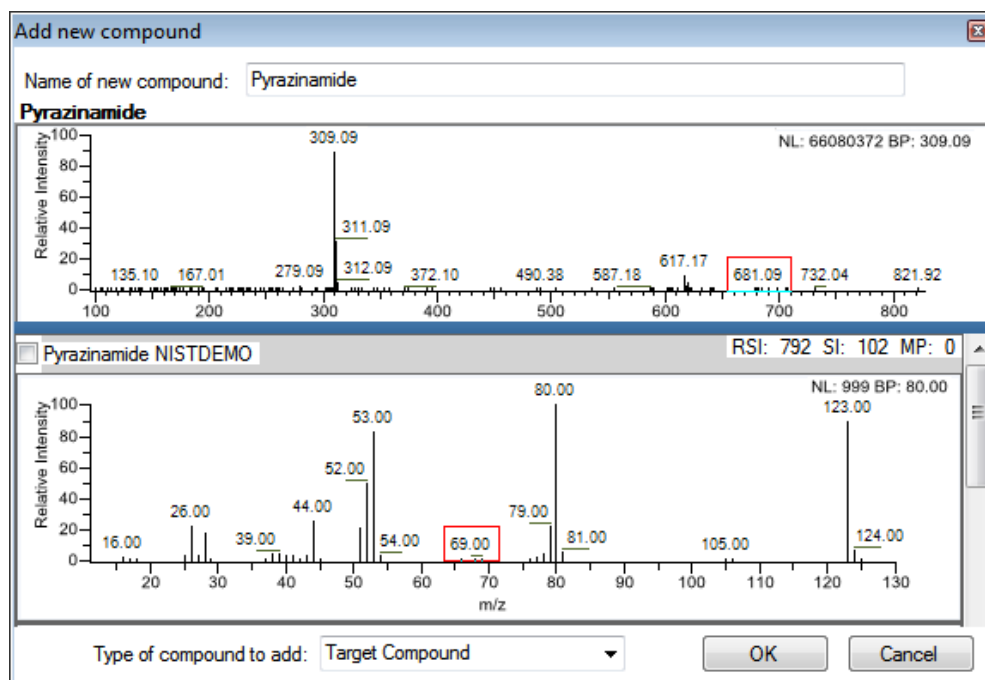
5 Using the Method Development Mode for Quantitation Methods

Editing a Master Method

The 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 quantitative peak, and the second and third largest ions as the confirming ion peaks.

- When the name of the first match does not exist in the method, the application adds this compound to the method and displays the name in the Compound list. You can now view and edit the parameters for this compound.
- When the name of the first match is already in the method, the Add New Compound dialog box opens (see [Add New Compound dialog box](#)). You cannot overwrite a compound name in the method. If the selected peak already exists in the method, you must give it a new name to add it to the method. Or, you can select a different compound to add to the method, following [step 10](#) through step 12.


Figure 38. Add New Compound dialog box



10. Do one of the following:

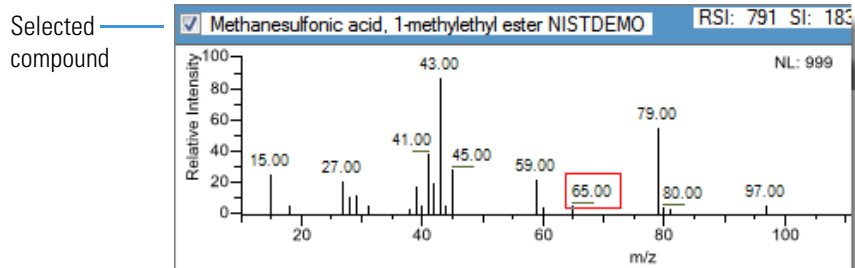
- Type a new name for the first matched compound.

The application displays a red warning when the selected compound name already exists in the method. You cannot overwrite the compound name, and you cannot create a duplicate name in the method. You must type a unique name.

Name of new compound: 

—or—

- To use a compound other than the first matched compound, scroll to the spectrum for that compound and select its corresponding check box in the title bar of the spectrum pane.



- In the Type of Compound To Add list, select a compound type.
- Click **OK**.

❖ To change the compound reference spectrum

- In the chromatogram pane, click a peak.

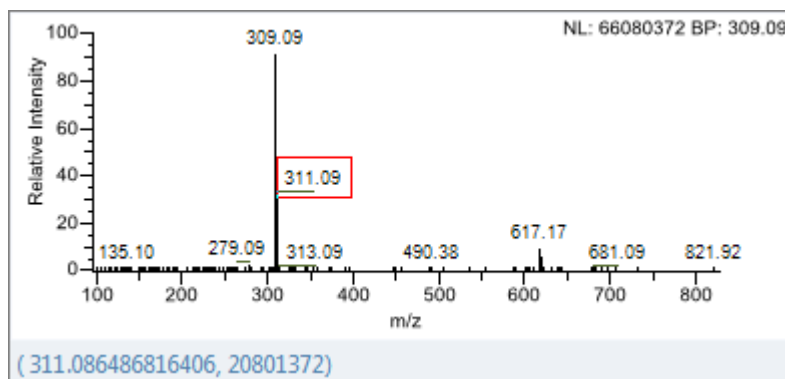
The application displays the spectrum for the selected peak in the spectrum pane.

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

❖ To replace a quantitation mass

- Click the data pane for the quantitation mass that you want to replace.
- In the spectrum pane, hold the cursor over a peak.

The red box indicates the selected peak.



- Right-click and choose **Set This Spectral Peak as Quan Value** from the shortcut menu.
- 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 ion peaks. See “Ratios” on page 202.

❖ **To add a mass to the existing quantitation mass ranges**

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

The red box indicates the selected peak.

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

The application adds the selected mass to the existing quantitation 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 ion peaks. See “Ratios” on [page 202](#).

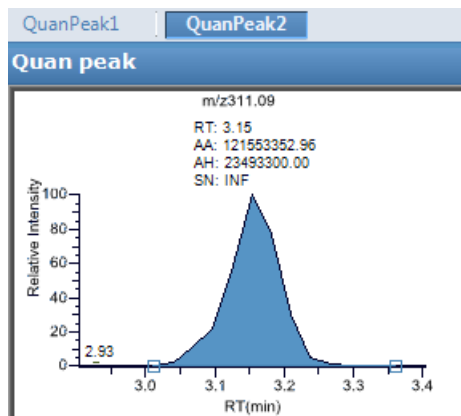
❖ **To add a quantitative peak**

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

The red box indicates the selected peak.

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

The application adds a new quantitative peak to the compound.



You can use the shortcut menu in the spectrum pane for this new quantitative peak to perform any of the tasks that you would perform on the original quantitative peak.

❖ **To add a spectral peak as a new compound**

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

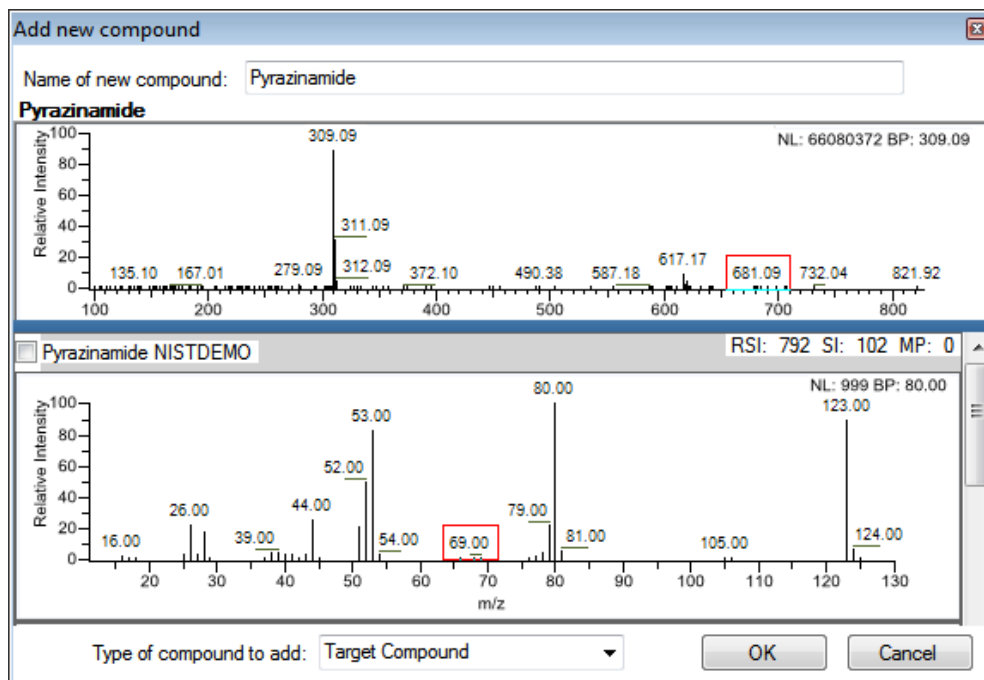
The red box indicates the selected peak.

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

The 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 quantitative peak, and the second and third largest ions as the confirming ion peaks.

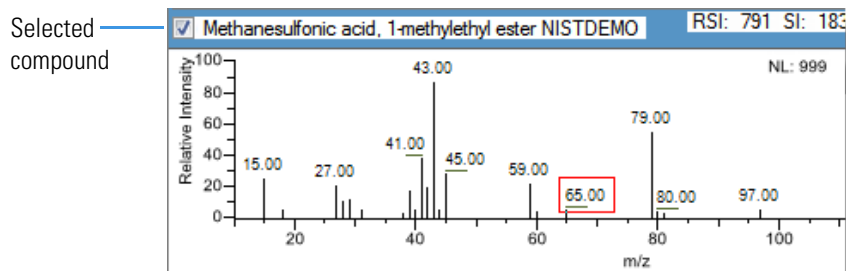
When there are multiple matches, the Add New Compound dialog box opens (see [Add New Compound dialog box](#)). If the name of the first match is already in the library, the dialog box opens with the matching compound selected.

Figure 39. Add New Compound dialog box



3. (Optional) Make any of the following changes:

- Change the name for the compound in the Name of New Compound box.
- Use a compound other than the compound chosen by the application by scrolling to the spectrum for that compound and selecting the compound name in the title bar of the spectrum pane.



- In the Type of Compound To Add list, select a compound type.

4. Click **OK**.

❖ **To replace a quantitative peak with a confirming ion peak**

1. When you have multiple quantitative peaks, select the quantitative peak that you want to replace.
2. Right-click the header bar for the confirming ion peak that you want to use as the quantitative peak, and choose **Swap with Quan Peak** from the shortcut menu.

The application swaps the quantitative peak and the confirming ion peak. The application replaces all information for the quantitative peak with information for the confirming ion. This includes the expected retention time that the confirming ion inherited from the original quantitative peak. The original quantitative peak replaces the confirming ion peak. The application recalculates the ratios for all confirming ion peaks.

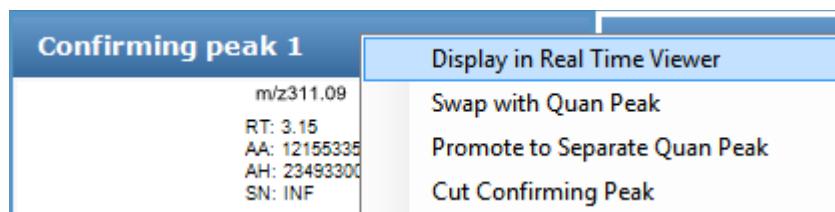
❖ **To set a confirming ion peak as an additional quantitative peak**

Right-click the header bar for the confirming ion peak and choose **Promote to Separate Quan Peak** from the shortcut menu.

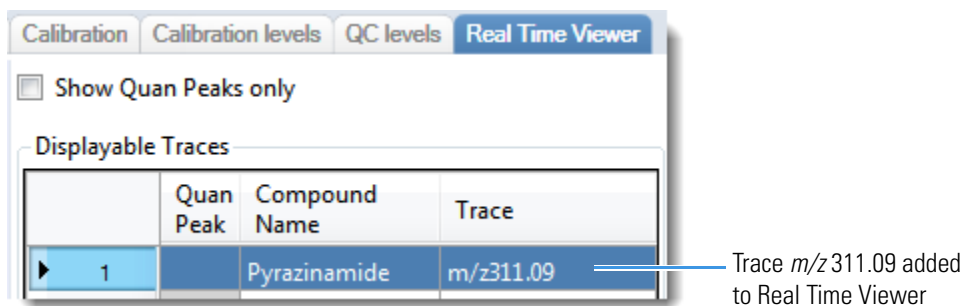
The application creates a new quantitative peak, using information from the confirming ion peak. This includes the expected retention time that the confirming ion peak inherited from the original quantitative peak. The application removes all references to the confirming ion peak from the method.

❖ **To add a trace to the Real Time Status pane**

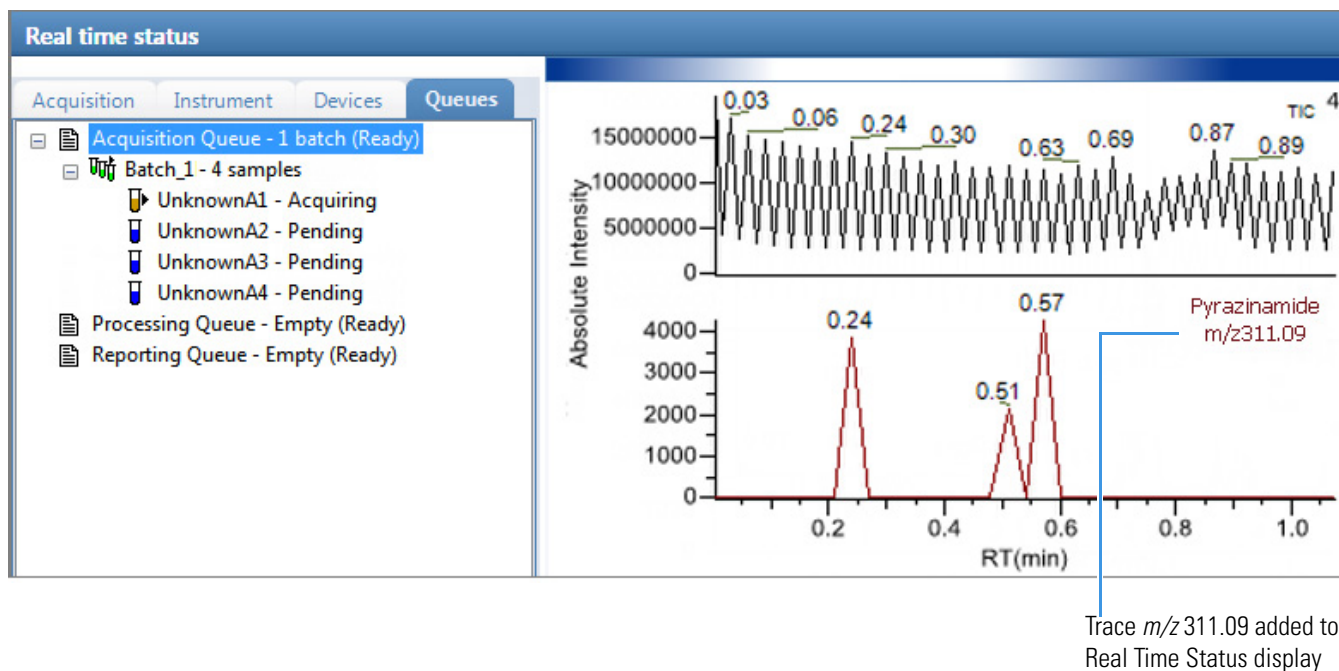
Right-click the header bar for the quantitative peak or confirming ion peak that you want to add to the Real Time Status pane and choose **Display in Real Time Viewer** from the shortcut menu.



The application moves the peak to the Traces To Display in Real Time Viewer pane on the Real Time Viewer page. See “[Real Time Viewer](#)” on page 211.



When you acquire samples with this method, the application displays the m/z 311.09 trace in addition to the TIC in the Real Time Status pane.



❖ To replace a confirming ion peak

1. Click the pane for the confirming ion peak 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 Spectral Peak as Confirming** from the shortcut menu.
The application replaces the confirming ion peak with the selected mass.

❖ To add a mass as a new confirming ion peak

1. In the spectrum pane, hold the cursor over a peak.
The red box indicates the selected peak.
2. Right-click and choose **Add This Spectral Peak as New Confirming** from the shortcut menu.
The application adds the confirming ion peak to the quantitative peak.

QuanPeak1	QuanPeak2
Quan peak	Confirming peak 1
m/z 309.09	m/z 311.09

You can use the shortcut menu in the spectrum pane for this new confirming ion peak to perform any of the tasks that you would perform on the original confirming ion peaks.

❖ To use the cut-and-paste feature on confirming ion peaks

1. Right-click the header bar for the confirming ion peak that you want to remove and choose **Cut Confirming Peak** from the shortcut menu.
2. Right-click the header bar for the confirming ion peak that you want to replace and choose **Paste Confirming Peak** from the shortcut menu.

The application pastes the confirming ion peak that you removed. You can paste a deleted peak back to the quantitative peak from which it was removed, or you can paste the confirming ion peak that was deleted to another quantitative peak for this compound.

❖ To save the new method

1. Choose **File > Save**.

The Save Master Method dialog box opens.

2. Type a new name for the master method and click **OK**, or select a method name to overwrite and click **Overwrite**.

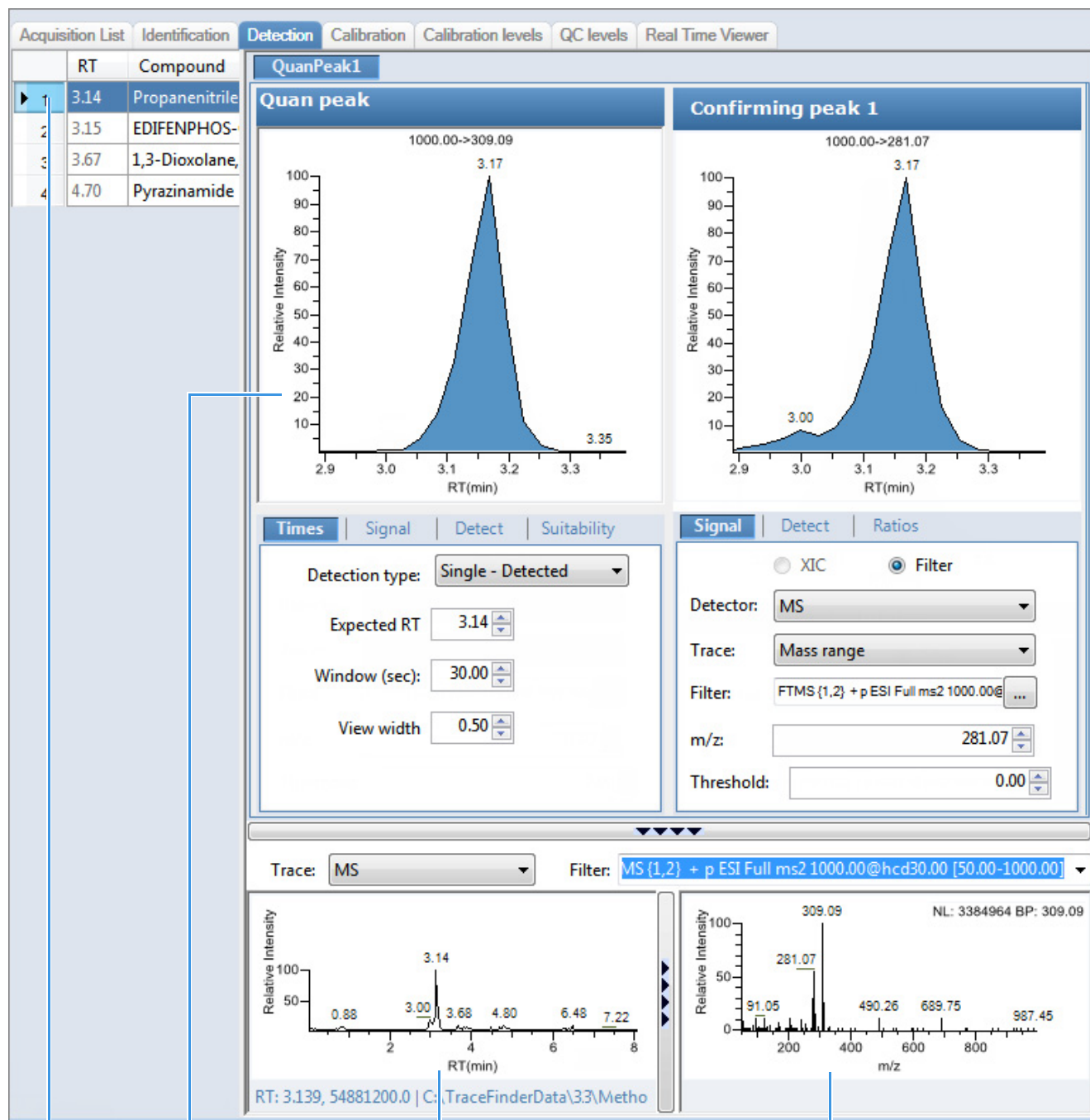
The application saves the new method data in the following folder:

```
...\TraceFinderData\3.3\Methods
```

Detection Page

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

Figure 40. Detection page




Selected compound data

Chromatogram pane

Spectrum pane

Selected compound

Table 21. Detection page panes

Pane	Description
Compound	Lists all compounds in the master method. The Compound list uses a right-click shortcut menu. See “Using the Shortcut Menu Commands” on page 212.
QuanPeak n	Displays a chromatogram for the quantitative peak and its confirming ion peaks. The quantitative peak and confirming peak panes include additional pages for retention time, signal, detection, spectrum, and ratio parameters for the selected compound.
Trace	<p>Displays a combination of the Detector and Trace values used for the raw data file.</p> <p>Do not confuse this Trace parameter with the Trace parameter on the Signal page. This Trace parameter combines both the Detector and Trace values specified on the Signal page. See “Signal page for a mass spectrometer detector” on page 173.</p> <p>Note When you select a detector option other than MS or PDA, the spectrum pane reports “Not Available.”</p>
Filter	Displays the filter used for the raw data file. Available only when you set the Trace parameter to MS.
Reference Chromatogram and Spectra	<p>Displays a reference chromatogram and spectra for the raw data file.</p> <p>When you view an analog trace, there is no spectra display. To close the spectra pane and use the full width to display the chromatogram, click .</p>
Additional pages	
Times	Defines the retention time and window for a quantitative peak. See Times.
Signal	Defines the detector and detection parameters used to display each chromatogram trace. See “Signal” on page 168.
Detect	Defines the peak detection algorithm and its options. See “Detect” on page 176.
Spectrum	Defines a reference mass spectrum for a quantitative peak or compound. See “Spectrum” on page 190.
Ratios	Defines the criteria for evaluating, confirming, or qualifying ions. See “Ratios” on page 202.

Times

Use the features on the Times page to define the expected retention time or a retention time range for a quantitative peak.

Figure 41. Times page

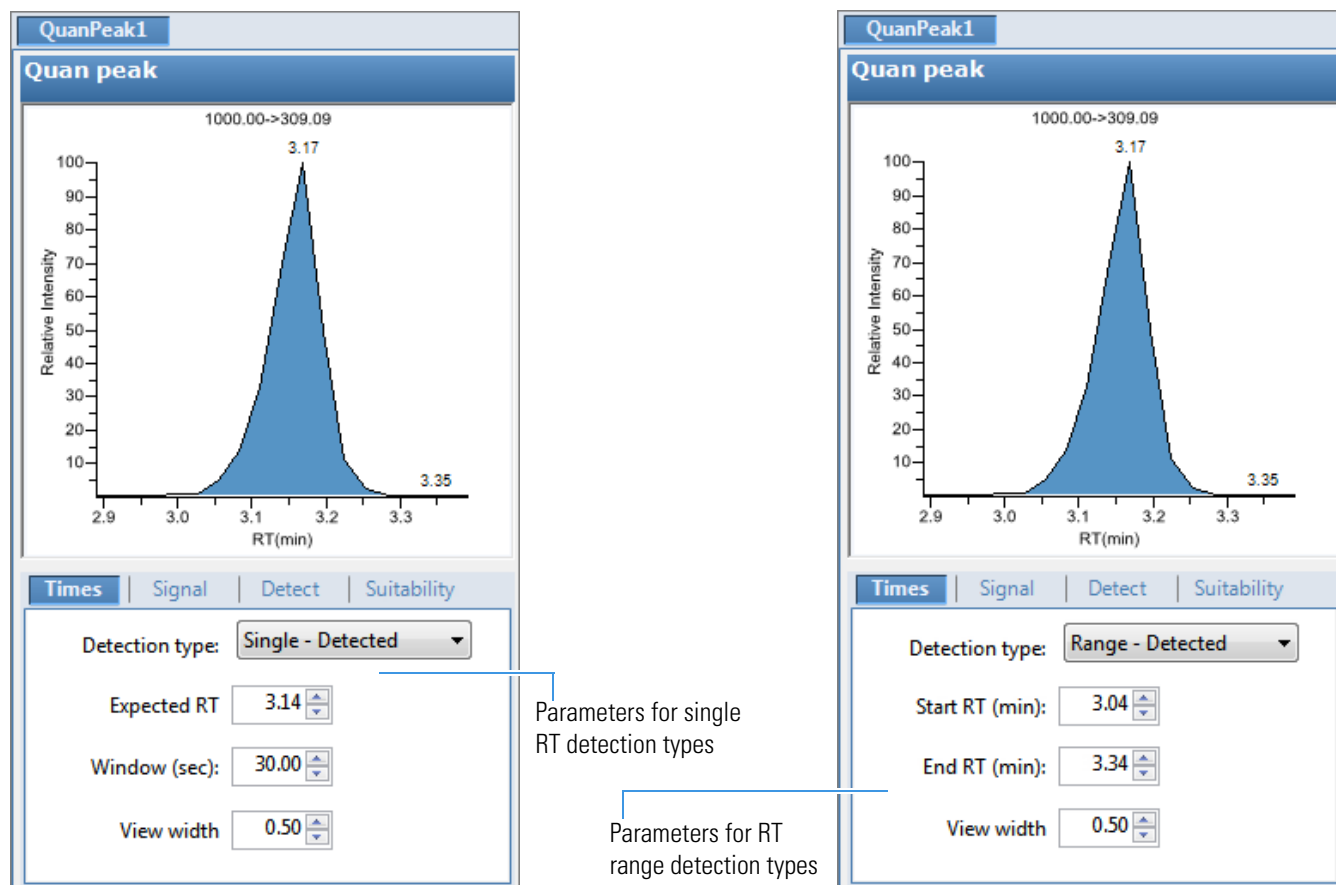


Table 22. Times page parameters (Sheet 1 of 2)

Parameter	Description
Detection Type	<p>Single - Detected: (Default) Specified as a centered retention time window. The application integrates a distinct peak. In reports, the application displays the expected retention time and actual retention time values as Method RT and Detected RT, respectively.</p> <p>Range - Detected: Specified as a retention time start/end range.</p> <p>Range - Integrated: Specified as a retention time start/end range. The application integrates all peaks within the specified time range.</p>
Expected RT (min)	Expected retention time for a single peak. Available only for the Single - Detected detection type.
Window (sec)	Width of the window (in seconds) to indicate how far around the expected retention time the system looks for a peak apex. Available only for the Single - Detected detection type.

Table 22. Times page parameters (Sheet 2 of 2)

Parameter	Description
Start/End RT (min)	Beginning and ending retention time window that can encompass multiple peaks. Available only for the Range - Detected and the Range - Integrated detection types. When you change from a Single - Detected detection type, these values default to the previous beginning and ending time calculated from the Expected RT and Window values.
View Width (min)	Viewable size of the ion chromatogram display. Changing the view width does not affect the peak detection process; the application uses it only for graphical display. When you select either Range - Detected or Range - Integrated as the detection type, you cannot select a View Width value less than the retention time range (<i>end time minus start time</i>).
Shortcut menu	
Set Peak Windows Settings to All Peaks in Compound	Copies the View Width and Window values to all quantitative peaks for the compound and updates the compound. Available only when a compound has multiple quantitative peaks.
Set Peak Windows Settings to All Peaks in Method	Copies the View Width and Window values to all quantitative peaks for the method and updates the method.

Signal

Use the Signal page to define the detector and filters as you display each chromatogram trace. For detailed descriptions of all the features on the Signal page, see “Signal Page” on page 173. The application can use both analog detectors and mass spectrometer detectors. See “Signal page for a mass spectrometer detector” on page 173 or “Signal page for an analog detector” on page 174.

Follow these procedures:

- [To specify ranges of ions for detection and integration](#)
- [To specify an XIC filter](#)
- [To specify an MS filter](#)

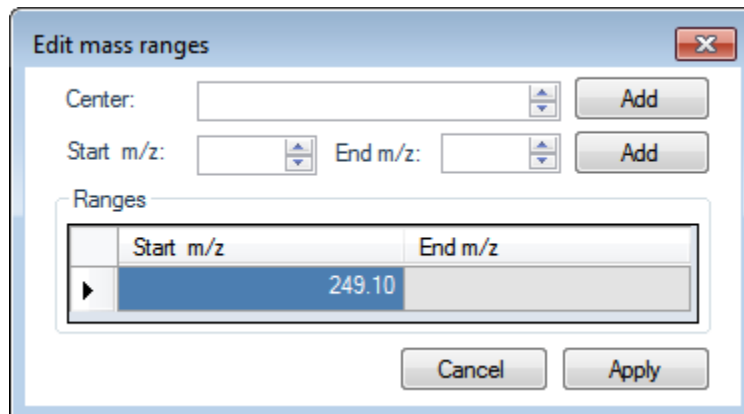
❖ To specify ranges of ions for detection and integration

1. Select **MS** from the Detector list.
2. Select **Mass Range** from the Trace list.
3. In the Ranges area, click **Edit**.

Note The parameters in the Ranges area are available only when you set the Detector parameter to MS and the Trace parameter to Mass Range.

The Edit Mass Ranges dialog box opens where you can define mass ranges using a center of mass value or start and end values.

Figure 42. Edit Mass Ranges dialog box



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

A new row with this value opens under Ranges. Center mass values are listed in the Start m/z column. The application uses a range of one amu that is centered on this value.

5. 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.

6. 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.

7. Click **Apply**.

The application applies the parameters to the list of ranges.

❖ To specify an XIC filter

1. Select **MS** from the Detector list.
2. Select **Mass Range** from the Trace list.
3. Select the **XIC** option.

Note The XIC option is available only when you set the Detector parameter to MS and the Trace parameter to Mass Range.

4. Click the Filter browse button, .

The XIC Filter dialog box opens. See [XIC Filter dialog box](#).

5. Specify your filter options.

6. Click **OK**.

The application updates the chromatogram data using the specified XIC filter options, and the Filter box indicates the parameters of the specified XIC filter, as in this example:

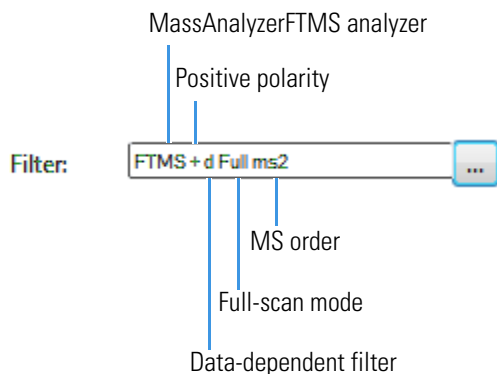


Figure 43. XIC Filter dialog box

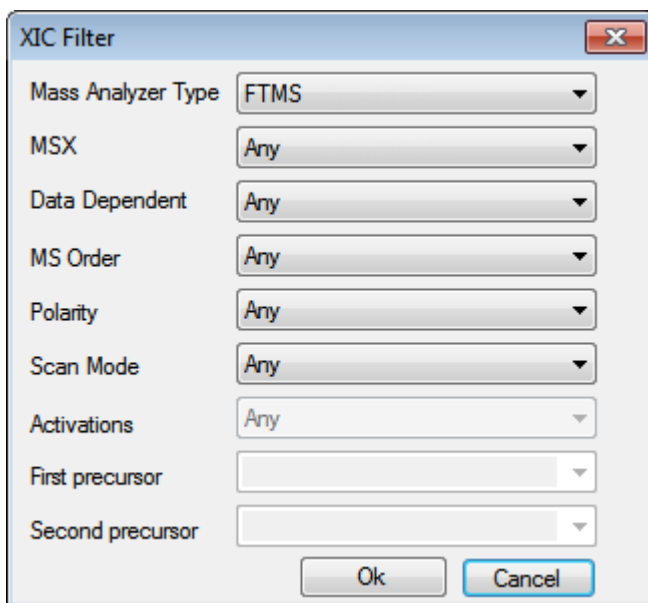


Table 23. XIC Filter dialog box parameters (Sheet 1 of 2)

Parameter	Description
Mass Analyzer Type	Any: Any mass analyzer. FTMS: Fourier Transform Mass Spectrometer ITMS: Ion Trap Mass Spectrometer Sector: Static electric or magnetic sectors, or a combination of the two SQMS: Single Quad Mass Spectrometer TOFMS: Time-of-Flight Mass Spectrometer TQMS: Triple Quad Mass Spectrometer
MSX	Any: Allows both MSX and non-MSX scans. On: Allows only MSX scans. Off: Allows only non-MSX scans.

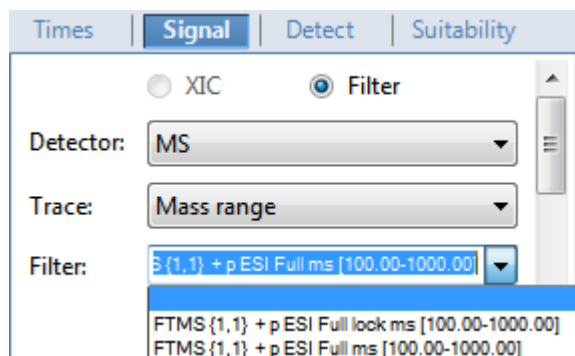
Table 23. XIC Filter dialog box parameters (Sheet 2 of 2)

Parameter	Description
Data Dependent	Any: Allows both data-dependent and non-data-dependent filters. On: Allows only data-dependent filters. Off: Allows only non-data-dependent filters.
MS Order	Any: Allows any MS order. MS: Single mass spec stage MS2-MS3: Multiple mass spec stages
Polarity	Any: Allows both positive and negative. Positive Negative
Scan Mode	Any: Allows any scan mode. Full: Full-scan mode SIM: Selective ion monitoring SRM: Selective reaction monitoring CRM: Consecutive reaction monitoring Q1MS: MS using quadrupole 1 Q3MS: MS using quadrupole 3
Activations	Any: Allows any activation method. CID: Collision-induced dissociation MPD: Multiple photodissociation ECD: Electron capture dissociation PQD: Pulsed dissociation ETD: Electron transfer dissociation HCD: Higher energy collision-induced dissociation This parameter is available only when the MS Order is set to MS2 or MS3 .
First Precursor	This parameter is available only when the MS Order is set to MS2 or MS3 .
Second Precursor	This parameter is available only when the MS Order is set to MS3 .

❖ **To specify an MS filter**

1. Select the **Filter** option.
2. Select **MS** from the Detector list.
3. Select a trace type from the Trace list.

4. Select a filter from the Filter list.



Filter types can be any of the following:

- MS
 - MS2
 - MS2 CID
 - MS2 HCD
5. To update the new filter selection, click outside the Signal pane.

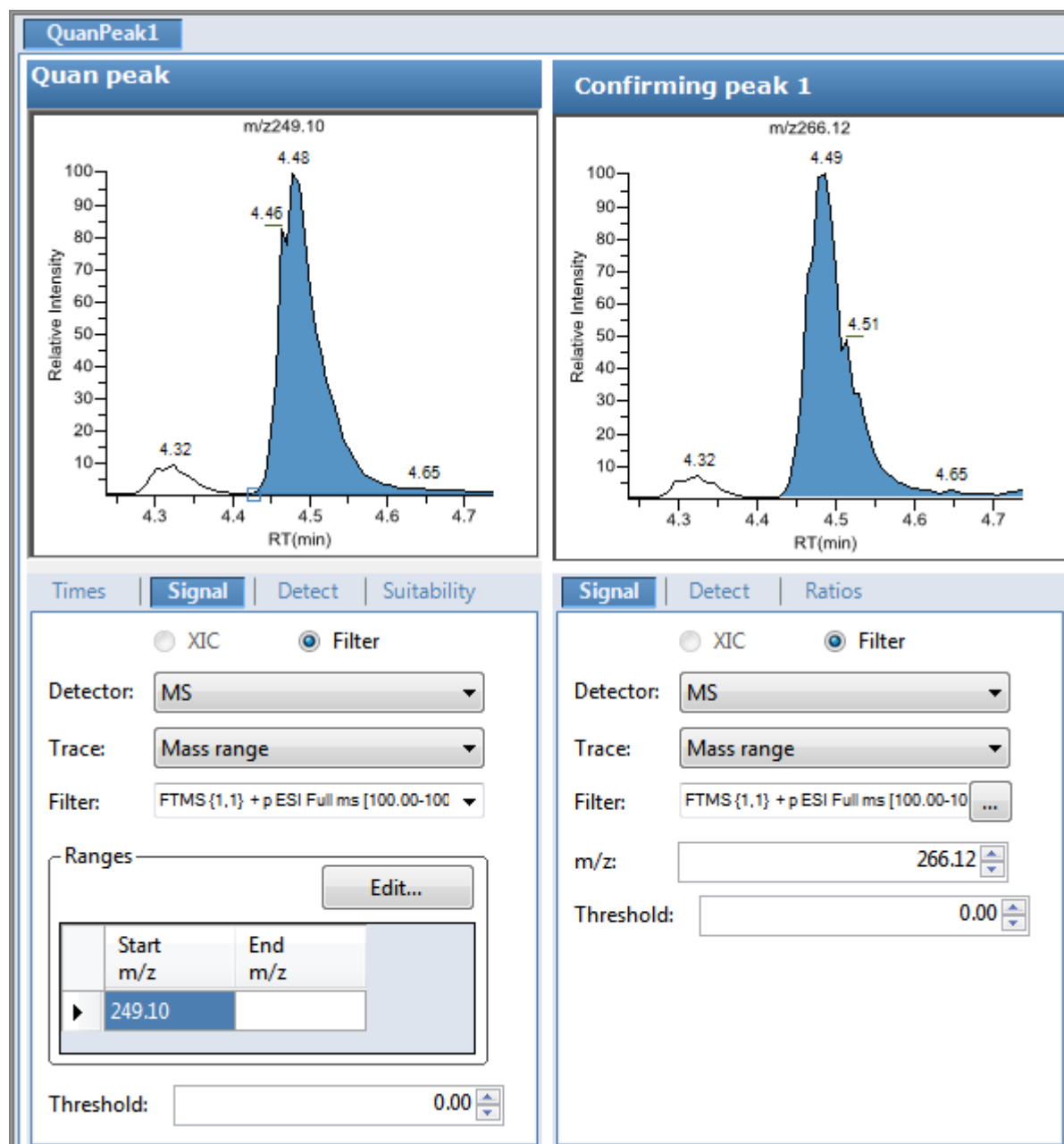
As long as the filter is highlighted blue, the new selection is not yet applied.
 6. (Optional for quantitative peaks) To apply this same quantitative peak filter to other peaks, right-click and choose one of the following from the shortcut menu:
 - **Set Filter Options on All Peaks in This Compound:** Applies this filter to all other peaks in the compound.
 - **Set Filter Options on All Compounds:** Applies this filter to all peaks for all compounds in the method.
 - **Set Quan Peak Filter Options on All Compounds:** Applies the filter specified for the quantitative peak to all quantitative peaks for all compounds in the method.
 7. (Optional for confirming peaks) To apply this same confirming peak filter to other peaks, right-click and choose one of the following from the shortcut menu:
 - **Set Filter Options on All Peaks in This Compound:** Applies this filter to all other peaks in the compound.
 - **Set Filter Options on All Compounds:** Applies this filter to all peaks for all compounds in the method.
 - **Set Confirm Peak Filter Options on All Compounds:** Applies the filter specified for the confirming peak to all confirming peaks for all compounds in the method.
 - **Set Confirm Peak 1 Filter Options on All Compounds:** Applies the filter specified for confirming peak 1 to the first confirming peak for all compounds in the method.

Signal Page

Use the features on the Signal page to define the detector and filters as you display each chromatogram trace for either analog detectors or mass spectrometer detectors. For detailed descriptions of all the parameters on the Signal page, see “Signal page parameters” on page 174.

- [Signal page for a mass spectrometer detector](#)
- [Signal page for an analog detector](#)

Figure 44. Signal page for a mass spectrometer detector



5 Using the Method Development Mode for Quantitation Methods

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Figure 45. Signal page for an analog detector

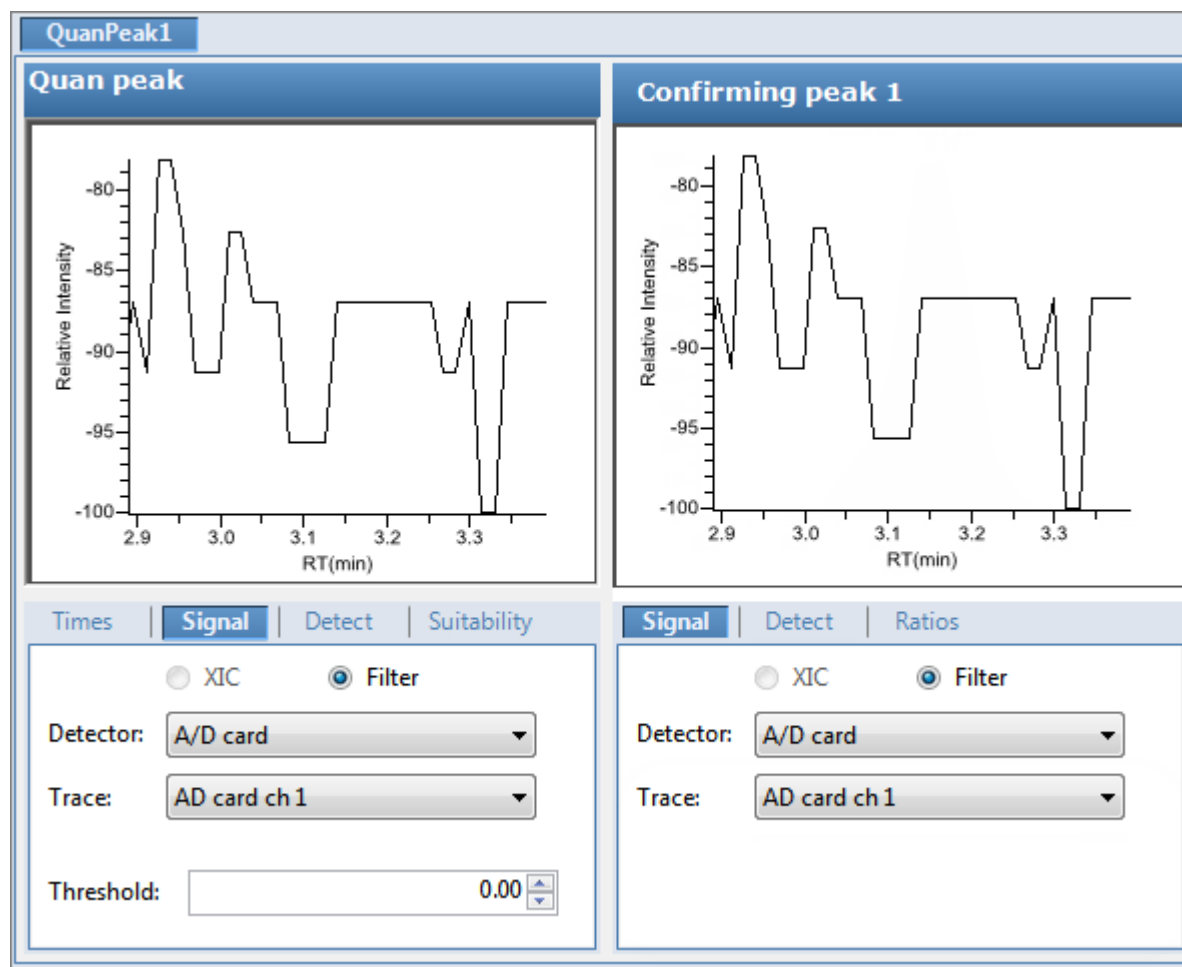


Table 24. Signal page parameters (Sheet 1 of 3)

Parameter	Description
XIC	Specifies an Extracted Ion Chromatogram experiment type that uses a single, full-scan mass filter that is post-processed to extract a peak for the ions of interest.
Filter	Select from the list of mass filters to use for processing the compound.

Table 24. Signal page parameters (Sheet 2 of 3)

Parameter	Description
Detector	<p>The detection options that are used to create the method determine the available detector options. The method can use the standard options (all the listed options) or only the detection options used to acquire an associated raw data file. To specify the available detector options, see “Specifying Default Peak Detection Parameters” on page 39.</p> <p>MS: Mass spectrometer that ionizes sample molecules and then separates the ions according to their mass-to-charge ratio (m/z).</p> <p>PDA: Photodiode array detector providing a linear array of discrete photodiodes on an integrated circuit chip. It is placed at the image plane of a spectrometer to allow simultaneous detection of a range of wavelengths.</p> <p>Analog: Supplemental detectors (for example, FID, ECD). When you select this detector, any reports that display a QIon value show the value as Analog and any reports that display spectra show the spectra as Not Available.</p> <p>A/D 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.</p> <p>UV: A UV spectrophotometer (for variable-wavelength detection) or photometer (for single-wavelength detection) equipped with a low-volume flow cell. This detector detects analytes that readily absorb light at a selected wavelength.</p>
Trace	<p>Represents a specific range of the data. The application uses the trace to identify the characteristic ions for a compound.</p> <p>MS detector options: Mass Range, TIC, or Base Peak. When you select Mass Range, you are prompted to enter the start and end m/z values for the ranges.</p> <p>PDA detector options: Spectrum Maximum, Wavelength Range, or Total Scan.</p> <p>Analog detector options: Analog 1, Analog 2, Analog 3, or Analog 4. You can configure these channel names in your instrument configuration.</p> <p>A/D Card detector options: AD Card ch1, AD Card ch2, AD Card ch3, or AD Card ch4. You can configure these channel names in your instrument configuration.</p> <p>UV detector options: Channel A, Channel B, Channel C, or Channel D. You can configure these channel names in your instrument configuration.</p>
Filter	<p>Available only when you select the MS detector. Represents a particular data acquisition channel. For example, the filter option + <i>c Full ms [35.00-500.00]</i> represents a positive ion centroid signal acquired in single-stage, full-scan mode from m/z 35 to 500.</p>

Table 24. Signal page parameters (Sheet 3 of 3)

Parameter	Description
Ranges	Available only when you select the Mass Range trace for an MS detector.
Edit	Opens the Edit Mass Ranges dialog box where you can specify a range of ions for detection and integration. See “To specify ranges of ions for detection and integration” on page 168.
Start <i>m/z</i> End <i>m/z</i>	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 <i>m/z</i> 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](#). Use the Genesis and Avalon sensitivity modes for mass spectrometry detection. You use the ICIS sensitivity mode primarily for analog detection.

On this page, you can specify how you want each mode to run. See the following for detailed descriptions of all the features on the Detect page:

- For Genesis sensitivity, see [“Detect page parameters for Genesis”](#) on page 177.
- For ICIS sensitivity, see [“Detect page parameters for ICIS”](#) on page 180.
- For Avalon sensitivity, see [“Detect page parameters for Avalon”](#) on page 183.

Figure 46. Detect page for Genesis

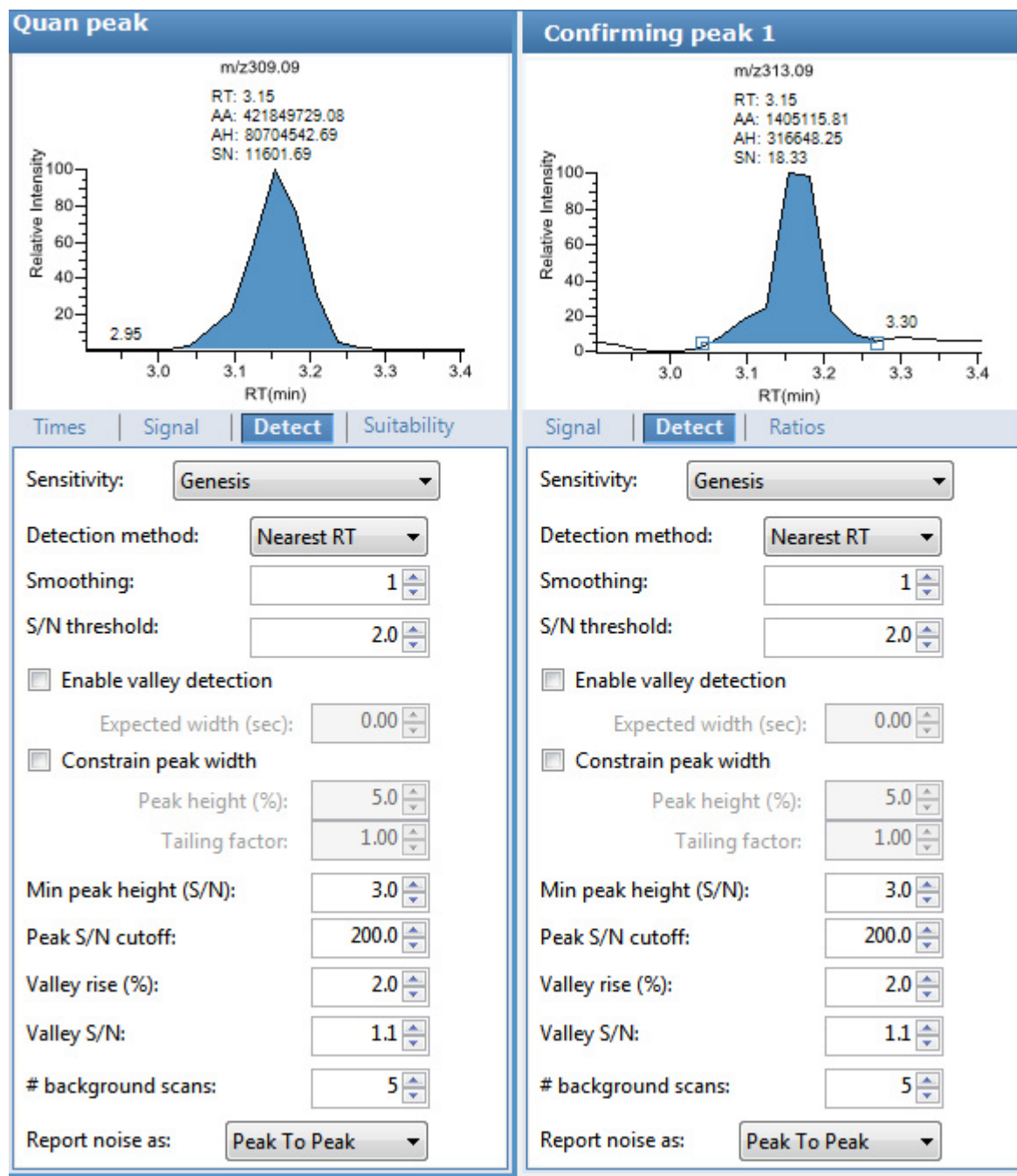


Table 25. Detect page parameters for Genesis (Sheet 1 of 3)

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.

Table 25. Detect page parameters for Genesis (Sheet 2 of 3)

Parameter	Description
Smoothing	<p>Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration.</p> <p>Valid values: Any odd integer from 1 through 15 points Default: 1</p>
S/N Threshold	<p>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.</p> <p>Valid range: 0.0 through 999.0</p>
Enable Valley Detection	<p>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.</p>
Expected Width (sec)	<p>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.</p> <p>With valley detection enabled, any valley points nearer than the <i>expected width</i>/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width.</p> <p>Valid range: 0.0 through 999.0</p>
Constrain Peak Width	<p>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 activates the Peak Height (%) and Tailing Factor options.</p>
Peak Height (%)	<p>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.</p> <p>Valid range: 0.0 through 100.0%</p>
Tailing Factor	<p>A factor that controls how the 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.</p> <p>Valid range: 0.5 through 9.0</p>

Table 25. Detect page parameters for Genesis (Sheet 3 of 3)

Parameter	Description
Min Peak Height (S/N)	<p>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 application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value.</p> <p>Valid range: 0.0 (all peaks) through 999.0</p>
Peak S/N Cutoff	<p>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 application defines the right and left edges of the peak when the S/N reaches a value less than 200.</p> <p>Valid range: 50.0 through 10000.0</p>
Valley Rise (%)	<p>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 the rise percentage, the application applies valley detection peak integration criteria. The application applies this test to both the left and right edges of the peak. The rise percentage criterion is useful for integrating peaks with long tails.</p> <p>Valid range: 0.1 through 500.0</p>
Valley S/N	<p>Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher.</p> <p>Valid range: 1.0 through 100.0 Default: 2.0</p>
# Background Scans	Number of background scans performed by the application.
Report Noise As	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or a peak-to-peak resolution threshold. Options are RMS or Peak to Peak.
Shortcut menu	
Apply to All Peaks in Method	Updates all compounds in the method with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks with Like Sensitivity Setting	Uses the current settings on the Detect page to update all compounds in the method that use the Genesis sensitivity mode. These updates apply to both quantitative and confirming ion peaks that use the Genesis sensitivity mode.
Apply to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.

5 Using the Method Development Mode for Quantitation Methods

Editing a Master Method

Figure 47. Detect page for ICIS

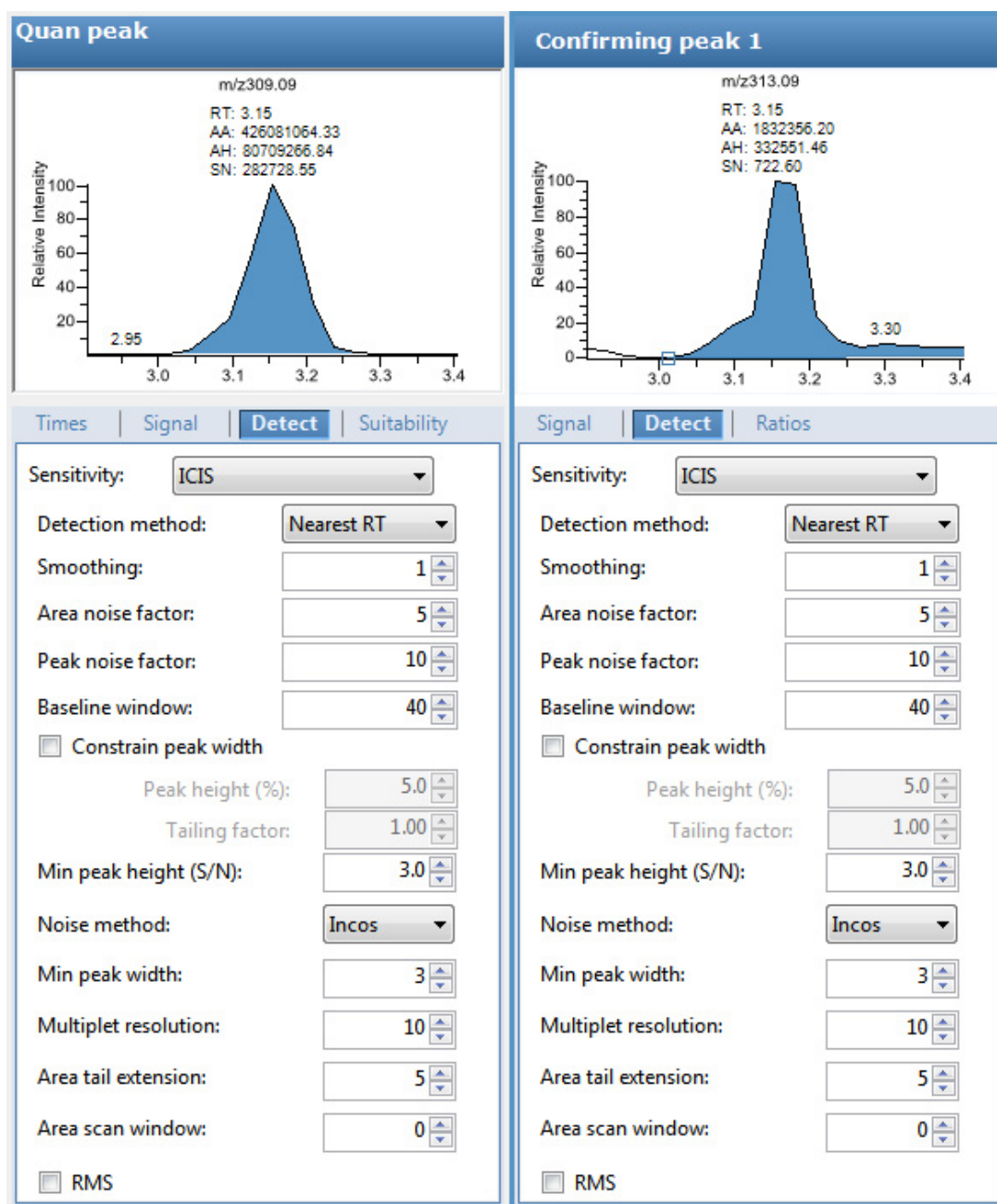


Table 26. Detect page parameters for ICIS (Sheet 1 of 3)

Parameter	Description
Sensitivity	Specifies the ICIS peak detection algorithm, used primarily with analog detectors.
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 26. Detect page parameters for ICIS (Sheet 2 of 3)

Parameter	Description
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Valid values: 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. Valid range: 1 through 500 Default: 5
Peak Noise Factor	The noise level multiplier used to determine the potential peak signal threshold. Valid range: 1 through 1000 Default: 10
Baseline Window	The application looks for a local minima over this number of scans. Valid 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 activates 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. Valid range: 0.0 through 100.0%
Tailing Factor	A factor that controls how the 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. Valid 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 application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Valid range: 0.0 (all peaks) through 999.0

Table 26. Detect page parameters for ICIS (Sheet 3 of 3)

Parameter	Description
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. Valid range: 0 through 100 scans Default: 3
Multiplet Resolution	The minimum separation in scans between the apexes of two potential peaks. This is a filter to determine if two peaks are resolved. Valid range: 1 through 500 scans Default: 10
Area Tail Extension	The number of scans past the peak endpoint to use in averaging the intensity. Valid range: 0 through 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. Valid range: 0 through 100 scans Default: 0
RMS	Specifies that the 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.
Shortcut menu	
Apply to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks in Method	Updates all compounds in the method with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks with Like Sensitivity Setting	Uses the current settings on the Detect page to update all compounds in the method that use the ICIS sensitivity mode. These updates apply to both quantitative and confirming ion peaks that use the ICIS sensitivity mode.

Figure 48. Detect page for Avalon

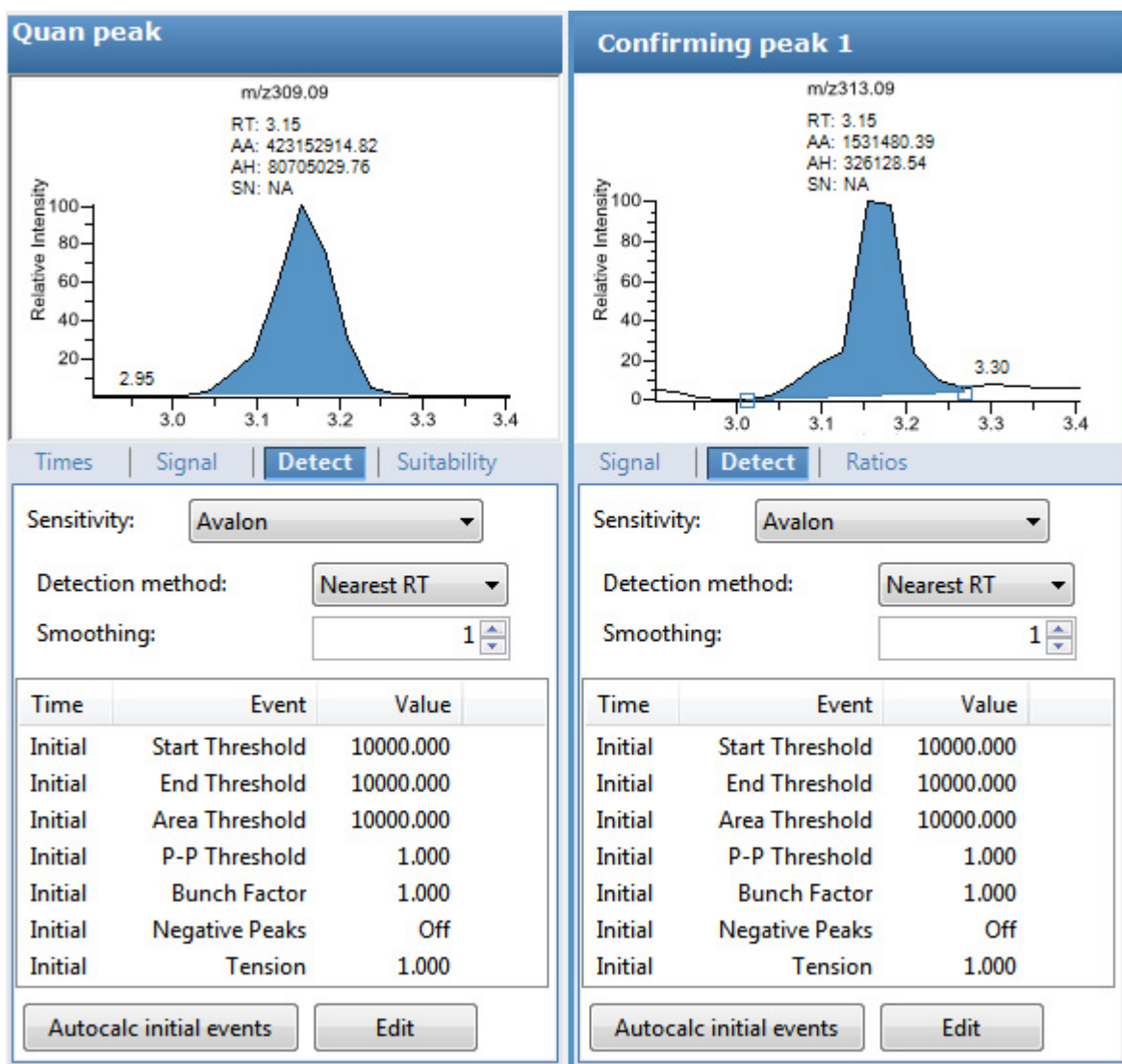


Table 27. Detect page parameters for Avalon (Sheet 1 of 2)

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.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Valid values: Any odd integer from 1 through 15 points Default: 1

Table 27. Detect page parameters for Avalon (Sheet 2 of 2)

Parameter	Description
Autocalc Initial Events	Automatically calculates the events in the Event list.
Edit	Opens the Avalon Event List dialog box. See Avalon Event List .
Shortcut menu	
Apply to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks in Method	Updates all compounds in the method with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks with Like Sensitivity Setting	Uses the current settings on the Detect page to update all compounds in the method that use the Avalon sensitivity mode. These updates apply to both quantitative and confirming ion peaks that use the Avalon sensitivity mode.

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. See [Avalon Event List dialog box parameters](#). For a detailed list of events and value ranges, see [Event types](#).

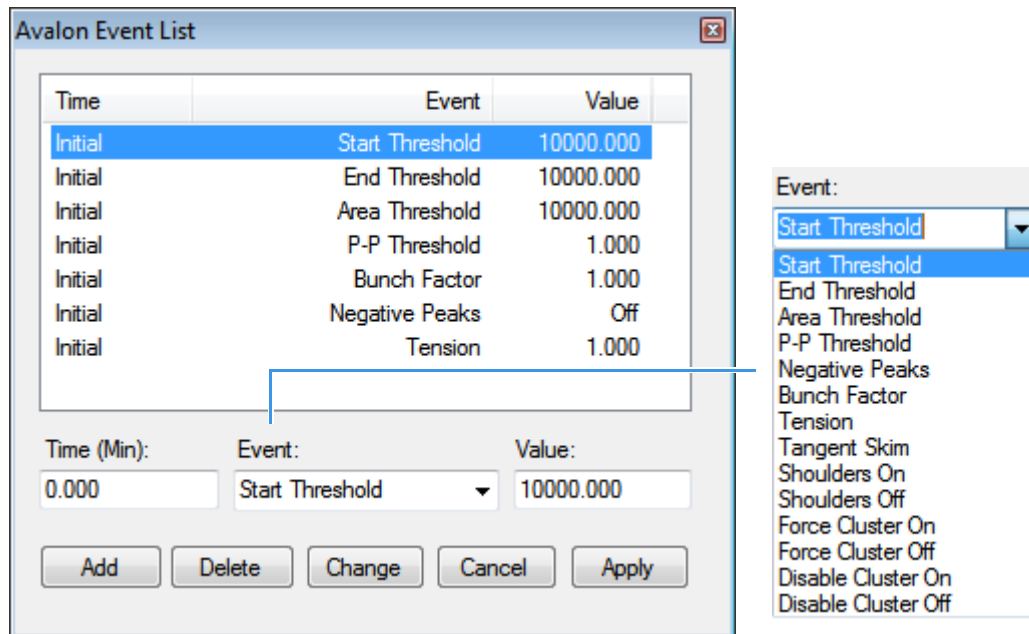
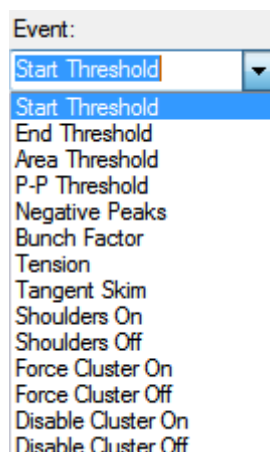
Figure 49. Avalon Event List dialog box

Table 28. 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.”
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 50. Event types**Table 29.** Event type descriptions (Sheet 1 of 2)

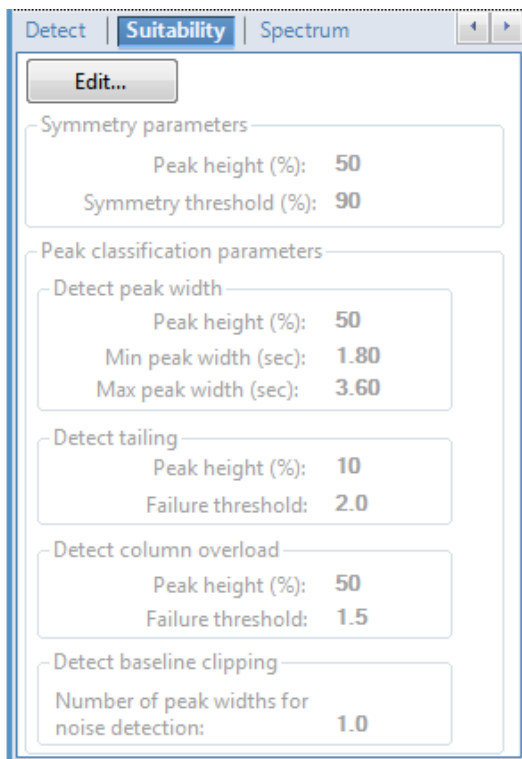
Event type	Description
Start Threshold	Specifies the threshold at the start of a peak. The Start Threshold is directly related to the RMS noise in the chromatogram. Valid range: 0 through 999 999 999
End Threshold	Specifies the threshold at the end of a peak. The End Threshold is directly related to the RMS noise in the chromatogram. Valid range: 0 through 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. Valid range: 0 through 999 999 999

Table 29. Event type descriptions (Sheet 2 of 2)

Event type	Description
P-P Threshold	<p>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.</p> <p>Valid range: 0.1 through 99.99</p>
Negative Peaks	<p>Permits detection of a negative going peak. Automatically resets after finding a negative peak.</p> <p>Valid values: On or Off</p>
Bunch Factor	<p>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.</p> <p>Valid range: 0 through 999</p>
Tension	<p>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.</p> <p>Valid range: 0 through 999.99 minutes</p>
Tangent Skim	<p>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.</p> <p>Valid range: 0 through 1</p>
Shoulders On	<p>Allows peak shoulders to be detected (peaks which are separated by an inflection rather than a valley) Sets a threshold for the derivative.</p>
Shoulders Off	<p>Disables peak shoulder detection.</p> <p>Valid range: 0 through 50</p>
Force Cluster On	<p>Force the following peaks to be treated as a cluster (single peak).</p>
Force Cluster Off	<p>End the forced clustering of peaks.</p>
Disable Cluster On	<p>Prevent any peaks from being clustered.</p>
Disable Cluster Off	<p>Permit clusters to occur again.</p>

Suitability

Use the Suitability page to determine if the column is degrading and to identify suspicious peaks eluting at the same time as the target compound. Suspicious peaks caused by highly retained compounds from a previous injection tend to have a broader than expected peak profile. Tailing peaks frequently indicate a degrading column. The Suitability page displays the parameter values to check the suitability of chromatographic peaks during processing. You can edit these parameters in the System Suitability dialog box. See “[System Suitability dialog box](#)” on page 189.



❖ To set system suitability parameters

1. Click **Edit**.

The System Suitability dialog box opens. See “[System Suitability dialog box](#)” on page 189.

2. To perform symmetry testing, do the following:
 - a. Select the **Symmetry Parameters** check box.
 - b. Type a peak height for symmetry testing in the Peak Height box.
 - c. Type a threshold for symmetry testing in the Symmetry Threshold box.
3. To carry out classification tests, do the following:
 - a. Select the **Peak Classification Parameters** check box.

- b. To adjust Xcalibur peak width testing thresholds, type parameters in the Detect Peak Width area as follows:
 - To enter a peak height for the test, type a value in the Peak Height box.
 - To enter a minimum peak width threshold, type a value in the Min Peak Width box.
 - c. To adjust the Xcalibur peak tailing test, type parameters in the Detect Tailing area:
 - To enter a peak height for the test, type a value in the Peak Height box.
 - To enter a threshold limit for peak tailing, type a value in the Failure Threshold box.
 - d. To adjust the Xcalibur column overload test, type parameters in the Detect Column Overload area:
 - To enter a peak height for the test, type a value in the Peak Height box.
 - To enter a threshold limit for peak tailing, type a value in the Failure Threshold box.
 - e. To adjust the Xcalibur baseline clipping test, type parameters in the Detect Baseline Clipping area:

To define the test window, type a value in the Number of Peak Widths for Noise Detection box.
4. To save your settings, click **OK**.

Figure 51. System Suitability dialog box

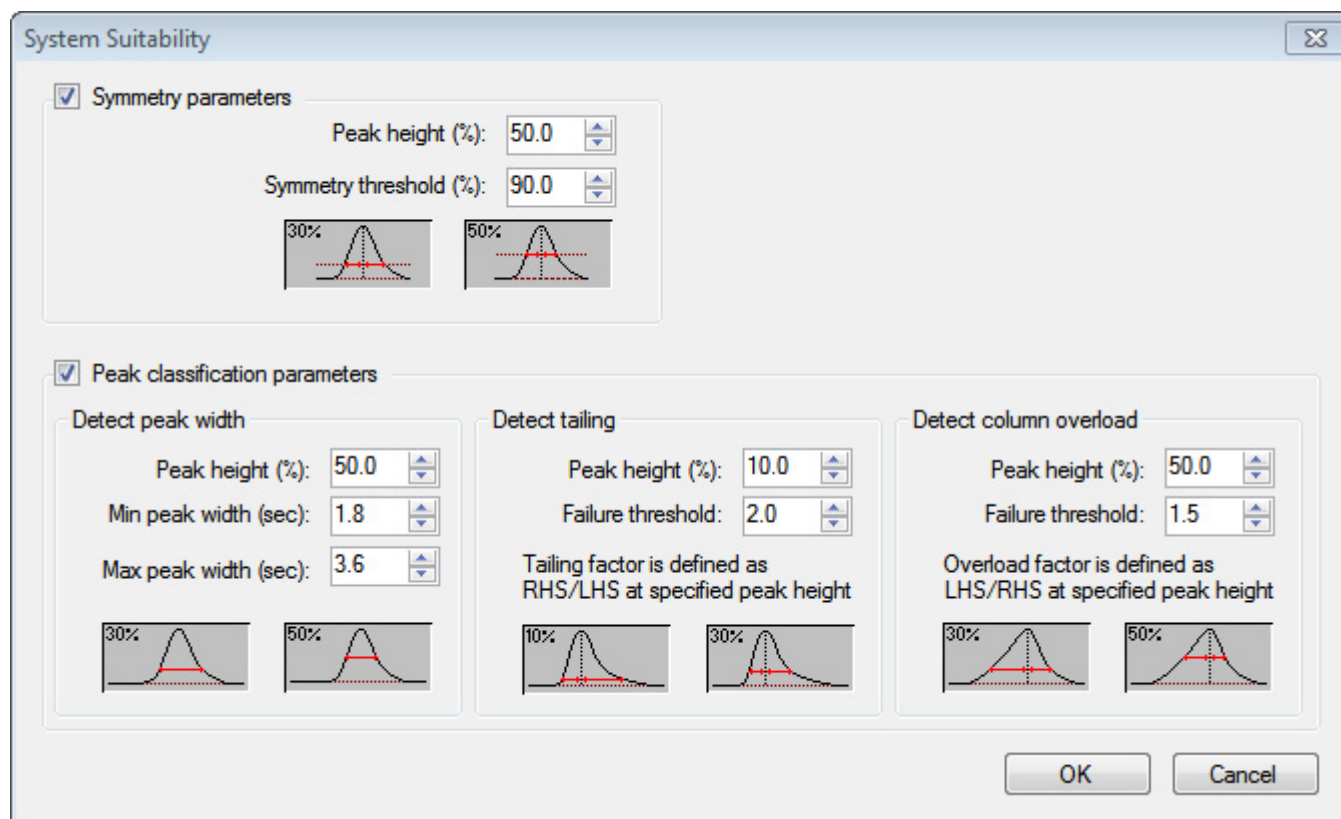


Table 30. System Suitability dialog box parameters (Sheet 1 of 2)


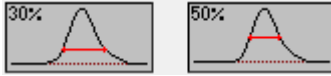
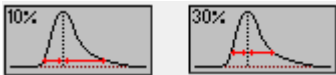

Parameter	Description
Symmetry Parameters	
Peak Height	The percentage of the peak height at which to compare the symmetry of the left and right peak widths. 
Symmetry Threshold	The minimum percentage difference to be considered symmetrical and pass the suitability test.
Peak Classification Parameters	
Detect Peak Width	Determines the minimum width of each side of the peak measured at the specified percentage of the peak height.
Peak Height	The percentage of the peak height at which to measure the full peak width. 
Min Peak Width	Minimum peak width (measured at the specified percentage of the peak height) required to pass the suitability test.

Table 30. System Suitability dialog box parameters (Sheet 2 of 2)

Parameter	Description
Max Peak Width	Maximum allowed peak width (measured at the specified percentage of the peak height) to pass the suitability test.
Detect Tailing	The width of the right side of the peak divided by the width of the left side of the peak at the specified percentage of the peak height.
Peak Height	The percentage of the peak height at which to measure the left and right sides of the peak. 
Failure Threshold	Minimum Detect Tailing value (RHS/LHS) required to pass the suitability test.
Detect Column Overload	The width of the left side of the peak divided by the width of the right side of the peak at the specified percentage of the peak height.
Peak Height	The percentage of the peak height at which to measure the left and right sides of the peak. 
Failure Threshold	Minimum Detect Column Overload value (LHS/RHS) required to pass the suitability test.

Spectrum

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

For detailed descriptions of all the shortcut menu commands on the Spectrum page, see “Spectrum Page” on page 195.

Follow these procedures:

- To create a reference spectrum
- To update confirming ion ratios
- To change the quantitation mass used for a quantitative peak
- To add ions together to get an accumulated signal
- To add a quantitative 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 create a reference spectrum

1. Click a peak in the quantitative peak chromatogram pane.

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

2. Right-click the Spectrum pane and choose **Apply Background Subtraction to Peak and Set as Reference Spectrum** from the shortcut menu.

The application uses the background-subtracted reference spectrum during quantitative processing and reports the background-subtracted reference spectrum (indicated with BS in the scan heading) as the last scan for each compound in the Quantitation Report - 2 report.

Note This command is available only when you select a background subtraction method on the Acquisition page in the master method. See [“Editing the Acquisition Page”](#) on page 137.

❖ To update confirming ion ratios

1. Click a peak in the quantitative 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 quantitative 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 mass-to-charge value for an ion.

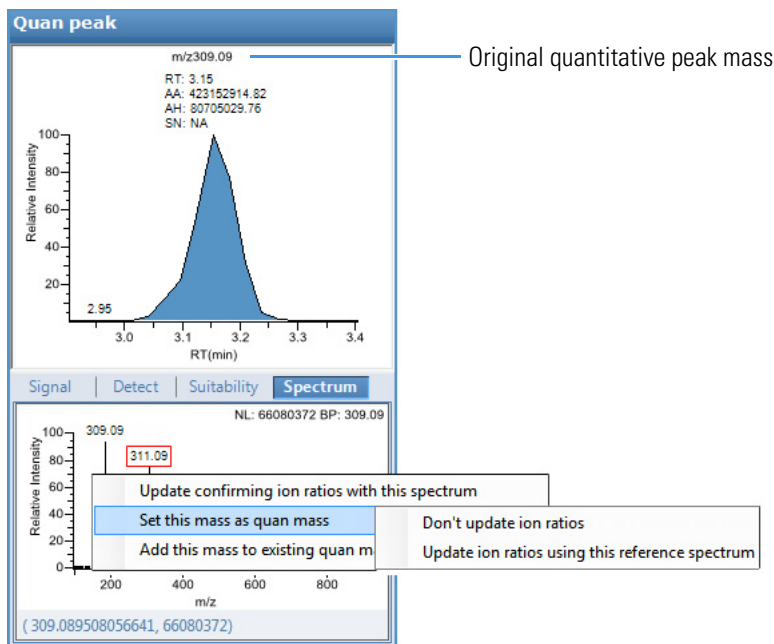
A red box around the ion's m/z value indicates that the ion is selected.

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**

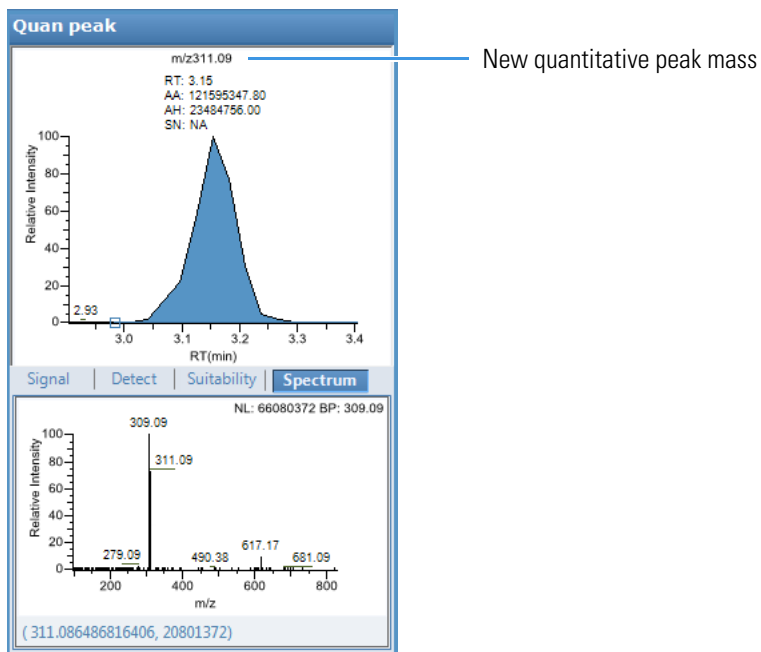
The following examples show an original quantitative peak and a quantitative peak with an updated quantitation mass.

Figure 52. Original quantitative peak mass example



The application replaces the original quantitation mass with the selected mass.

Figure 53. Updated quantitative 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 quantitative peak signal.

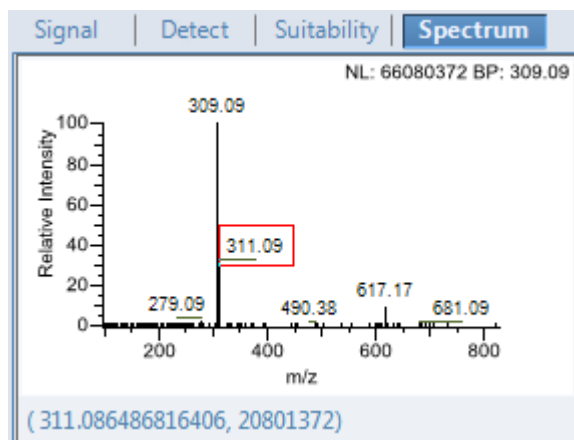
❖ **To add a quantitative peak to an existing compound**

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

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

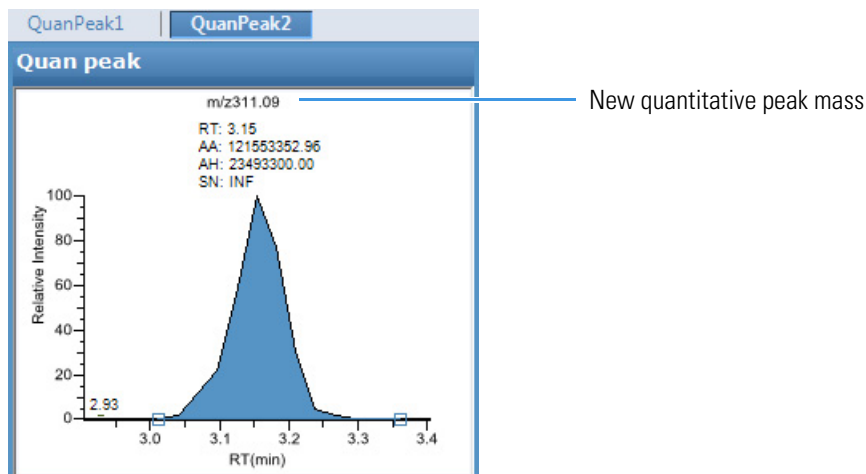
2. In the Spectrum pane, hold the cursor over the m/z value for an ion.

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 application adds this ion as a new quantitative peak.



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

1. Click the quantitative peak in the chromatogram pane.

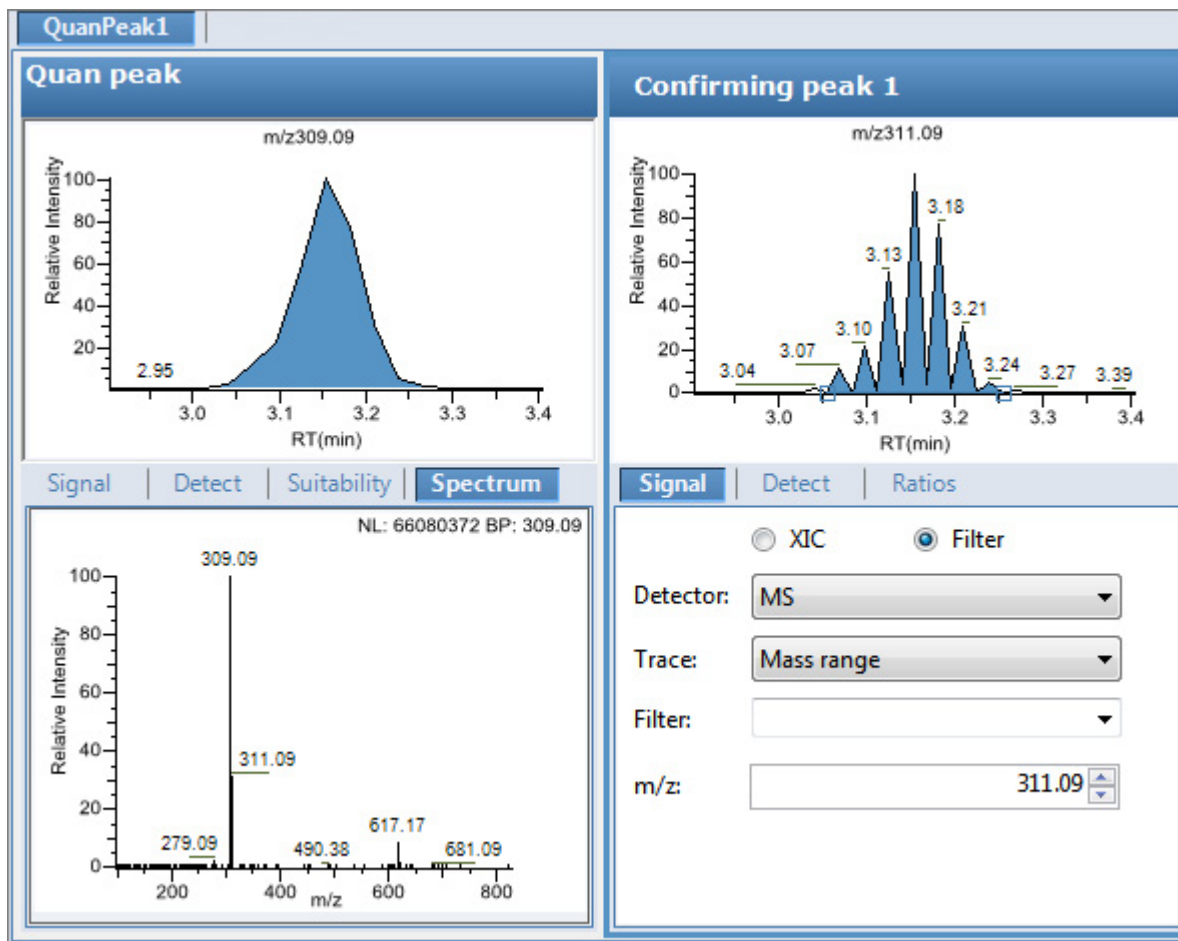
The mass spectrum for the peak is displayed in the Spectrum pane.

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 application adds the selected mass as a confirming peak for this quantitative 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.

Spectrum Page

Use the shortcut menu commands on the Spectrum page to store a reference mass spectrum for a quantitative peak or compound.

Figure 54. Spectrum page

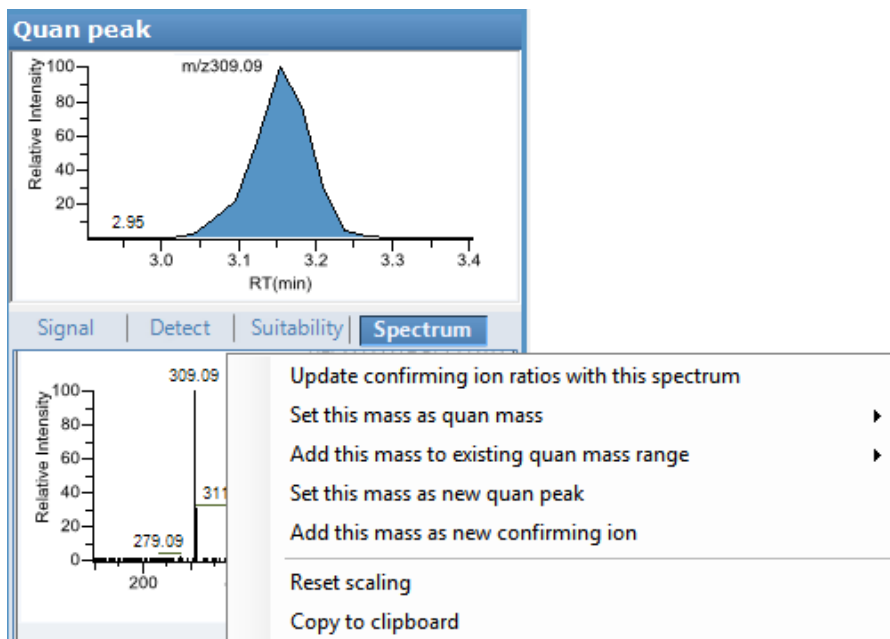


Table 31. Spectrum page shortcut menu commands

Command	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 quantitation mass of the selected ion to the quantitation mass used for the quantitative 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 quantitation mass range. You can choose to update the ion ratios to adjust the confirming ion comparisons to the new summed quantitative peak signal.
Set This Mass as New Quan Peak	Adds a new quantitative peak to an existing compound.
Add This Mass as New Confirming Ion	Adds one or more confirming ion peaks to an existing compound.
Reset Scaling	Returns the chromatogram or spectrum display to its original size.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Library

Use the Library page to define the criteria for library matching. For detailed descriptions of all the features on the Library page, see [Library page](#).

❖ To activate library matching

1. Select the **Enable** check box.
2. From the Library Search Type list, select the type of library to use for matching.
 - **NIST:** Uses the NIST library that you installed with the TraceFinder application. See “Installing the NIST and QED Libraries” on page 14.

Note Because the NIST library is large, using this library can slow sample processing.

- **Library Manager:** Uses the library that you specified in the Configuration console. See “Screening Libraries” on page 59.
- **NIST High Resolution:** Uses an installed NIST library that contains an EI accurate ion m/z or MS/MS spectra.

The application searches the library, matches the fragment ion spectrum in the library to the compound’s ion spectrum, and returns the highest score (best match).

Figure 55. Library page

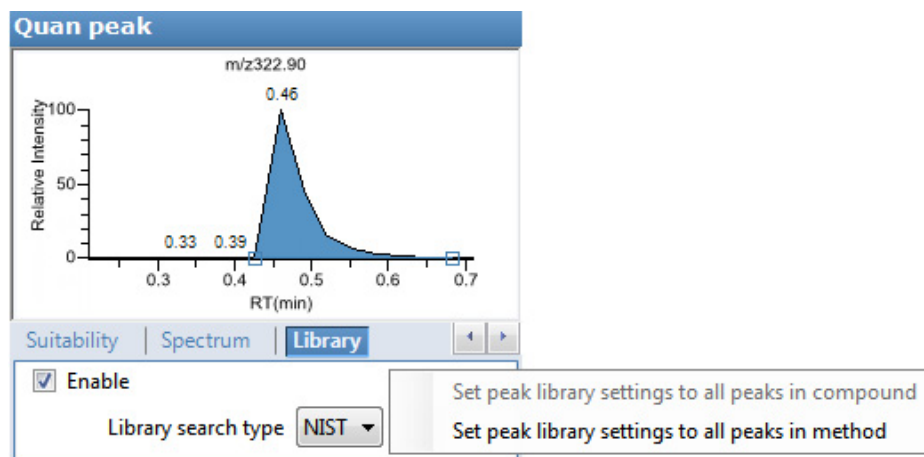


Table 32. Library page parameters

Command	Description
Library Search Type	Specifies the type of library to use for matching. <ul style="list-style-type: none"> • NIST: Uses the NIST library that you installed with the TraceFinder application. • Library Manager: Uses the library that you specified in the Configuration console. • NIST High Resolution: Uses a NIST library that contains an EI accurate ion m/z or MS/MS spectra.
Shortcut menu	
Set Peak Library Settings to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Library page. These updates apply to both quantitative and confirming ion peaks. The application reprocesses all peaks in the compound and performs a new library search.
Set Peak Library Settings to All Peaks in Method	Updates all compounds in the method with the current settings on the Library page. These updates apply to both quantitative and confirming ion peaks. When you use this command in the local method for a processed batch, the application prompts you to reprocess the batch to update the library settings.

Isotopes

Use the Isotopes page to define the criteria for identifying an isotope peak. To identify an isotopic pattern, the application must detect the compound for at least one of its defined adduct ions. The application identifies the elemental composition to match using the formula that is associated with the most intense adduct peak. The application then generates an isotopic pattern score (as a percentage value) for the match between the measured and expected isotopic patterns of the calculated elemental composition.

For detailed descriptions of all the features on the Isotopes page, see [Isotopes page](#).

❖ To specify isotope criteria

1. Select the **Enable** check box to activate the isotopes features.
2. In the Fit Threshold box, type the fit threshold percentage.

The resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

3. In the Allowed Mass Deviation box, type the parts per million to use as the minimum deviation from the expected m/z .

The isotopic pattern algorithm considers an isotope peak as found if its measured m/z is less than this amount away from its expected m/z . For best results, set this value to a number that causes up to 98 percent of all mass deviations to be smaller than the allowed mass deviation value.

4. In the Allowed Intensity Deviation box, type a value to specify the allowed intensity deviation of the mass spectrometer relative to the monoisotopic ion, as a percentage of the base peak height.

The isotopic pattern algorithm considers an isotope peak as not found if its intensity, relative to the monoisotopic ion's intensity, is more than the deviation percentage from the theoretical relative intensity of the isotope ion. For best results, set this value to a number that causes up to 98 percent of all intensity deviations to be smaller than the allowed intensity deviation value.

5. To specify that isotopic pattern calculations use internal mass calibration instead of external mass calibration, select the **Use Internal Mass Calibration** check box.

With this check box selected, the application applies a requirement that an isotope's m/z must be closer to its theoretical value to avoid a score penalty.

Figure 56. Isotopes page

Table 33. Isotopes page parameters (Sheet 1 of 2)

Parameter	Description
Fit Threshold %	To identify a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage. Default: 90%
Allowed Mass Deviation (ppm)	Specifies the allowed mass deviation in the spectrum data. The TraceFinder isotopic pattern algorithm considers an isotope peak as found if its measured m/z is less than this amount away from its expected m/z . For best results, set this value to a number that causes up to 98 percent of all mass deviations to be smaller than the allowed mass deviation value. Valid range: 3 through 100 ppm Default: 3 ppm

Table 33. Isotopes page parameters (Sheet 2 of 2)

Parameter	Description
Allowed Intensity Deviation (%)	<p>Specifies the allowed intensity deviation of the mass spectrometer, relative to the monoisotopic ion, as a percentage of the base peak height.</p> <p>The TraceFinder isotopic pattern algorithm considers an isotope peak as not found if its intensity relative to the monoisotopic ion's intensity is more than this deviation percentage from the theoretical relative intensity of the isotope ion. For best results, set this value to a number that causes up to 98% of all intensity deviations to be smaller than the allowed intensity deviation value.</p> <p>Default: 10%</p>
Use Internal Mass Calibration	Specifies that the application require an isotope's m/z to be closer to its theoretical value to avoid a score penalty.
Shortcut menu	
Set Peak Isotope Settings to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Isotopes page. These updates apply to both quantitative and confirming ion peaks. The application reprocesses all peaks in the compound and performs a new library search.
Set Peak Isotope Settings to All Peaks in Method	Updates all compounds in the method with the current settings on the Isotopes page. These updates apply to both quantitative and confirming ion peaks. When you use this command in the local method for a processed batch, the application prompts you to reprocess the batch to update the library settings.

Fragments

Use the Fragments page to define the criteria for identifying a fragment ion.

To use fragment ions, the application requires the following conditions:

- The selected compound databases contain the charged mass for each defined fragment ion of interest for the compounds in the target list.
- The HCD (higher energy collision-induced dissociation), source CID (source collision-induced dissociation), or AIF (all ions fragmentation) ion spectra exist at a time point within the compound's elution time range.

For detailed descriptions of all the features on the Fragments page, see [Fragments page](#).

❖ **To specify fragment ion options**

1. Select the **Enable** check box.
2. To ignore the Fragment Ions options when no fragment is defined in the compound database, select the **Ignore If Not Defined** check box.

When the compound database does not define fragments for a compound, the application does not include the results for fragment ions in the results.

- When the Ignore If Not Defined option is selected, the application does not perform filtering for the Fragment Ions and, in the Data Review view, the FI column is blank.
 - When the Ignore If Not Defined option is not selected, the application considers that this target compound is not identified. The Fragment Ions filter fails.
3. In the Min. # of Fragments box, type the minimum number of fragments required to identify a compound.

The application uses the number of fragment masses defined in the compound database when it processes a sample for fragment ions. The value you specify for Min. # of Fragments cannot be greater than the number of fragments defined in the compound database.

4. In the Intensity Threshold box, type the intensity threshold value.

The intensity of a fragment must be above this threshold for the application to identify it.

5. In the Mass Tolerance box, type a mass tolerance value and then select **ppm** or **mmu** for the mass tolerance units.

This mass tolerance value indicates the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value for the fragment ions. It is separate from the mass tolerance value specified for the parent peak.

Note When using ion trap data, the application uses 300 mmu regardless of the value you enter here.

Figure 57. Fragments page

The screenshot shows the 'Fragments' configuration page. At the top, there are four tabs: 'Spectrum', 'Library', 'Isotopes', and 'Fragments'. The 'Fragments' tab is selected. Below the tabs, there are several settings:

- Enable:** A checked checkbox.
- Ignore if Not Defined:** An unchecked checkbox.
- Min. # of Fragments:** A numeric input field with a spinner, set to 1.
- Intensity Threshold:** A numeric input field with a spinner, set to 10000.
- Mass Tolerance:** A numeric input field with a spinner set to 5, and a dropdown menu set to 'ppm'.

Table 34. Fragments page parameters

Parameter	Description
Ignore If Not Defined	Ignores the values you specify when no fragment is defined in the compound database, and does not include the results for fragment ions in the Data Review results.
Min. # of Fragments	Specifies the minimum number of fragments required to find the compound. Valid range: 1 through 5 Default: 1
Intensity Threshold	Specifies the minimum height of a fragment ion peak. The peak of a fragment ion must be above this intensity threshold for the application to find it. Valid range: 1 through 1e9 Default: 10 000
Mass Tolerance	Specifies the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value for the fragment ions and is separate from the mass tolerance specified for the parent (see “Editing the Acquisition Page” on page 137). Valid range: 0 through 500 Default: 5 ppm Unit: mmu or ppm Note When using ion trap data, the application uses 300 mmu regardless of the value you enter here.
Shortcut menu	
Set Fragment Settings to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Fragments page. These updates apply to both quantitative and confirming ion peaks. The application reprocesses all peaks in the compound and performs a new library search.
Set Fragment Settings to All Peaks in Method	Updates all compounds in the method with the current settings on the Fragments page. These updates apply to both quantitative and confirming ion peaks. When you use this command in the local method for a processed batch, the application prompts you to reprocess the batch to update the library settings.

Ratios

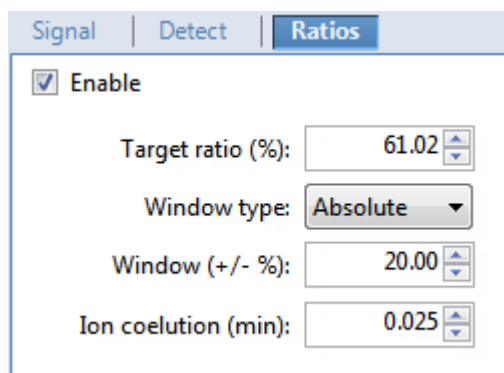
Use the Ratios page to define the criteria for evaluating the confirming or qualifying ions. The application detects compounds that have confirming ion values outside their acceptable window and flags them in the Acquisition mode and in reports.

For detailed descriptions of all the features on the Ratios page, see [Ratios page](#).

❖ To specify ion ratio criteria

1. Select the **Enable** check box to activate 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 peak is 41.02–81.02%.



The screenshot shows the 'Ratios' tab in a software interface. It contains the following settings:

- Enable**
- Target ratio (%): 61.02
- Window type: Absolute
- Window (+/- %): 20.00
- Ion coelution (min): 0.025

However, if 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 peak is 48.82–73.22%.

Figure 58. Ratios page

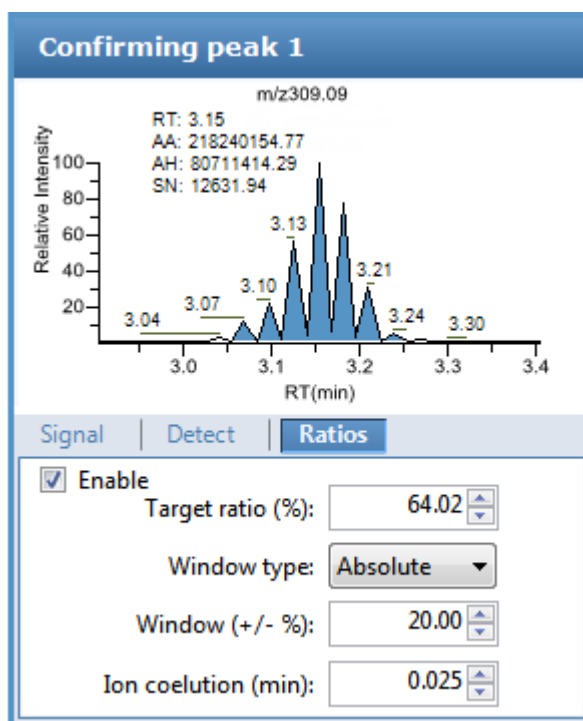


Table 35. Ratios page parameters

Parameter	Description
Enable	Makes the ion ratio criteria available.
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.
Ion Coelution (min)	Specifies the maximum difference in retention time between a confirming ion peak and the quantification ion peak. Valid range: 0.025 through 0.1
Shortcut menu commands	
Set Ion Ratio to All Confirming Peaks in Compound	Copies the Window Type, Window, and Ion Coelution values to all confirming ion peaks for the compound and updates the compound. Available only when a compound has multiple confirming ion peaks.
Set Ion Ratio to All Confirming Peaks in Method	Copies the Window Type, Window, and Ion Coelution values to all quantitative peaks for the method and updates the method.

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.

Typically, general quantitation uses a measured response (area or height) to determine the amount of a compound contained in a sample. The application compares the response of an unknown, target compound to the response of a calibration sample that contains a known amount of the compound by building a calibration curve to interpolate the amount in the target compound.

To use a semi-quantitative process, you specify the compound's standard type as Estimated and then identify another compound as the linked compound. Instead of using the target compound to create a calibration curve, the application uses a calibration curve from the linked compound to calculate the amount in the target compound.

To use a real sample for the calibration procedure, you specify the compound's standard type as Std Addition. The autosampler divides the sample into multiple portions (one unspiked portion and at least two spiked portions). To maintain consistent conditions across all samples, the autosampler adds selected amounts of standard into the vials and adds a volume of a solvent calculated to maintain constancy in the total volume of liquid in each vial.

For detailed descriptions of all the features on the Calibration page, see [“Calibration Page”](#) on [page 206](#).

Follow these procedures:

- [To specify an internal standard type for a compound](#)
- [To specify an estimated standard type for a compound](#)
- [To specify a standard addition standard type for a compound](#)

❖ **To specify an internal standard type for a compound**

1. On the Identification page, specify at least one compound in the method as an internal standard compound type. See [“Identification”](#) on [page 152](#).
2. On the Calibration page, do the following:
 - a. In the Standard Type column, select **Internal**.
 - b. In the ISTD column, select the compound that you want to use as the internal standard for this compound.

The application lists only compounds specified as internal standards on the Identification page.

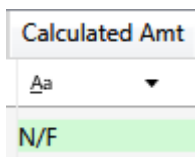
To view the internal standard peak in Data Review, see [“Compound Details”](#) on [page 498](#).

❖ **To specify an estimated standard type for a compound**

1. In the Standard Type column, select **Estimated**.
2. In the Linked Compound column, select any other compound in the method that you want to link to this compound.

The Estimation Method value defaults to Ext Curve and is read-only.

The Compound Results in Data Review display the Calculated Amt value as “N/F” (not found) highlighted in green.



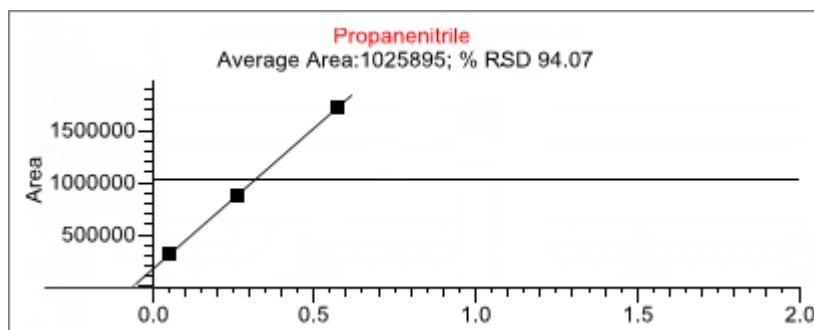
❖ **To specify a standard addition standard type for a compound**

In the Standard Type column, select **Std Addition**.

- The Curve Type column value defaults to Linear and is read-only.
- The Origin column value defaults to Ignore and is read-only.
- The Weighting column value defaults to Equal and is read-only.

When you process this sample, the application divides the sample into multiple portions: one portion is not spiked and at least two portions are spiked. The application calculates the analyte concentration as *intercept/slope*, where *intercept* is the *y*-intercept of the regression line and *slope* is the slope of the regression line.

When you use the Std Addition calibration, the *y*-intercept on the calibration curve might not be at 0, as shown in the following figure:



The Compound Results in Data Review display the following:

- The Calculated Amt value is the spiked amount from the calibration curve.
- The Theoretical Amt value is the level defined in the method.
- The Sample Amt value is the actual amount in the standard spike plus the spiked amount in each standard.

Calibration Page

Use the features on the Calibration page to define the mathematical model used for preparing the initial calibration evaluation for one or more calibration standards.

Figure 59. Calibration page

Acquisition List Identification Detection Calibration Calibration levels Chk Std levels Real Time Viewer								
	RT	Compound	Compound type	Standard type	Response via	Curve type	Origin	Weighting
1	0.00	Naphthalene, 1,5-dichlor...	Target Compound	Internal	Area	Linear	Ignore	Equal
2	0.01	Pyrazinamide	Target Compound	External	Area	Linear	Ignore	Equal
3	1.07	Methyl 2-furoate	Target Compound	Estimated				
4	1.32	Methyl 2-furoate *2*	Target Compound	Std Addition	Area	Linear	Ignore	Equal

Table 36. Calibration 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.
Compound Type	Displays the compound type as a Target Compound or an Internal Standard.
Standard Type	Specifies Internal, External, Estimated, or Std Addition standards.
Response Via	The use of area or height. When you set the standard type to Estimated, this column is inactive.
Curve Type	Specifies Linear, Quadratic, or AverageRF curve types. When you set the standard type to Estimated, this column is inactive. When you set the standard type to Std Addition, this column value defaults to Linear and is read-only.
Origin	The origin treatment is Ignore, Include, or Force. The Origin and Weighting columns are available only when you use Linear or Quadratic curve types. When you set the standard type to Estimated, this column is inactive. When you set the standard type to Std Addition, this column value defaults to Ignore and is read-only.
Weighting	Specifies the weighting as Equal, 1/X, 1/X ² , 1/Y, or 1/Y ² . When you set the standard type to Estimated, this column is inactive. When you set the standard type to Std Addition, this column value defaults to Equal and is read-only.
Units	The units to be displayed with the calculated values.
ISTD	The internal standard (ISTD) for a target compound or surrogate. The list displays all compounds with the compound type of Internal Standard. This column is available only when you set the standard type to Internal.
Amount	The amount of the internal standard for ISTD compounds. When you set the standard type to Estimated, this column is inactive.
Linked Compound	This column is available only when the standard type is set to Estimated. The list of available compounds to be linked does not include any compounds whose standard type is set to Estimated.

Table 36. Calibration page parameters (Sheet 2 of 2)

Parameter	Description
Estimation Method	This column is unavailable for editing when the standard type is set to Estimated. <ul style="list-style-type: none"> When the compound type for the associated linked compound is Target Compound, the estimation method is automatically set to Ext Curve. When the compound type for the associated linked compound is Internal Standard, the estimation method is automatically set to Ratio.
Shortcut menu	The Calibration page uses a right-click shortcut menu. See “Using the Shortcut Menu Commands” on page 212.

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.

For detailed descriptions of all the features on the Calibration Levels page, see [Calibration Levels page](#).

You can use the copy-and-paste functions in the shortcut menu to copy calibration levels from one column to another or from one master method to another. For detailed instructions, see [“Copying and Pasting Column Values”](#) on page 213.


❖ To specify calibration levels and concentrations

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

	RT	Compound			
▶ 1	3.15	Pyrazinamide			
2	3.67	1,3-Dioxolane, 2-heptyl-			
3	4.70	Pyrazinamide *2*			

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

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

	Level
1	Cal1
 2	Cal2
* 3	

3. Continue adding calibration levels.

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

4. To enter the concentrations in the table, do the following:
 - a. Select the first calibration level table cell.

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- 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 that you want to copy, right-click, and choose **Copy Down** from the shortcut menu.

Figure 60. Calibration Levels page

Acquisition List	Identification	Detection	Calibration	Calibration levels	Chk Std levels	Real Time
	RT	Compound		Cal1	Cal2	Cal3
1	3.14	Propanenitrile		5.000	10.000	15.000
2	3.15	Pyrazinamide				
▶ 3	3.67	1,3-Dioxolane, 2-heptyl-				
4	4.70	Pyrazinamide *2*				

Manage Calibration levels	
	Level
1	Cal1
2	Cal2
3	Cal3

Table 37. 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.
<i>CalLevel_1–CalLevel_n</i>	User-defined calibration levels for the compound. The names you enter here become the column headers for the calibration levels.
Manage Calibration Levels	Defines values for each of the calibration level values for the selected compound.
Shortcut menu	The Calibration Levels page uses a right-click shortcut menu. See “Using the Shortcut Menu Commands” on page 212.

Chk Std Levels

Use the Chk Std Levels page for a master method to define the standards for Chk Std levels. You can edit Chk Std levels for master methods only. The contents of this page are read-only when you are editing a local method. For detailed descriptions of all the features on the Chk Std Levels page, see “Chk Std Levels page” on page 210.

You can use the copy-and-paste functions in the shortcut menu to copy Chk Std levels from one column to another or from one master method to another. For detailed instructions, see “Copying and Pasting Column Values” on page 213.

❖ To specify Chk Std levels and concentrations

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

	RT	Compound			
▶ 1	3.15	Pyrazinamide			
2	3.67	1,3-Dioxolane, 2-heptyl-			
3	4.70	Pyrazinamide *2*			

2. In the Manage Chk Std Levels area, type a name for the first Chk Std level.

The application adds a new, empty Chk Std level row below the edited row.

3. Type a value for the % Test.

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

	Level	% Test
1	Level1	5.00
* 2		NA

4. Continue adding Chk Std levels and values for the percentage test.

	Level	% Test
1	Level1	5.00
2	Level2	5.00
▶ 3	Level3	5.00

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

5. To enter the concentration values in the table, do the following:
 - a. Select the first Chk Std level table cell.
 - b. Click the cell again to make it editable.
 - c. Type a concentration value.
6. Repeat [step 5](#) for all Chk Std levels associated with the first compound.

Acquisition List	Identification	Detection	Calibration	Calibration levels	Chk Std levels	Real Time Vie
	RT	Compound	Level1	Level2	Level3	
1	3.14	Propanenitrile	5.000	10.000	15.000	
2	3.15	Pyrazinamide				

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

Figure 61. Chk Std Levels page

Acquisition List	Identification	Detection	Calibration	Calibration levels	Chk Std levels	Real Time
	RT	Compound	Level1	Level2	Level3	
▶ 1	3.14	Propanenitrile	5.000	10.000	15.000	
2	3.15	Pyrazinamide	5.000	10.000	15.000	
3	3.67	1,3-Dioxolane, 2-heptyl-	5.000	10.000	15.000	

Manage Chk Std levels		
	Level	% Test
▶ 1	Level1	5.00
2	Level2	5.00
3	Level3	5.00

Table 38. 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.
<i>Level_1–Level_n</i>	User-defined quality control levels for the compound.
Manage Levels	
Level	User-defined quality control level names. The names you enter here become the column headers for the levels.
% Test	A value for the acceptable difference (as a percentage) between the known amount and calculated (measured) amount of each level.
Shortcut menu	The Levels page uses a right-click shortcut menu. See “Using the Shortcut Menu Commands” on page 212.

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. See “Real Time Status Pane” on page 388.

Figure 62. Real Time Viewer page

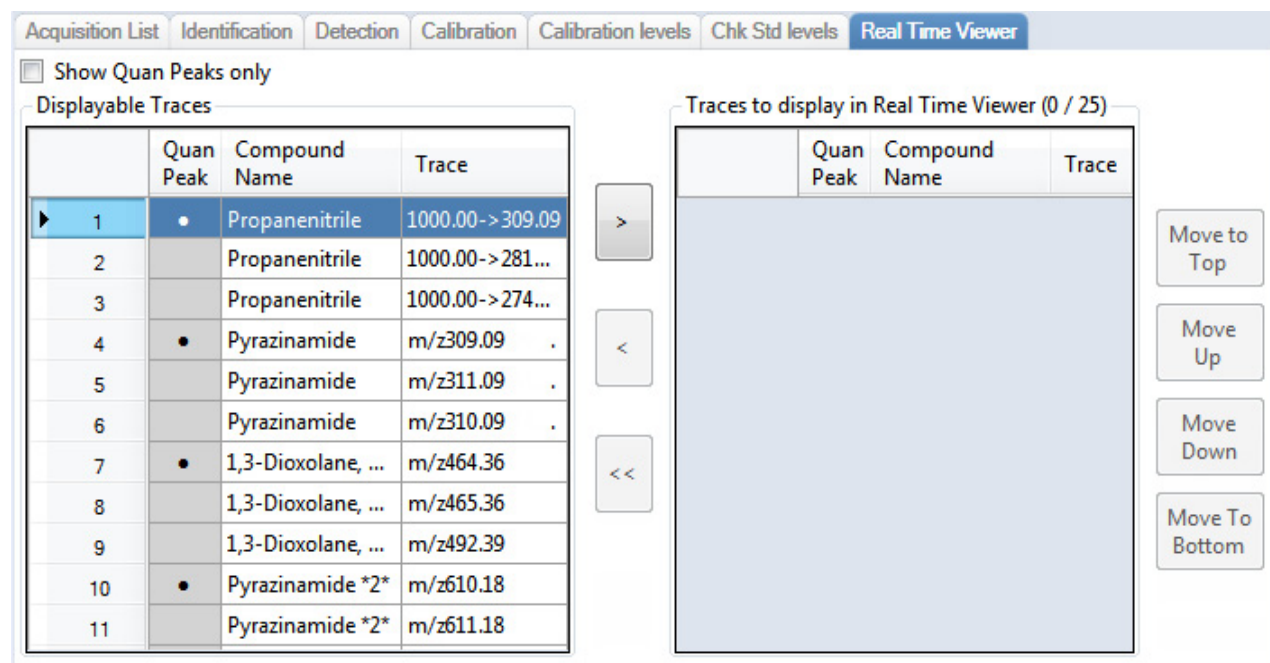


Table 39. Real Time Viewer page parameters (Sheet 1 of 2)

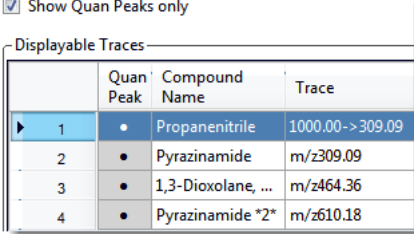




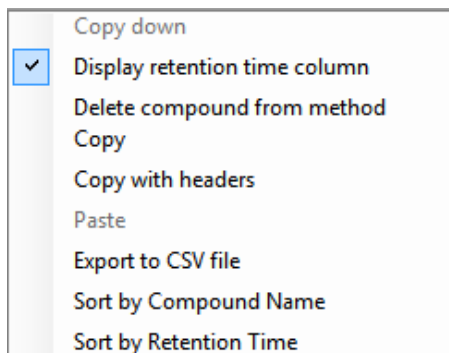
Parameter	Description
Show Quan Peaks Only	Displays only quantitative peaks in the compounds list. Quantitative peaks are indicated with a black dot in the Quan Peak column. <input checked="" type="checkbox"/> Show Quan Peaks only 
Displayable Traces	
Quan Peak	Dots indicate quantitative peak traces. Unmarked traces indicate confirming ion peaks.
Compound Name	Names of all compounds in the method.
Trace	Lists the simple mass or precursor mass for all traces—both quantitative peak and confirming ion peak—for each compound.
	Moves the selected trace to the Traces to Display in Real Time Viewer pane.

Table 39. Real Time Viewer page parameters (Sheet 2 of 2)

Parameter	Description
	Moves the selected trace to the Displayable Traces pane.
	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 (n/25)	List the traces to be displayed and the display order used in the real-time display in the Acquisition mode. See “ Real-Time Trace Display ” on page 402. 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 in the Acquisition mode.
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 and Real Time Viewer pages) 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 40.** Compounds page shortcut menu commands (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 C, “Using Copy Down and Fill Down.”
Display Retention Time Column	Displays or hides the RT column in the compound list.

Table 40. Compounds page shortcut menu commands (Sheet 2 of 2)

Command	Description
Delete Compound From Method	Removes the selected compound from the current master method.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy compound information to a text editor or spreadsheet application. You cannot paste this data back into the method development compound 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 a text editor or spreadsheet application. You cannot paste this data back into the method development compound list.
Paste	Pastes a single column of copied data from a text editor or spreadsheet application 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.
Sort by Compound Name	Sorts the compounds alphabetically from A to Z.
Sort by Retention Time	Sorts the compounds from shortest retention time to longest retention time.

Copying and Pasting Column Values

You can use the copy-and-paste functions in the shortcut menu to copy column values within a master method or from one master method to another. You can use these copy-and-paste techniques on any pages with grids of data in the Compounds and QAQC views.

After you copy grid values to the Clipboard, you can paste them into a text application such as Notepad, an email, a spreadsheet, other grid cells in the same master method, or into another master method.

Tip When copying data into an application other than a TraceFinder master method grid, use the Copy with Headers command instead of the Copy command in the shortcut menu to preserve the column headers.

Follow these procedures:

- [To copy a value from one cell to another cell](#)
- [To copy all values in a column to another column](#)
- [To copy multiple columns](#)
- [To copy an entire grid to another master method](#)

❖ **To copy a value from one cell to another cell**

1. Select a cell value to copy to the Clipboard.

You can select either an entire table cell or just a cell value.



2. Right-click and choose **Copy** from the shortcut menu.

The application copies either the selected cell value or the selected cell to the Clipboard.

3. In this or another master method, select the cell value or table cell that you want to overwrite.
 - If you copied a cell value, you can select the cell value or simply click in the cell.
 - If you copied an entire cell, you must select a table cell to overwrite.
4. Right-click and choose **Paste** from the shortcut menu.

The application replaces the selected value with the value copied to the Clipboard.

❖ **To copy all values in a column to another column**

1. Use the SHIFT key to select the column to copy.

Cal_1
5.000
5.000
5.000
5.000

2. Right-click and choose **Copy** from the shortcut menu.
3. In this or another master method, use the SHIFT key to select the column to overwrite.

Cal_3
10.000
10.000

4. Right-click and choose **Paste** from the shortcut menu.

The application overwrites the selected cells with the cells that you copied to the Clipboard.

Cal_3
5.000
5.000
5.000
5.000

❖ **To copy multiple columns**

1. Use the SHIFT key to select the columns to copy.

Cal_1	Cal_2
5.000	10.000
5.000	10.000
5.000	10.000
5.000	10.000

2. Right-click and choose **Copy** from the shortcut menu.
3. In this or another master method, use the SHIFT key to select the columns to overwrite.

Cal_A	Cal_B

4. Right-click and choose **Paste** from the shortcut menu.

The application overwrites the selected cells with the cells that you copied to the Clipboard.

Cal_A	Cal_B
5.000	10.000
5.000	10.000
5.000	10.000
5.000	10.000

❖ **To copy an entire grid to another master method**

1. Use the SHIFT key to select all the columns in the grid.

LOD (Detection limit)	LOQ (Quantitation limit)	LOR	ULOL (Linearity limit)	Carryover limit
10.000	20.000	30.000	0e0	0e0
10.000	20.000	30.000	0e0	0e0

2. Right-click and choose **Copy** from the shortcut menu.

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Editing a Master Method

3. In another master method, use the SHIFT key to select the columns to overwrite.

LOD (Detection limit)	LOQ (Quantitation limit)	LOR	ULOL (Linearity limit)	Carryover limit
0.000	0.000	0.000	0e0	0e0
0.000	0.000	0.000	0e0	0e0

4. Right-click and choose **Paste** from the shortcut menu.

The application overwrites the selected cells with the cells that you copied to the Clipboard.

Note When the Clipboard contains more cells of data than there are selected target cells for the paste operation, the application overwrites the selected cells and reports that the Clipboard contents were truncated to fit the grid.

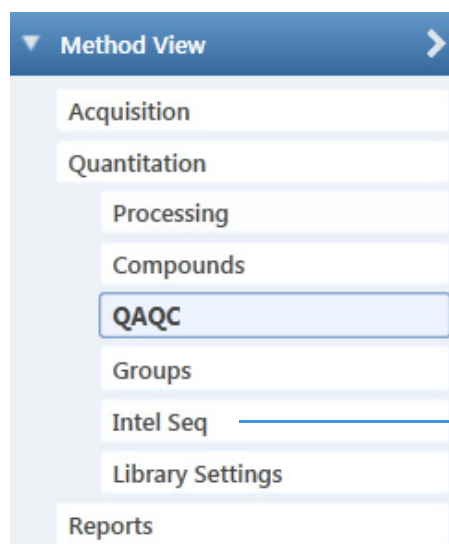
Editing the QAQC Page

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

On most QAQC pages, you can use the copy-and-paste functions in the shortcut menu to copy grid values from one column to another or from one master method to another. For detailed instructions, see “Copying and Pasting Column Values” on page 213.

❖ To open the QAQC page

Click **QAQC** in the Method View navigation pane.



Available only when you activate the Intelligent Sequencing option in the Configuration console

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

- [Limits](#)
- [Calibration](#)
- [Chk Std](#)
- [Matrix Blank](#)
- [ISTD](#)
- [Solvent Blank](#)
- [Threshold](#)

Limits

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

Figure 63. Limits page

Limits	Calibration	Chk Std	Matrix Blank	ISTD	Solvent Blank	Threshold		
	RT	Compound	LOD (Detection limit)	LOQ (Quantitation limit)	LOR	ULOL (Linearity limit)	Carryover limit	
▶ 1	3.14	Propanenitrile	0.000	0.000	0.000	0e0	0e0	

Table 41. 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	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 application compares the initial calibration results for each compound found in the sample to the values defined on this page.

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

Figure 64. Calibration page

Limits	Calibration	Chk Std	Matrix Blank	ISTD	Solvent Blank	Threshold	
	RT	Compound	R ² threshold	Max RSD (%)	Min RF	Max Amt Diff (%)	CV Test (%)
1	3.14	Propanenitrile	0.9900	20.00	0.000	20.00	0.000

Table 42. 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). Note This RSD value is not the same value used in Data Review or the Compound Calibration Report. The application uses this RSD value when you select AverageRF as the curve type for the method. See “Calibration Page” on page 206.
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).
CV Test (%)	Coefficient of Variance test. The coefficient of variance percentage is the standard deviation of the multiple samples of one level, multiplied by 100, and then divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.

Chk Std

Use the Chk Std page to review the calibration on an ongoing basis. The application compares the quality check standard results for each compound in the sample to the initial calibration using values defined on this page.

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

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

Figure 65. Chk Std page

Limits	Calibration	Chk Std	Matrix Blank	ISTD	Solvent Blank	Threshold
	RT	Compound	Max RF Diff (%)	Min RF	CV Test (%)	
1	3.14	Propanenitrile	20.00	0.000	0.00	

Table 43. 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 QC Std sample and the average response factor from the calibration (when in average RF mode).
Min RF	The minimum response factor for the QC Std sample (when in average RF mode).
CV Test (%)	Coefficient of Variance test. The coefficient of variance percentage is the standard deviation of the multiple samples of one level, multiplied by 100, and then divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.

Matrix Blank

Use the Matrix Blank page to define acceptable levels of target compounds in blank samples. The application compares 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.

For detailed descriptions of all the features on the Matrix Blank page, see [Matrix Blank page parameters](#).

In 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

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

❖ To specify the maximum concentration

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

Figure 66. Matrix Blank page

Limits Calibration Chk Std Matrix Blank ISTD Solvent Blank Threshold						
	RT	Compound	Method	Percentage	Max Conc	
▶ 1	3.14	Propanenitrile	Concentration		0.000	
2	3.15	Pyrazinamide	None		0.000	
3	3.67	1,3-Dioxolane, 2-heptyl-	Concentration		0.000	
4	4.70	Pyrazinamide *2*	% of LOD		0.000	
			% of LOQ			
			% of LOR			

Table 44. Matrix 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 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.

ISTD

Use the ISTD page to review the response and retention time of internal standards (when available). The application compares 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 if you have not identified any compounds as internal standards, this page does not show any values.

Figure 67. ISTD page

Limits	Calibration	Chk Std	Matrix Blank	ISTD	Solvent Blank	Threshold	
	RT	Compound	Min recovery (%)	Max recovery (%)	Min RT (-min)	Max RT (+min)	CV Test (%)
▶ 1	3.14	Propanenitrile	50.00	150.00	0.25	0.25	

Table 45. 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 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 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. The coefficient of variance percentage is the standard deviation of the multiple samples of one level, multiplied by 100, and then divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.

Solvent Blank

Use the Solvent Blank page to view or edit QC values for solvent reporting. The application compares the calculated response for each compound in the sample to the maximum response defined on this page.

In the Solvent Blank report, the application flags the calculated values for target compounds that exceed these limits.

Figure 68. Solvent Blank page

Limits		Calibration		Chk Std		Matrix Blank		ISTD		Solvent Blank		Threshold	
	RT	Compound		Method		Upper Limit							
1	3.14	Propanenitrile		None									
2	3.15	Pyrazinamide		All Ion RT		0							
3	3.67	1,3-Dioxolane, 2-heptyl-		Quan Ion RT		0							

Table 46. 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 quantitation ion only (Quan Ion RT) or as a summed response for the quantitation 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.

Threshold

Use the Threshold page (see “[Threshold page](#)” on [page 225](#)) to specify how to create a threshold guide to overlay on compounds in the Comparative View in the Data Review mode. For each compound, you can specify an absolute value or you can specify a percentage of the peak height. The application uses the selected threshold method and the specified amount to create a threshold guide in the Comparative View chromatograms. See “[Comparative View](#)” on [page 468](#).

When you create a batch, you can group samples and then specify a sample in the group as the threshold sample to use in the Comparative View. For instructions about specifying a threshold sample, see “[Threshold Samples Page](#)” on [page 446](#).

5 Using the Method Development Mode for Quantitation Methods

Editing a Master Method

In the following figures, the threshold for the dibutyl phthalate compound is 50 percent of the peak height in the threshold sample ([Threshold page in Method View](#)), the samples Benzo26473, Benzo25557, and Benzo26154 are members of groupB ([Samples page in Batch View](#)), and the threshold sample for the group is Benzo26473 ([Threshold Samples page in Batch View](#)). In the Comparative Data view ([Comparative View in Data Review](#)), you can easily see that the peak height of dibutyl phthalate in the other samples in the group is less than 50 percent of the peak height in the threshold sample.

Figure 69. Threshold page in Method View

Master method: <u>Benzos1</u>													
Limits		Calibration		Chk Std		Matrix Blank		ISTD		Solvent Blank		Threshold	
	RT	Compound	Method	Threshold	Percentage								
	1.91	Benzoic acid, 2-[[[4-(ace...	% of Thresh...		50								
▶	2.72	Dibutyl phthalate	% of Thresh...		50								

Figure 70. Samples page in Batch View

	Status	Groups	Filename
1	●	groupb	Benzo26473
2	●	groupb	Benzo25557
▶ 3	●	groupb	Benzo26154

Figure 71. Threshold Samples page in Batch View

Group	Sample
▶ groupb	Benzo26473

Figure 72. Comparative View in Data Review

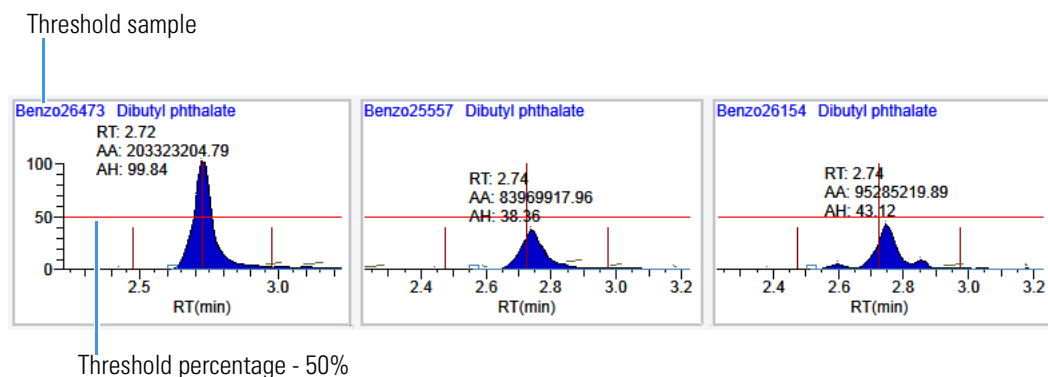


Figure 73. Threshold page

Limits							Calibration							Chk Std							Matrix Blank							ISTD							Solvent Blank							Threshold						
	RT	Compound	Method				Threshold	Percentage																																								
▶	3.14	Propanenitrile	Threshold ▼				1.000																																									
	3.15	Pyrazinamide	Threshold ▼				1.000																																									
	3.67	1,3-Dioxolane, 2-heptyl-	% of Threshold Sample ▼					0.1																																								
	4.70	Pyrazinamide *2*	% of Threshold Sample ▼					0.1																																								

Table 47. Threshold 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	Specifies the threshold method as a specific peak height value (Threshold) or as a percentage of the peak height in the threshold sample (% of Threshold Sample).
Threshold	Specifies the absolute peak height value to use when you select the Threshold method. This value represents the default threshold value to use when you do not specify a Threshold Sample for a group of samples. Default: 1.000
Percentage	Specifies the percentage of the peak height value to use when you select the % of Threshold Sample method. This value represents a percentage of the actual peak height in the Threshold Sample you select for a group of samples. For instructions about specifying a Threshold Sample, see “Threshold Samples Page” on page 446. Valid range: 0.1 through 100.1 Default: 0.1

Editing the Groups Page

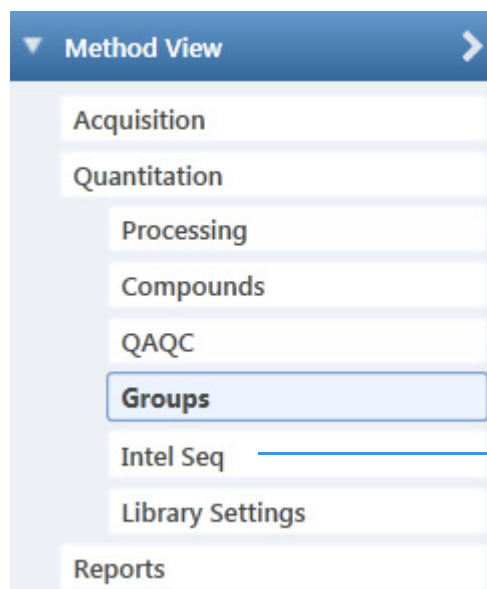
Use the Groups page of the Method View to organize compounds into functional or logical groups. You can use these groups for creating a subset of target compounds. For detailed descriptions of all the features on the Groups page, see “Groups Page.”

For quantitative processing, the 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 open the Groups page

Click **Groups** in the Method View navigation pane.

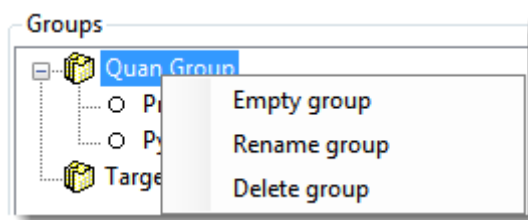


Available only when you activate the Intelligent Sequencing option in the Configuration console

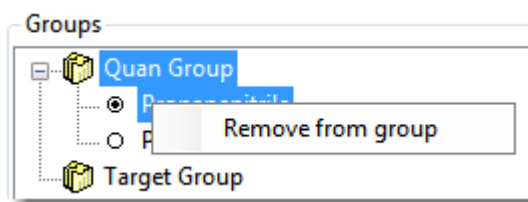
❖ To create a group

1. At the bottom of the Groups area, click **Add Group**.
The Add a New Group dialog box opens.
2. Type a name for the new group and click **OK**.
The new group appears in the Groups area.
3. Drag a compound from the Compounds area onto a group name (as if you were moving files into a folder).

4. 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.



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



Groups Page

Use the features on the Groups page to organize compounds into functional or logical groups.

Figure 74. Groups page

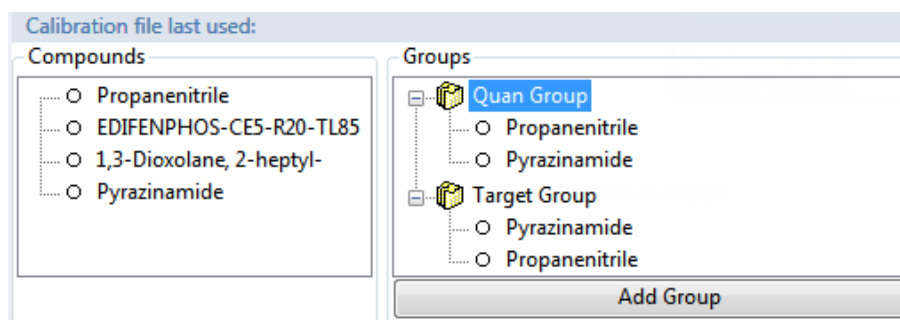


Table 48. Groups page parameters

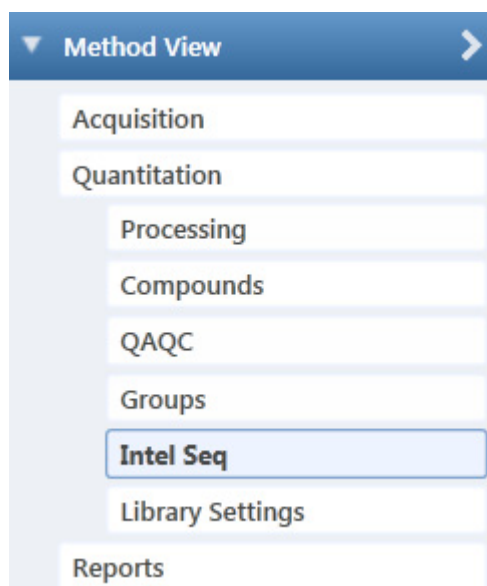
Parameter	Description
Compounds	Lists all available compounds.
Groups	Lists all available groups.
Add Group	Opens the Add a New Group dialog box where you can create a new group.
Shortcut menu	
Empty Group	Removes all compounds from the selected group.
Rename Group	Changes the name of the selected group.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

Editing the Intelligent Sequencing Page

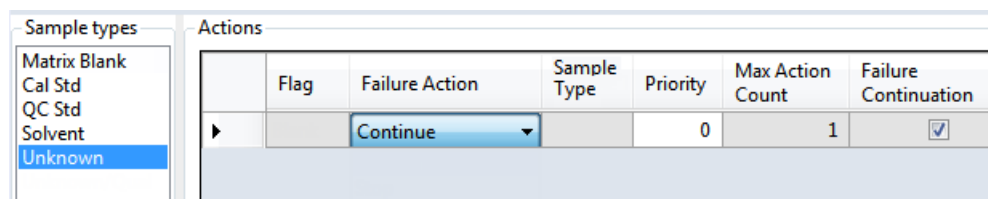
Use the Intelligent Sequencing page to specify the actions you want the application to take when there are acquisition failures with each sample type. The Intelligent Sequencing page is available only when you activate the Intelligent Sequencing option in the Configuration console. See “[Intelligent Sequencing](#)” on [page 62](#).

❖ To open the Intelligent Sequencing page

Click **Intel Seq** in the Method View navigation pane.



The Intelligent Sequencing page opens.

A screenshot of the Intelligent Sequencing page. On the left is a 'Sample types' list with 'Unknown' selected. On the right is an 'Actions' table with one row for the selected sample type.

	Flag	Failure Action	Sample Type	Priority	Max Action Count	Failure Continuation
▶		Continue		0	1	<input checked="" type="checkbox"/>

❖ To specify actions for sample acquisition failures

1. In the Sample Types list, select a sample type.

Each sample type has a specific set of failure flags. See “[Sample-Specific Failure Flags](#)” on [page 231](#).

2. For each failure flag, select a failure action.

The failure action choices are the same for each failure flag except flags for Solvent or Matrix Blank sample types. The Solvent and Matrix Blank sample types do not have Auto Sample or Auto Sample and Reinject failure actions.

Sample types	Actions					
	Flag	Failure Action	Sample Type	Priority	Max Action Count	Failure Continuation
Matrix Blank		Continue		0	1	<input checked="" type="checkbox"/>
Cal Std		Continue				
QC Std		Stop				
Solvent		Auto Sample				
Unknown		Reinject				
		Auto Sample and Reinject				

Each Failure Action requires one or more of the following values:

- Sample Type
- Priority
- Max Action Count
- Failure Continuation

For a detailed description of each of these parameters, see [Actions](#).

3. Select a sample type to use for the failure action.

This value is available only for Auto Sample and Auto Sample and Reinject failure actions. When you create your samples list on the Auto Samples page, you must include at least one sample with this sample type for the autosampler to use when it encounters this error condition. See “[Auto Samples Page](#)” on [page 443](#).

4. In the Priority column, type a priority value for this action.

The priority value can be any positive or negative integer.

- The application performs the failure action for the highest priority failure it encounters and ignores all others.
- When you assign the same priority to two or more failures, the application performs the failure action for the first failure it encounters and ignores all others.

5. In the Max Action Count column, type a value for the maximum number of times the application should repeat a sample.

6. In the Failure Continuation column, do one of the following:

- Select the check box to skip this sample and continue to the next sample when this sample exceeds the Max Action Count value.
- Clear the check box to stop the batch when this sample exceeds the Max Action Count value.

Example

The following example shows the actions that the application uses when the acquisition for a sample fails.

Flag	Failure Action	Sample Type	Priority	Max Action Count	Failure Continuation
Ion Ratio Failure	Auto Sample and Reinject	Solvent	0	2	<input checked="" type="checkbox"/>
Carryover	Continue			1	<input type="checkbox"/>

1. The acquisition encounters an Ion Ratio Failure error on a sample.
2. The application runs a Solvent sample.
3. The application reinjects the original sample.
4. This action is priority 0 in the Acquisition queue.
5. The application repeats this autosample and reinject process two times.
6. After repeating the failure action two times, the application skips the sample and continues to the next sample.

Actions

Use the Actions pane to specify what action the application takes when it encounters a submission failure for the type of failure flag associated with each sample type.

Flag	Failure Action	Sample Type	Priority	Max Action Count	Failure Continuation
Blank	Continue		0	1	<input checked="" type="checkbox"/>

Table 49. Actions parameters (Sheet 1 of 2)

Parameter	Description
Flag	Flag (error) types specific to each sample type. See Sample-Specific Failure Flags . Each flag type has a set of user-specified actions that the application follows when it encounters this error.
Failure Action	In the event of a failed sample, the application does one of the following: <ul style="list-style-type: none"> • Continue: Continues to the next sample in the batch. • Stop: Stops the batch. • Auto Sample: Injects the sample type specified for the Auto Sample Type parameter and continues to the next sample. • Reinject: Reinjects the current sample by inserting a “reinject” sample in the batch. • Auto Sample and Reinject: Injects the sample type specified for the Auto Sample Type parameter and then reinjects the failed sample.

Table 49. Actions parameters (Sheet 2 of 2)

Parameter	Description
Sample Type	<p>Specifies either a Solvent or Matrix Blank sample type to use for the auto sample injection.</p> <p>Default: Solvent</p>
Priority	<p>The priority value can be any positive or negative integer.</p> <p>When two or more failures have the same priority, the application performs the failure action for the first failure it encounters and ignores all others.</p> <p>The application performs the failure action for the highest priority failure and ignores all others.</p>
Max Action Count	<p>Specifies the maximum number of times the application should repeat a sample before it continues to the next sample or stops the sequence, as determined by the value in the Failure Continuation parameter.</p> <p>Default: 1</p>
Failure Continuation	<p>When this check box is selected, samples that exceed the value specified for the Max Action Count parameter cause the application to skip the sample and continue to the next sample.</p> <p>When this check box is cleared, samples that exceed the value specified for the Max Action Count parameter cause the application to stop the batch.</p> <p>Default: Selected</p>

Sample-Specific Failure Flags

Each sample type has a specific set of failure flags.

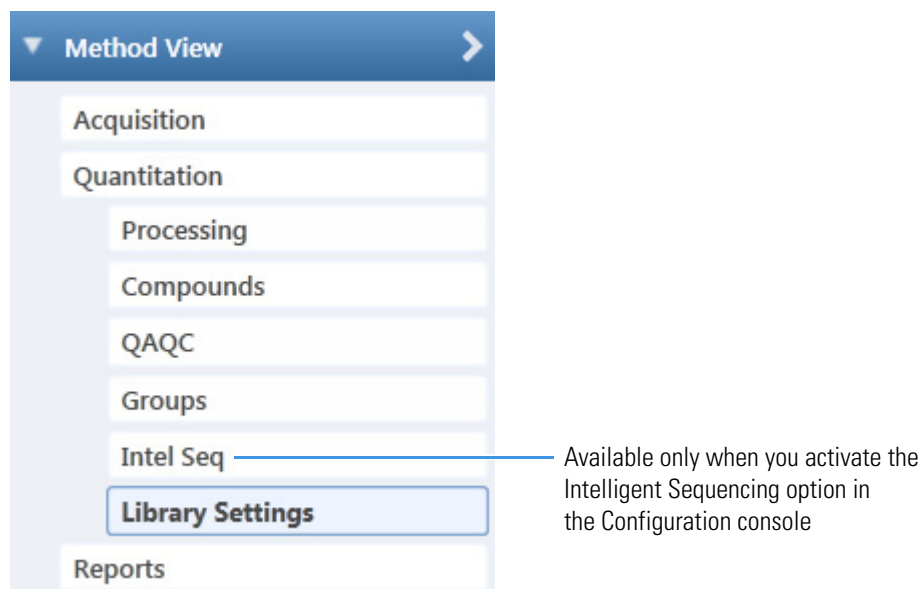
Sample Type	Flag
Matrix Blank	<ul style="list-style-type: none"> Blank
Cal Std	<ul style="list-style-type: none"> Out of Range Ion Ratio Failure Carryover
QC Std	<ul style="list-style-type: none"> Ion Ratio Failure Carryover Out of Range
Solvent	<ul style="list-style-type: none"> Solvent Flag
Unknown	<ul style="list-style-type: none"> Ion Ratio Failure Carryover

Editing the Library Settings Page

Use the Library Settings page to specify settings to use for library searches.

❖ To open the Library Settings page

Click **Library Settings** in the Method View navigation pane.



The Library Settings page opens. See [Library Settings page](#).

Figure 75. Library Settings page

The screenshot shows the Library Settings page with the following parameters:

- General Library Settings:**
 - MS Order: MS (dropdown)
 - Use Isolation Width:
- NIST Settings:**
 - Search Type: Normal (dropdown)
 - Precursor tolerance: 1.60 (spin box)
 - Product tolerance: 1.60 (spin box)
 - Ignore Precursor:
 - Use alt peak matching:
 - Reverse Search:
 - Presearch: Default (dropdown)
 - SI Threshold: 250 (spin box)
 - RSI Threshold: 250 (spin box)
 - Probability Threshold: 10.00 (spin box)
- Library Manager Settings:**
 - Spectrum Tolerance: 5.00 (spin box)
 - Score Threshold: 80.00 (spin box)
 - Ignore Precursor:
 - Reverse Search:

Table 50. Library Settings page parameters (Sheet 1 of 3)

Parameter	Description
General Library Settings	
MS Order	Specifies that the confirming peaks come from the same scan (MS), are fragments from an adjacent scan (MS2), or come from the Source CID (MS–In Source CID).
Use Isolation Width	Specifies that the application use the isolation width to determine if there is an MS/MS within the same peak RT window that includes the precursor fragments. Available only when you set the MS Order to MS2 .

Table 50. Library Settings page parameters (Sheet 2 of 3)

Parameter	Description
NIST Settings	
Search Type	<p>Normal: Uses a more extensive set of presearch screenings—a total of four different criteria.</p> <p>MS/MS: Searches for an MS/MS spectrum in a library of MS/MS spectra.</p> <p>In-source HiRes: Searches for an in-source/EI with an accurate ion m/z or an MS/MS spectrum in a library that contains in-source/EI accurate ion m/z or MS/MS spectra.</p>
Precursor Tolerance	<p>Specifies the precursor m/z tolerance range as either amu or ppm.</p> <p>Valid range: 0.015 through 100 000 Default: 1.60</p> <p>Available only when you select MS/MS or In-source HiRes search types.</p>
Product Tolerance	<p>Specifies the mass spectral peak tolerance range as either amu or ppm.</p> <p>Valid range: 0.015 through 100 000 Default: 1.60</p> <p>Available only when you select MS/MS or In-source HiRes search types.</p>
Ignore Precursor	<p>Ignores mass spectral peaks within the specified precursor tolerance range.</p> <p>Available only when you select MS/MS or In-source HiRes search types.</p>
Use Alt Peak Matching	<p>Specifies that the application use alternate peak matching.</p> <p>Available only when you select MS/MS or In-source HiRes search types.</p>
Reverse Search	<p>Specifies that the NIST library search use the reverse search method. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).</p>
Presearch	<p>Specifies that the application use presearch screening before calculating the spectrum-by-spectrum match factor.</p>

Table 50. Library Settings page parameters (Sheet 3 of 3)

Parameter	Description
SI Threshold	The lower threshold value for the search index method that is used to search the NIST library. The application does not return results below this value. Valid range: 0 through 999 Default: 250
RSI Threshold	The lower threshold value for the reverse search index method that is used to search the NIST library. The application does not return results below this value. Valid range: 0 through 999 Default: 250
Probability Threshold	Threshold value for the match probability.
Library Manager Settings	
Spectrum Tolerance	Specifies the spectrum tolerance as either amu or ppm. Valid range: 0.1 through 1000.0 Default: 5.00 ppm
Score Threshold	The application does not return results below this value. Valid range: 0 through 100 Default: 80.00
Ignore Precursor	Ignores mass spectral peaks within the specified precursor tolerance range.
Reverse Search	Specifies that the Library Manager search use the reverse search method. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).

Editing the Reports Page

Use the Reports page to specify how you want to save or print your reports. For detailed descriptions of the features on the Reports page, see [Reports Page](#).

For the quantitation report types, you can modify quantitation limits flags, user interface options, and quantitation flag options on the Quan Report Settings page.

See the instructions for the following tasks:

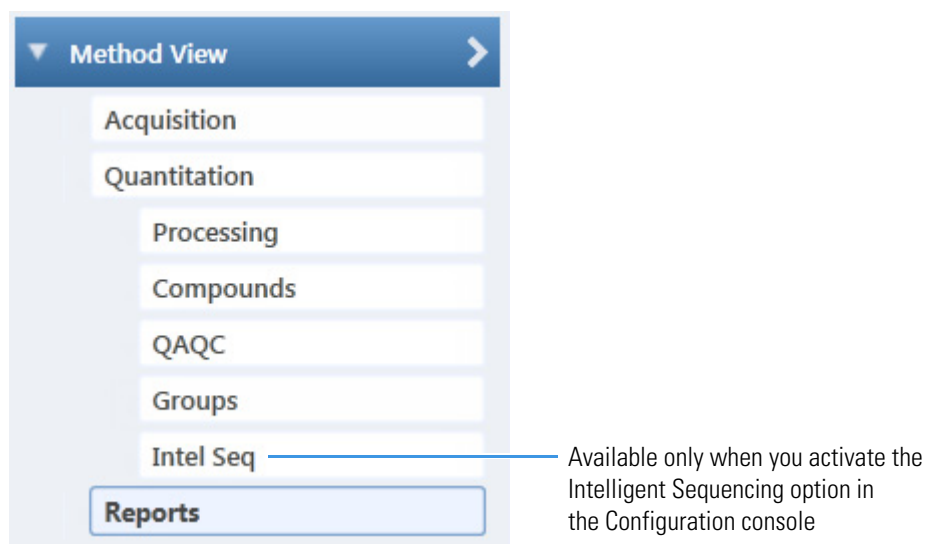
- [Specifying Report Formats](#)
- [Specifying Quan Report Settings](#)

Specifying Report Formats

For each report type, you can create a hard-copy printout, a PDF file, a CSV file, or an Excel file.

❖ To open the Reports page

Click **Reports** in the Method View navigation pane.



The Reports page opens with a list of all configured reports.

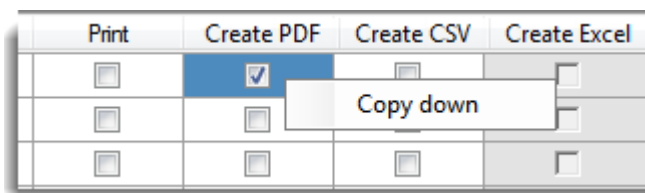
To configure which reports are available when you create a master method or which reports create a batch-level report, see [“Specifying the Reports”](#) on [page 71](#).

❖ To specify report types and output formats

1. To edit the Report Title, double-click the name and type your new custom title.

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

- To specify the type of report output to create for each report type, select the check box in the appropriate column.
- To duplicate an output type for all reports, click the cell to select it, and 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.

Reports Page

Use the features on the Reports page to specify how you want to save or print your reports.

Figure 76. Reports page

	Report	Print	Create PDF	Create CSV	Create Excel	Exists
	Batch Report	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	Blank Report	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	Calibration Report	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Table 51. Reports page parameters

Parameter	Description
Report list columns	
Report	The name of a report.
Print	Sends reports to the default printer.
Create PDF	Saves reports as PDF files.
Create CSV	Saves reports as CSV files.
Create Excel	Saves reports as Excel files.
Exists	Indicates that the report template is identified in the C:\TraceFinderData\3.3\Templates\ReportTemplates folder.

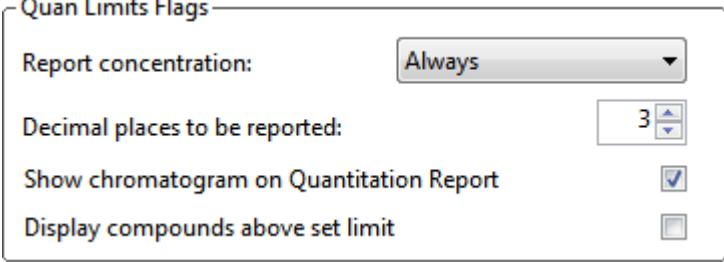
Specifying Quan Report Settings

Use the options on the Quan Report Settings page to choose parameters for flagging values and displaying information in reports. See “[Quan Report Settings Page](#)” on [page 240](#).

Follow these procedures:

- [To specify quantitation limits](#)
- [To specify user interface options](#)
- [To specify quantitation flag options](#)

❖ To specify quantitation limits



Quan Limits Flags

Report concentration: Always

Decimal places to be reported: 3

Show chromatogram on Quantitation Report

Display compounds above set limit

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 “[Editing the QAQC Page](#)” on [page 217](#).

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

User Interface Options	
Shade row when sample is outside of evaluation criteria	<input type="checkbox"/>
Separate ion overlay display	<input checked="" type="checkbox"/>
Use alternate calibration report format	<input type="checkbox"/>

1. To shade a compound row in 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 seven calibration standards, select the **Use Alternate Calibration Report Format** check box.

❖ To specify quantitation flag options

Quan Flag Options	
Flag values below LOD	<input checked="" type="checkbox"/>
Flag values below LOQ	<input checked="" type="checkbox"/>
Flag values above LOR	<input checked="" type="checkbox"/>
Flag values above ULOL	<input checked="" type="checkbox"/>
Flag values above Carryover	<input checked="" type="checkbox"/>
Flag values between LOD and LOQ	<input checked="" type="checkbox"/>

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

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

These flags appear in a variety of reports and are defined in “[Quan Report Settings page parameters](#)” on [page 240](#).

Quan Report Settings Page

Use the features on the Quan Report Settings page to specify parameters for flagging values and displaying information in reports.

Figure 77. Quan Report Settings page

Table 52. 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 in the quantitation report.
Display Compounds Above Set Limit	Prints reports for only the compounds that are found in a sample. If a compound is above the specified Quan Flag Options limits, the application reports the compound. This prevents generating “empty” reports for the compounds that are not found.
User Interface Options	
Shade Row When Sample is Outside of Evaluation Criteria	Shades a compound row in any of the reports if a value fails one of the criteria used for evaluation.

Table 52. Quan Report Settings page parameters (Sheet 2 of 2)

Parameter	Description
Separate Ion Overlay Display	Separates the ion overlay pane from the confirming ion plots in an analysis.
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 seven calibration standards).
Quan Flag Options	Values that are above or below limits defined on the Limits page. These flags appear in 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.

Saving a Master Method to a New Name

You can save any method to a new name, or you can use the current method data to overwrite an existing method. The new method contains all the data of the saved method.

❖ To save a method to a new name

1. From the main menu, choose **File > Save As**.

The Save Master Method As dialog box opens, displaying all available methods.

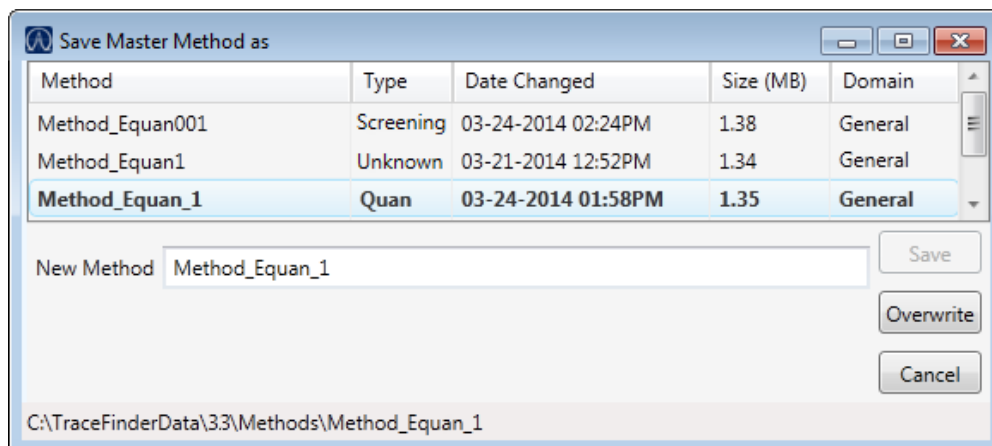


Table 53. Save Master Method As dialog box parameters

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan, Screening, or Unknown Only.
Date Changed	Date the method was last updated.
Size	Size of the method in megabytes.
Domain	TraceFinder domain for which the method was created.
New Method	Name of the new method to create.
<i>Path</i>	Path to the selected method in the Methods folder.

2. Do one of the following:
 - In the New Method box, type a name for the new method.
The application enables the Save button.
 - In the Method column, select a method to overwrite.
The application enables the Overwrite button.
3. Click **Save** or **Overwrite**.

The application saves all the method data using the specified name and opens the Acquisition page of the new method.

Creating a Method Template

In the TraceFinder application, you can create a processing method using a method template that contains common settings. You can create a method template that specifies peak detection criteria, screening libraries, confirming ion criteria, compound calibration, and qualitative peak processing. For a complete description of the features in the Method Template Editor, see “[Method Template Editor](#)” on [page 249](#).

The application uses the settings in the method template to identify the data to display in the Qualitative View. See “[Qualitative View](#)” on [page 475](#).

Only quantitation methods use method templates.

Follow these procedures:

- [To open the Method Template Editor](#)
- [To specify peak criteria](#)
- [To identify the peaks](#)
- [To specify confirming ions](#)
- [To calibrate the compounds](#)
- [To save the method template](#)

❖ To open the Method Template Editor

1. Click **Method Development** in the navigation pane.

The Method Development navigation pane opens.

2. Click **Method View**.



3. From the main menu, choose **File > New > Method Template**.

The Method Template Editor opens. See “[Method Template Editor](#)” on [page 249](#).

❖ To specify peak criteria

Find the peaks*

Sensitivity: Genesis

Limit the retention time range:
Min RT (min): 0.00
Max RT (min): 999.00

Enable peak threshold
% of largest peak: 10
 By height
 By area

Only select top peaks
Select the top: 10
 By height
 By area

Note Parameters in the Find the Peaks* area might also be used for qualitative peak processing.

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 provides 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 application uses the Enable Peak Threshold filter to determine which peaks meet the specified percentage of the height or area 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

Identify the peaks*

Use these libraries

- NISTDEMO
- QED NIST Library

Limit library hits: 3

Best match method: Reverse Search Index

Note Parameters in the Identify the Peaks* area might also be used for qualitative peak processing.

- In the Use these Libraries box, select the libraries that you want to search.
All libraries loaded on your instrument are displayed in the Use these Libraries box.
- To limit the number of matches returned when the system searches a spectrum against the selected libraries, set a value in the Limit Library Hits box.
- To specify how to sort the library searches, select a value from the Best Match Method list.

❖ To specify confirming ions

Handle confirming ions

- Include confirming ions
 - Number of confirming ions: 2
- Specify default ion ratio ranges
 - Ion coelution (min): 0.025
 - Window type: Absolute
 - Window(+/- %): 20.00
- Include compound peak spectrum as reference spectrum

- 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. You can set this value to integers from 1 through 10, inclusive. This value defaults to 2 because you typically perform a 3-ion experiment with one quantitation 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

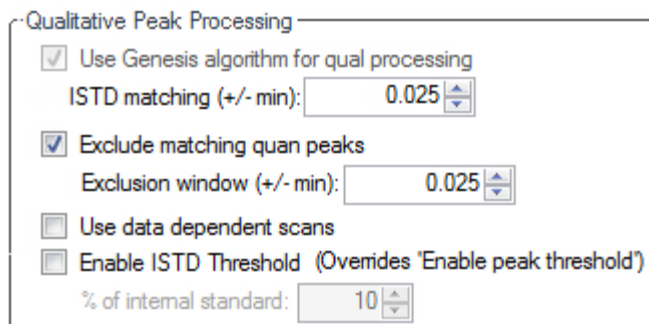
Calibrate the compounds

Calibration method:	External
Curve type:	Linear
Origin:	Ignore
Weighting:	Equal
Response via:	Area

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, the Weighting parameter is unavailable.
 - **Quadratic**: All other settings are available with this exception: When you select Include in the Origin list, the Weighting parameter is unavailable.
 - **Average RF**: The Weighting and Origin parameters are unavailable.
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/X²:** 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/Y²:** 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 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**



Qualitative Peak Processing

Use Genesis algorithm for qual processing
ISTD matching (+/- min): 0.025

Exclude matching quan peaks
Exclusion window (+/- min): 0.025

Use data dependent scans

Enable ISTD Threshold (Overrides 'Enable peak threshold')

% of internal standard: 10

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 that you specify. For additional information about the Genesis algorithm, see [“Genesis Detection Method”](#) on page 43.

This parameter is available only when you set the Sensitivity parameter in the Find the Peaks area to ICIS or Avalon. When you select the Use Genesis Algorithm for Qual Processing check box, the application ignore the Sensitivity parameter in the Find the Peaks area.

2. Select or clear the **Exclude Matching Quan Peaks** check box and specify a value for the exclusion window.

The application excludes quantitative peaks in a range plus or minus the value that 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 MSⁿ scan.

This option constrains the Data Review to only data-dependent scan spectra. See [“Working in the Local Method View”](#) on page 526.

In addition to the peak information, the TIC Report and TIC Summary Report display information about the data-dependent filtered data.

4. To indicate whether to select peaks above a minimum percentage of the nearest internal standard peak that results in compound selection, select the **Enable ISTD Threshold** check box and specify a minimum percentage.

To consider a peak for a processing method, the application uses the Enable ISTD Threshold filter to determine which peaks meet the specified percentage of the height of the nearest internal standard peak.

When you select the Enable ISTD Threshold parameter, the method ignores values set for the Enable Peak Threshold and Only Select Top Peaks parameters. See [“To specify peak criteria”](#) on page 244.

Note When you create a method with the Method Forge, the application ignores the parameters in the Qualitative Peak Processing area.

❖ 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 application saves the new method template in the following folder:

... \TraceFinderData\3.3\Templates\Methods\General

Saved method templates are available when you create a method using Method Forge. See [“Creating a New Method with Method Forge”](#) on page 118.

Method Template Editor

Use the features in the Method Template Editor to specify peak detection criteria, screening libraries, confirming ion criteria, compound calibration, and qualitative peak processing.

Figure 78. Method Template Editor dialog box

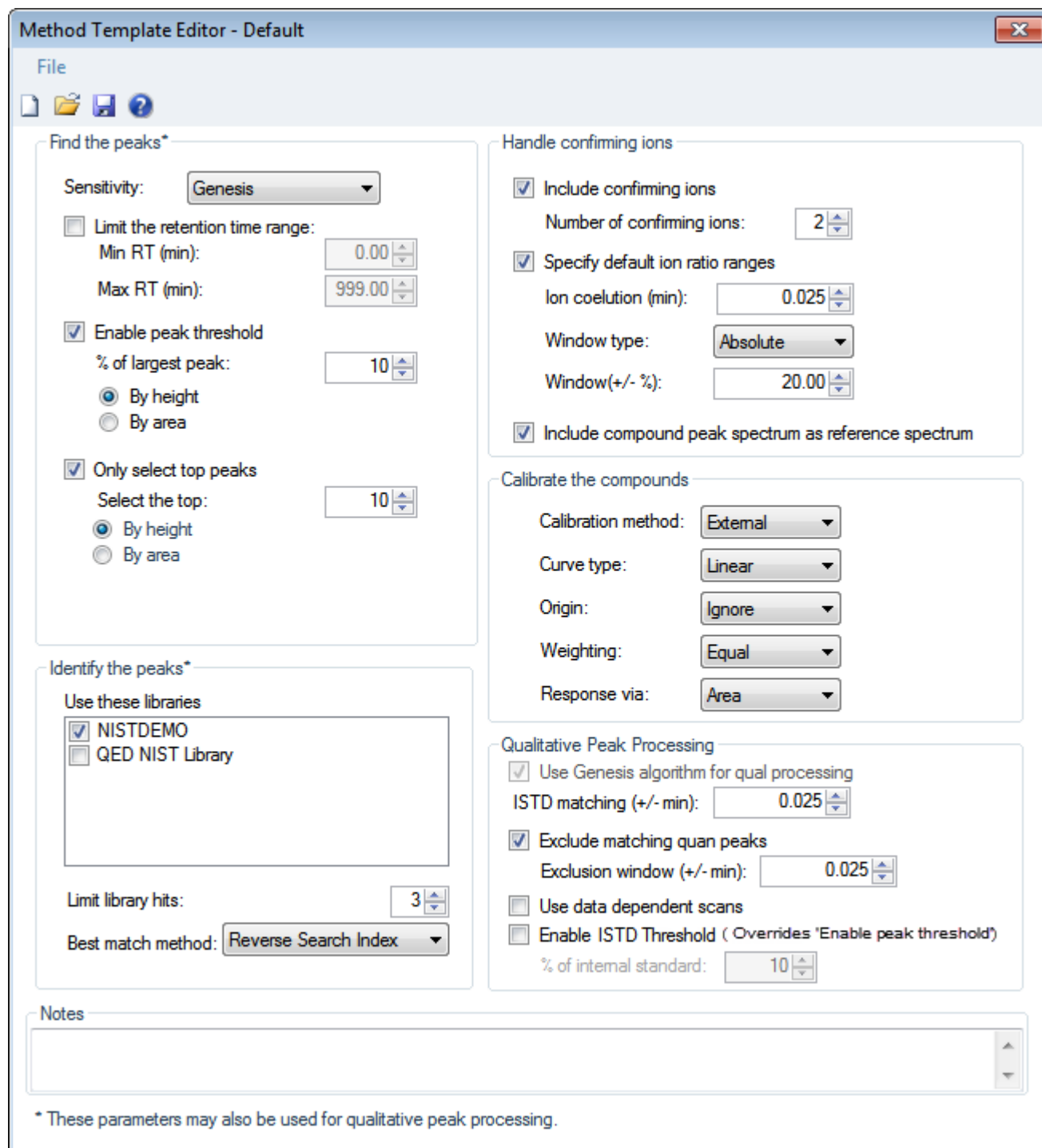


Table 54. Method Template Editor dialog box parameters (Sheet 1 of 3)

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 that you can search.
Limit Library Hits	Specifies the number of matches 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 quantitation mass and two confirming ions. Valid values: Integers from 1 through 10, inclusive.
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 54. 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. <ul style="list-style-type: none"> 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. <ul style="list-style-type: none"> 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/X²: Specifies a weighting of 1/X² 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/Y²: Specifies a weighting of 1/Y² for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).
Response Via	Specifies if the application uses area or height in response calculations. <ul style="list-style-type: none"> 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.
Exclude Matching Quant 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 that you specify.

5 Using the Method Development Mode for Quantitation Methods

Creating a Method Template

Table 54. Method Template Editor dialog box parameters (Sheet 3 of 3)

Parameter	Description
Use Data Dependent Scans	Constrains the Data Review to only data-dependent scan spectra. See “Working in the Local Method View” on page 526. In addition to the peak information, the TIC Report and TIC Summary Report display information about the data-dependent filtered data.
Enable ISTD Threshold	Specifies that, when identifying a peak, qualitative peak processing use the minimum threshold specified as a percentage of the nearest internal standard peak, rather than the threshold specified in the Enable Peak Threshold and Only Select Top Peaks parameters. See Enable Peak Threshold or Only Select Top Peaks in this parameter table.
% of Internal Standard	Percentage of the nearest internal standard peak to use as the minimum threshold for identifying a peak.

Exporting Mass Data

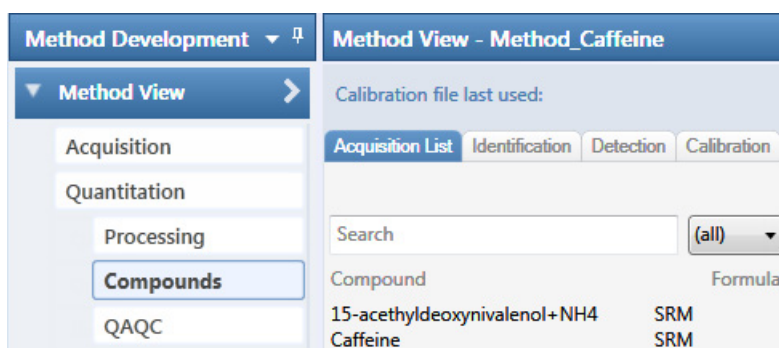
You can export the mass data list from the Compounds page to an XML file that can be read by the TSQ, ISQ, Q Exactive, TSQ Endura, or TSQ Quantiva applications. You can export mass data only from quantitation methods.

❖ To export mass data list to an XML file

1. Open the master method whose mass data list you want to export.

If you make changes to the method, you must save it before you can export the mass data list.

2. To view a list of your mass data, click the **Acquisition List** tab on the Compounds page.



You do not have to display the Acquisition List to export the data, but the compounds in the Acquisition List must contain at least one experiment type appropriate to the export file format. For information about displaying the Acquisition List, see [“Acquisition List”](#) on [page 150](#). For information about editing the experiment type for a compound, see [“Editing Compounds in the Database”](#) on [page 84](#).

3. Choose **Method View > Export Mass List** from the main menu.

IMPORTANT If you have neither a TSQ, an ISQ, a Q Exactive, a TSQ Endura, nor TSQ Quantiva instrument configured, a message asks which format you want to export: Triple Quadrupole, Q Exactive, TSQ Quantiva/Endura SIM, or TSQ Quantiva/Endura SRM.

The application writes the mass data in the Acquisition List to the following folder, using a format compatible with your configured instrument:

...\\TraceFinderData\3.3\Methods\Methodname

For examples of exported mass lists, see the following:

- [“Triple Quadrupole Format”](#) on [page 79](#)
- [“Q Exactive Format”](#) on [page 79](#)
- [“TSQ Quantiva/Endura SIM Format”](#) on [page 79](#)
- [“TSQ Quantiva/Endura SRM Format”](#) on [page 80](#)

Using the Method Development Mode for Target Screening Methods

This chapter includes method development tasks for creating and editing screening master methods. (See [Method Development navigation pane](#).) When user security is activated, you must have Method Development Access permission to use these features.

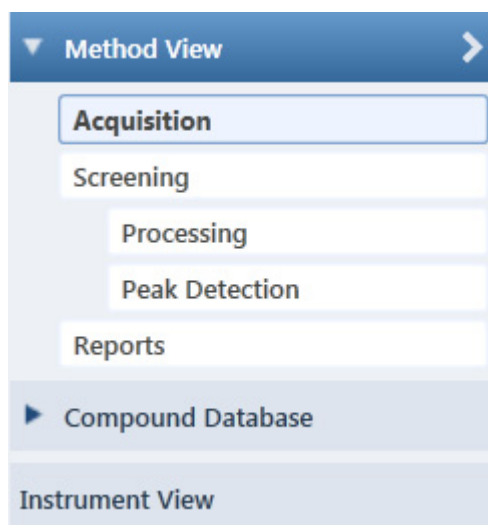
Contents

- [Opening a Master Method](#)
- [Starting a Target Screening Master Method](#)
- [Editing a Master Method](#)
- [Saving a Master Method to a New Name](#)

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

When you create a master method, the application uses the method to determine how the application 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 displays the results, and how the reporting functionality defines the output for your data and results.

The 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.

Figure 79. Method Development navigation pane**Table 55.** Method Development navigation pane commands

Command	Description
Method View	
Acquisition	Displays the Acquisition page of the Method View. Use the features on the Acquisition page to define basic information about the master method. See “Editing the Acquisition Page” on page 261.
Screening	
Processing	Displays the Processing page of the Method View. Use the features on the Processing page to specify peak filter settings, screening databases, and identification and confirmation settings for a target screening method. See “Editing the Processing Page” on page 264.
Peak Detection	Displays the Peak Detection page of the Method View. Use the features on the Peak Detection page to specify any of the following peak detection algorithms: Genesis, ICIS, or Avalon. See “Editing the Peak Detection Page” on page 286.
Reports	Displays the Reports page of the Method View. See “Editing the Reports Page” on page 297.
Compound Database	See “Working with the Compound Database” on page 74.
Instrument View	See “Working with Instrument Methods” on page 108.

Opening a Master Method

A target screening master method contains compound databases, identification and confirmation criteria used in detecting and processing, and settings for reporting compounds.

When you open a target screening master method, the Method View navigation pane displays the available pages for target screening methods. For descriptions of all the features in the Method Development navigation pane, see [“Starting a Target Screening Master Method”](#) on page 259.

❖ To open a target screening method in the Method Development mode

1. Click **Method Development** in the navigation pane.

The Method Development navigation pane opens.

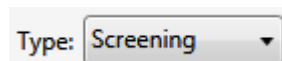


2. Choose **File > Open > Master Method** from the main menu.

The Open Master Method dialog box opens, displaying all available methods.

Tip You can also open one of your most recently used master method files. Choose **Files > Recent Files > Method**.

3. Select **Screening** in the Type list.



The method list displays only target screening methods. See [Open Master Method dialog box](#).

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

The Acquisition page for the selected method opens. To edit the master method, see [“Editing a Master Method”](#) on page 261.

The navigation pane displays the available pages for target screening methods. For descriptions of all the features in the Method Development navigation pane, see [“Starting a Target Screening Master Method”](#) on page 259.

6 Using the Method Development Mode for Target Screening Methods

Opening a Master Method

Figure 80. Open Master Method dialog box

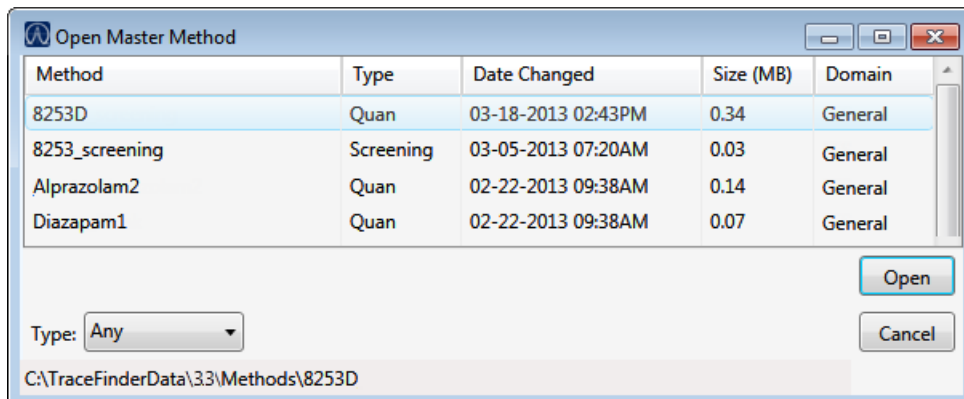


Table 56. Open Master Method dialog box parameters

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan, Screening, or Unknown Only.
Date Changed	Date the method was last updated.
Size	Size of the method in megabytes.
Domain	TraceFinder domain for which the method was created.
Type	Type of method to display: Quan, Screening, Unknown Only, or Any.
<i>Path</i>	Path to the selected method in the TraceFinderData\3.3\Methods\General folder.

Starting a Target Screening Master Method

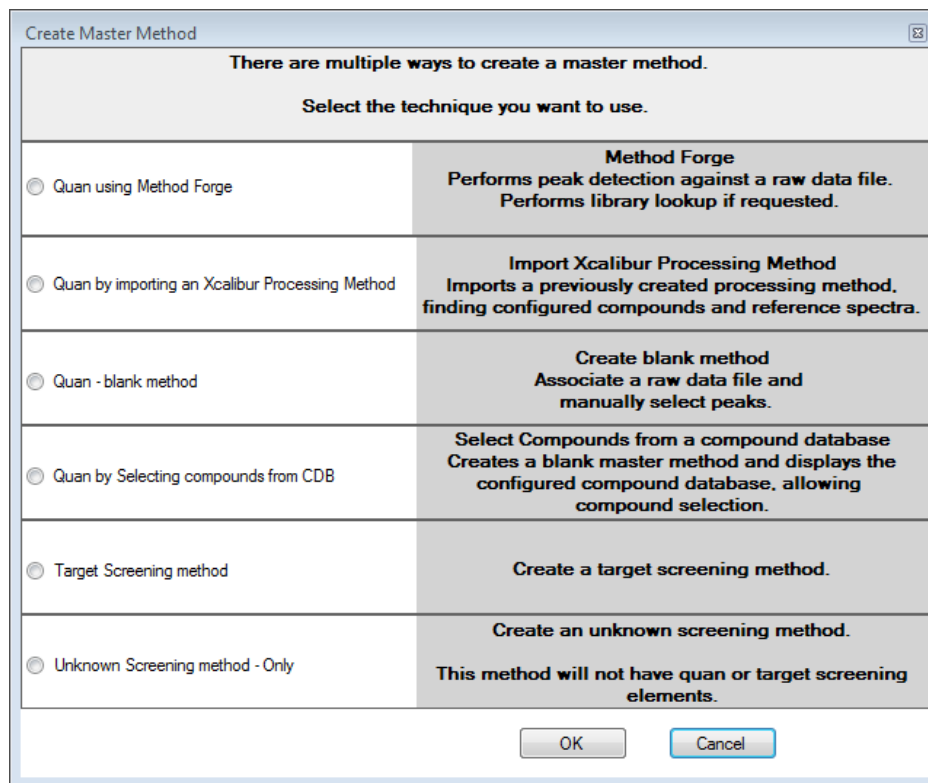
The following procedure includes the basic parameters you must define to create and save a target screening master method. For a detailed description of how to modify all parameters in a master method, see [“Editing a Master Method”](#) on page 261.

❖ To create a new method

1. Choose **File > New > Master Method** from the main menu.

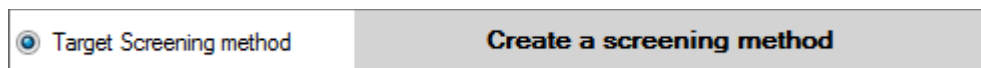
The Create Master Method dialog box opens.

Figure 81. Create Master Method dialog box



IMPORTANT The Unknown Screening Method - Only feature is available only when you select the Allow Unknown Screening option in the application configuration console. See [“Processing Options”](#) on page 62.

2. Select the **Target Screening Method** option and click **OK**.

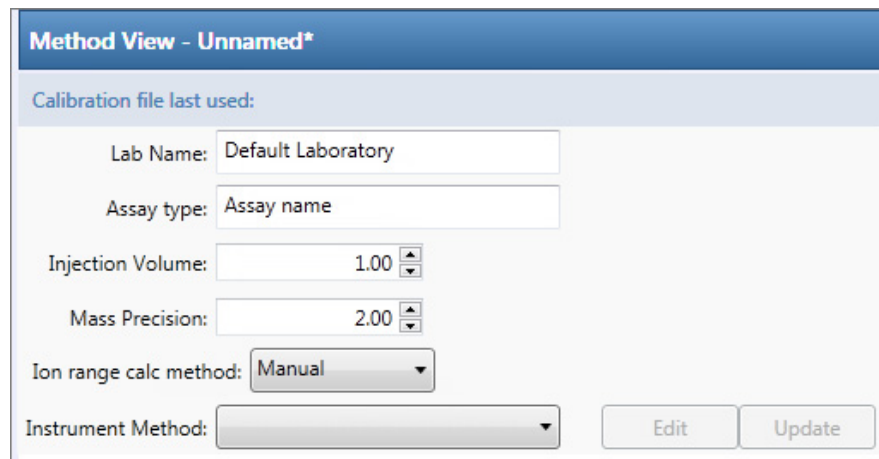


The Method View for a target screening method includes the Acquisition, Processing, Peak Detection, and Reports pages.

6 Using the Method Development Mode for Target Screening Methods

Starting a Target Screening Master Method

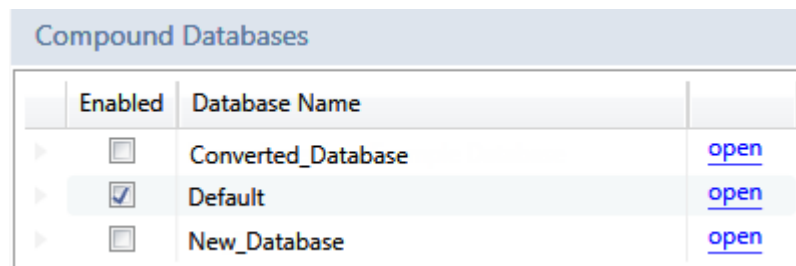
The Acquisition page for the method opens.



3. From the Instrument Method list, select an instrument method.
4. Click **Processing** in the Method View navigation pane.

The Processing page for the method opens. The application lists the compound databases (.cdb) that are stored in the following folder:

...\\Thermo\\TraceFinder\\3.3\\General\\Databases



Enabled	Database Name	
<input type="checkbox"/>	Converted_Database	open
<input checked="" type="checkbox"/>	Default	open
<input type="checkbox"/>	New_Database	open


5. Select the **Enabled** check box for at least one compound database.

You must select at least one compound database before you can save the method. The target screening method uses only the target list of compounds in the selected compound databases to identify the compounds in the samples.

6. To save the new method, choose **File > Save** from the main menu.
7. In the Save Master Method dialog box, type a name for the method and click **OK**.

For a detailed description of how to modify a master method, see [Editing a Master Method](#).



This animation shows how to create a new target screening method. To view the animation, click , and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.

Editing a Master Method

You can open a master method to specify method instructions, reporting options, peak filter settings, screening databases, identification and confirmation settings, and peak detection parameters.

See the instructions for the following tasks:

- [Editing the Acquisition Page](#)
- [Editing the Processing Page](#)
- [Editing the Peak Detection Page](#)
- [Editing the Reports Page](#)

Editing the Acquisition Page

Use the features on the Acquisition page to define basic information about the master method.

❖ To edit the parameters on the Acquisition page

1. Click **Acquisition** in the Method View navigation pane.

The Acquisition page for the method opens. See “[Acquisition Page](#)” on [page 263](#).

2. 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.

3. In the Assay Type box, type the assay type to be targeted by the method.
4. From the Injection Volume box, select the injection volume (in μL) to be used for sample injection.

Valid range: 0.1 through 2000 μL

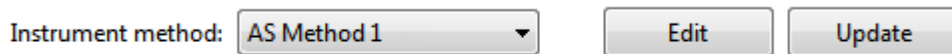
Use the up/down arrows to change the volume in increments/decrements of 1.0 μL , or use the keyboard to enter non-integer injection volumes.

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

5. From the Mass Precision box, select the number of decimal places to be used in reports and in peak and spectrum displays.

Valid values: Integers from 2 through 6, inclusive

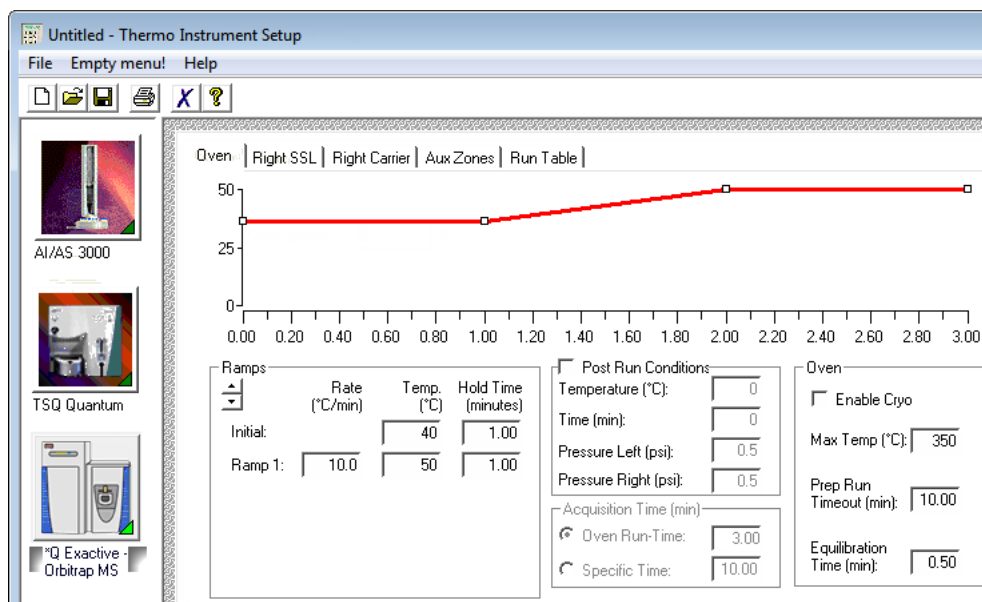
- From the Instrument Method list, select an instrument method.



- To edit the instrument method, click **Edit**.

The Thermo Instrument Setup window opens. This example of an instrument setup shows multiple configured instruments. (See [Thermo Instrument Setup window](#).)

Figure 82. Thermo Instrument Setup window



- Edit the values on the instrument page for your instrument.
- From the main menu in the Thermo Instrument Setup window, choose **File > Save** and then choose **File > Exit**.

The application returns you to the Acquisition page of the Method View.

Acquisition Page

Use the features on the Acquisition page to define basic information about the master method.

Figure 83. Acquisition page for a target screening method

The screenshot shows a software interface titled "Method View - Method_Screening_Alprazolam". Below the title bar, there is a section for "Calibration file last used:". The main area contains several input fields: "Lab name" with the value "Default Laboratory", "Assay type" with the value "Assay name", "Injection volume" with a spinner set to "10.00", and "Mass Precision" with a spinner set to "2". At the bottom, there is a dropdown menu for "Instrument method" set to "Instrument1", and two buttons labeled "Edit" and "Update".

Table 57. Acquisition page parameters (Sheet 1 of 2)

Parameter	Description
Lab Name	<p>The laboratory name to be displayed on the top of each printed, saved, or exported report.</p> <p>Default: Default Laboratory</p> <p>To specify this default laboratory name, see “Specifying Application Defaults” on page 37.</p>
Assay Type	<p>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).</p>
Injection Volume	<p>The system uses the injection volume (in μL) for sample injection. For a more detailed explanation, refer to the documentation for the autosampler.</p> <p>The injection volume in the master method overrides the injection volume in the instrument method.</p> <p>The injection volume in the batch overrides the injection volume in the master method.</p> <p>Valid range: 0.1 through 2000 μL</p>

Table 57. Acquisition page parameters (Sheet 2 of 2)

Parameter	Description
Mass Precision	Number of decimal places used in reports and in peak and spectrum displays. Valid values: Integers from 2 through 6, inclusive
Instrument Method	Instrument method used for acquiring samples.
Edit	Opens the Thermo Instrument Setup window where you can edit the instrument method.
Update	Choose one of the following: <ul style="list-style-type: none">• Send to System Methods: Overwrites the instrument method in the C:\TraceFinderData\3.3\Methods folder with the current instrument method.• Get From System Methods: Overwrites the current instrument method with the instrument method in the C:\TraceFinderData\3.3\Methods folder.

Editing the Processing Page

Use the features on the Processing page to specify peak filter settings, screening databases, and identification and confirmation settings for a master method.

Follow these procedures:

- [To open the Processing page](#)
- [To specify peak filter settings for limiting the display of unwanted data](#)
- [To add unknown screening to the method](#)
- [To specify compound databases](#)
- [To specify identification and confirmation settings](#)

❖ To open the Processing page

Click **Processing** in the Method View navigation pane.

The Processing page for the method opens. See “[Processing Page](#)” on [page 271](#).

❖ To specify peak filter settings for limiting the display of unwanted data

Peak Filter Settings			
Use RT Limits	<input type="checkbox"/>	Search from	<input type="text" value="0.00"/> minutes
		to	<input type="text" value="999.00"/> minutes
Use Matrix Blank	<input type="checkbox"/>	Amplifier	<input type="text" value="1.00"/>
Chromatogram View Width			<input type="text" value="0.75"/> minutes
Use Source CID Scans	<input type="checkbox"/>		
Show all compounds	<input type="checkbox"/>		

- To set a retention time range that excludes searching for peaks outside the range, do the following:
 - Select the **Use RT Limits** check box.
- To use one or more matrix blank samples for subtraction to filter the resulting peaks, do the following:
 - Select the **Use Matrix Blank** check box.

The application activates the Search From and To options.

- In the Search From box, enter the lower limit; in the To box, enter the upper limit.

The application activates the Amplifier option.

During automatic processing, the application subtracts the areas of the peaks in the matrix blank samples from the matching areas in the unknown samples.

To determine the pair of peaks to subtract from each other, the application selects the two peaks with the mass and the retention time that are closest to each other (as defined in the compound database), within the mass tolerance specified in the method.

When the same compound peak (same mass and retention time within the predefined tolerance windows) is in multiple selected matrix blank samples, the application subtracts only the one with the highest area.

When a compound peak in one matrix blank sample has the same primary ion as another peak in a different matrix blank sample but has different adducts, the application uses all the adducts from both these peaks for subtraction purposes. For example, if a compound has the M+H and M+Na ions in one matrix blank sample, and this same compound has the M+H and M+NH₄ ions in another matrix blank sample, the application uses for subtraction the area that results from all of these ions.

When no matrix blank sample exists in the sequence, or if one or more matrix blank samples exist but you do not select the Use Matrix Blank check box, then subtraction does not occur. If subtraction occurs and the subtracted area is less than 0, the application sets the subtracted area to 0.

- b. In the Amplifier box, type an amplifier value.

Use the up/down arrows to change the value in increments/decrements of 1 unit, or use the keyboard to enter non-integer values.

The application multiplies a matrix blank area by this value before performing subtraction. The larger the amplifier value, the more peaks the application filters from the final results.

In the Batch View for sequences created with this method, you can select which matrix blank samples to use for subtraction. See “Blank Subtraction” on page 535.

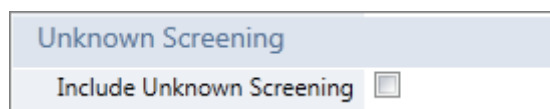
3. In the Chromatogram View Width box, type a value to define the chromatogram viewing range in the Data Review view.
4. To use source CID scans for target screening confirmation (fragment ion or library search), select the **Use Source CID Scans** check box.

When you select this check box, the application uses the source CID scans when they are available in the data file. If they are not available, then the application uses AIF or MS/MS scans when available.

5. To display all compounds from the compound databases in the Data Review display (regardless of whether there is a match in the samples), select the **Show All Compounds** check box.

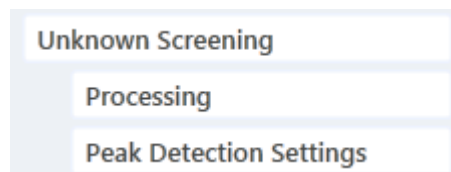
❖ To add unknown screening to the method

1. Select the **Include Unknown Screening** check box.



IMPORTANT The Include Unknown Screening check box is available only when you select the Allow Unknown Screening option in the application configuration console. See “Processing Options” on page 62.

The application adds the Unknown Screening features to the Method View navigation pane.



2. To specify unknown screening settings for peaks, libraries, databases, elements, and ChemSpider searches, click **Processing**.

For further instructions, see “Editing the Processing Page” on page 264.

3. To specify unknown screening peak detection settings, click **Peak Detection Settings**.

For further instructions, see “Editing the Peak Detection Page” on page 286.

The application indicates that a target screening method includes unknown screening in the following locations:

- In the Batch View in the Analysis mode, when you create a batch using a target screening method, the title bar indicates that the method includes unknown screening.

Batch View - Batch_X [Screening with Unknown]

- In the Analysis navigation pane, the application displays access to local methods for both target screening and unknown screening.
- In the Submit Options dialog box, when you submit a batch, the Process Data area shows all processing method types for the batch.

<input checked="" type="checkbox"/> Process data			
Quantitation :	<input type="checkbox"/> Peak Detect	<input type="checkbox"/> Quantitate	
Unknown Screening :	<input type="checkbox"/> Peak Detect	<input type="checkbox"/> Identify	<input type="checkbox"/> With RT Alignment

You can select the detection options for each processing method that you want to use when you submit the batch.

❖ To specify compound databases

Compound Databases		
Enabled	Database Name	
<input type="checkbox"/>	Converted_Database	open
<input checked="" type="checkbox"/>	Default	open
<input type="checkbox"/>	New_Database	open

1. Select the **Enabled** check box for at least one compound database.

The Compound Databases pane displays all compound databases stored in the ...\\Thermo\\TraceFinder\\3.3\\General\\Databases folder.

2. (Optional) To edit a database, click **Open** and do the following:
 - a. Edit the database.
See “Editing Compounds in the Database” on page 84.
 - b. When you finish editing the database, click **Processing** in the Method View navigation pane to return to the Processing page.

❖ To specify identification and confirmation settings

Note The Identification and Confirmation Settings pane displays parameters for identifying or confirming compounds. For additional information about the confirmation and identification process, see “Understanding the Identification and Confirmation Process” on page 279.

Identification and Confirmation Settings			
Peaks	<input checked="" type="checkbox"/> <i>m/z</i>	Threshold Override	<input type="checkbox"/> 5,000
		S/N Ratio Threshold	5.0
		Mass Tolerance:	5 ppm
Retention Time	<input checked="" type="checkbox"/> Identify <input type="checkbox"/> Confirm	Ignore if Not Defined	<input type="checkbox"/>
		Window Override (sec)	<input type="checkbox"/> 30
Fragment Ions	<input checked="" type="checkbox"/> Identify <input type="checkbox"/> Confirm	Ignore if Not Defined	<input type="checkbox"/>
		Min. # of Fragments	1
		Intensity Threshold	10,000
		Mass tolerance	5 ppm
Isotopic Pattern	<input checked="" type="checkbox"/> Identify <input type="checkbox"/> Confirm	Fit Threshold (%)	90
		Allowed Mass Deviation (ppm)	5
		Allowed Intensity Deviation (%)	10
		Use Internal Mass Calibration	<input type="checkbox"/>
Library Search		Library Search Type:	NIST
	<input checked="" type="checkbox"/> Identify <input type="checkbox"/> Confirm	Score Threshold (%)	80
		Use Reverse Library Searching Only	<input type="checkbox"/>

1. To set a target threshold override and include only peaks with areas above this designated threshold, do the following:

- a. Select the **Threshold Override** check box.
- b. In the associated box, type the threshold as an area value.

This threshold overrides the Response Threshold value set in the compound database. The application ignores the peaks with areas below your specified threshold.

- c. To include only peaks with signal-to-noise ratios (S/Ns) that are above a specified value, in the S/N Ratio Threshold box, type the threshold as a ratio value.

The application ignores the peaks with S/Ns that are below the specified threshold.

2. In the Mass Tolerance box, type a mass tolerance value and then select **ppm** or **mmu** for the mass tolerance units.

The application applies this mass tolerance to the extracted chromatograms.

3. To specify the Retention Time option, do the following:
 - a. Select either the **Identity** or **Confirm** check box.
 - b. Select the **Window Override** check box and type the window value.

This window overrides the RT Window value that was set in the compound database and includes only peaks within this designated window. The application identifies or confirms the presence of a compound only when its measured retention time matches the target compound's expected retention time within the specified Window Override retention time.

For additional information about how the application identifies retention time, see ["Retention Time"](#) on page 281.

4. To specify the Fragment Ions option, do the following:
 - a. Select either the **Identity** or **Confirm** check box.
 - b. To ignore the Fragment Ions options when no fragment is defined in the compound database, select the **Ignore if Not Defined** check box.

When the compound database does not define fragments for a compound, the application does not include the results of identification or confirmation for fragment ions in the target screening results.

- c. In the Min. # of Fragments box, type the minimum number of fragments required to identify or confirm the presence of a compound.
 - d. In the Intensity Threshold box, type the intensity threshold value.

The intensity of a fragment must be above this threshold to be identified or confirmed.

- e. In the Mass Tolerance box, type a mass tolerance value and then select **ppm** or **mmu** for the mass tolerance units.

This mass tolerance value indicates the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value for the fragment ions. It is separate from the mass tolerance value specified for the parent peak.

Note When using ion trap data, the application uses 300 mmu regardless of the value you enter here.

For additional information about how the application identifies fragment ions, see ["Fragment Ions"](#) on page 281.

5. To specify the Isotopic Pattern option, do the following:

- a. Select either the **Identity** or **Confirm** check box.
- b. In the Fit Threshold box, type the fit threshold percentage.

To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

- c. In the Allowed Intensity Deviation box, type a value to specify the allowed intensity deviation of the mass spectrometer relative to the monoisotopic ion, as a percentage of the base peak height.

The TraceFinder isotopic pattern algorithm considers an isotope peak as not found if its intensity, relative to the monoisotopic ion's intensity, is more than the deviation percentage from the theoretical relative intensity of the isotope ion. For best results, set this value to a number that causes up to 98% of all intensity deviations to be smaller than the allowed intensity deviation value.

- d. To specify that isotopic pattern calculations use internal mass calibration instead of external mass calibration, select the **Use Internal Mass Calibration** check box.

When this check box is selected, the application applies a requirement that an isotope's m/z must be closer to its theoretical value to avoid a score penalty.

For additional information about how the application calculates isotopic pattern scores, see [“Isotopic Pattern”](#) on [page 282](#).

6. To specify the Library Search option, do the following:

- a. Select either the **Identity** or **Confirm** check box.
- b. Select a Library Search Type, either **NIST** or **Library Manager**.
- c. Type the threshold value in the Score Threshold box.

The resulting score percentage from a library search match must be higher than your entered threshold value to identify or confirm the presence of a compound.

- d. To compare a library entry to an unknown compound, select the **Use Reverse Library Searching Only** check box.

A forward search compares the mass spectrum of an unknown compound to a mass spectral library entry.

For additional information about how the application performs library searches, see [“Library Search”](#) on [page 283](#).

Processing Page

The Processing page includes the following panes:

- Settings

Use the features in the Settings pane to specify peak filter settings. See [Settings pane on the Processing page](#).

- Target Screening Settings

Use the features in the Target Screening Settings pane to specify screening databases and identification and confirmation settings. See [“Target Screening Settings pane on the Processing page” on page 273](#).

Figure 84. Settings pane on the Processing page

Table 58. Settings pane parameters (Sheet 1 of 2)

Parameter	Description
Peak Filter Settings	
Use RT Limits	Specifies a lower and upper limit for searches. Valid range: 0.00 through 999.99 minutes Default: 0.00 minutes for lower limit; 999.00 minutes for upper limit
Use Matrix Blank	Specifies that during automatic processing, the application subtracts the areas of the peaks in the selected matrix blank samples from the matching areas in the unknown samples.
Amplifier	The application multiplies a matrix blank area by this value before performing subtraction. The larger the amplifier value, the more peaks the application filters from the final results. Valid range: .01 through 1000.00 Default: 1.00

Table 58. Settings pane parameters (Sheet 2 of 2)

Parameter	Description
Chromatogram View Width	Specifies a window width to define the chromatogram viewing range in the Data Review view. Valid range: 0.10 through 999.00 minutes Default: 0.75 minutes
Use Source CID Scans	Specifies that the application use the source CID scans when they are available in the data file. If they are not available, then the application uses AIF or MS/MS scans when available.
Show All Compounds	Displays results for all compounds in the method, regardless of whether they are found in any samples.
Unknown Screening	
Include Unknown Screening	Adds unknown screening features to the target screening method.

Figure 85. Target Screening Settings pane on the Processing page

▼ Target Screening Settings

Compound Databases

	Enabled	Database Name	
▶	<input checked="" type="checkbox"/>	Converted_Database	open
▶	<input type="checkbox"/>	Default	open

Identification and Confirmation Settings

Peaks *m/z*

Retention Time Identify Confirm

Fragment Ions Identify Confirm

Isotopic Pattern Identify Confirm

Library Search Identify Confirm

Threshold Override 5,000

S/N Ratio Threshold 5.0

Mass Tolerance: 5.00 ppm ▼

Ignore if Not Defined

Window Override (sec) 30

Ignore if Not Defined

Min. # of Fragments 1

Intensity Threshold 10,000

Mass tolerance 5.00 ppm ▼

MS Order MS2 ▼

Fit Threshold (%) 90

Allowed Mass Deviation (ppm) 5

Allowed Intensity Deviation (%) 10

Use Internal Mass Calibration

Library Search Type: NIST ▼

General Library Settings

MS Order MS ▼

Use Isolation Width

NIST Settings

Search Type Normal ▼

Precursor tolerance 1.60 ppm ▼

Product tolerance 1.60 ppm ▼

Ignore Precursor Use alt peak matching

Reverse Search

Presearch Default ▼

SI Threshold 250 ▼

RSI Threshold 250 ▼

Probability Threshold 10.00 ▼

Library Manager Settings

Spectrum Tolerance 5.00 ▼

Score Threshold 80.00 ▼

Ignore Precursor Reverse Search

Table 59. Target Screening Settings pane parameters (Sheet 1 of 5)

Parameter	Description
Compound Databases	
Enabled	Specifies databases to use for target screening processing.
Database Name	Lists available databases in the Databases folder.
Identification and Confirmation Settings	
Peaks	Specifies that the application use the mass-to-charge ratio (<i>m/z</i>) for filtering compound peaks.
Threshold Override	<p>Overrides the Response Threshold value set in the compound database. The application ignores the peaks with areas below this specified threshold.</p> <p>Valid range: 1000 through 1 000 000 000 Default: 5000</p>
S/N Ratio Threshold	<p>Includes only peaks with signal-to-noise ratios (S/Ns) above the specified value.</p> <p>Valid range: 1.0 through 100 000 Default: 5.0</p>
Retention Time	Specifies either the Identify or Confirm option for a retention time search. To identify a compound, the application searches the specified RT window for a match. To confirm a compound, the application searches the entire raw data file.
Ignore if Not Defined	Ignores the values you specify for Retention Time options when no retention time is defined in the compound database, and does not include the results of identification or confirmation for retention time in the Data Review target screening results.
Window Override	<p>Specifies the number of seconds to override the RT Window value set in the compound database and include only peaks within this designated window. The application identifies or confirms the presence of a compound only when its measured retention time matches the target compound's expected retention time within the specified Window Override retention time.</p> <p>Valid range: 0 through 999 seconds Default: 30 seconds</p>

Table 59. Target Screening Settings pane parameters (Sheet 2 of 5)

Parameter	Description
Fragment Ions	Specifies either the Identify or Confirm option for a fragment ion match. To identify a fragment, the application searches the specified RT window for a match. To confirm a fragment, the application searches the entire raw data file.
Ignore if Not Defined	Ignores the values you specify for Fragment Ions options when no fragment is defined in the compound database, and does not include the results of identification or confirmation for fragment ions in the Data Review target screening results.
Min. # of Fragments	Specifies the minimum number of fragments required to identify or confirm the presence of a compound. Valid range: 1 through 5 Default: 1
Intensity Threshold	Specifies the minimum height of a fragment ion peak. The peak of a fragment ion must be above this intensity threshold to be identified or confirmed. Valid range: 1 through 1e9 Default: 10 000
Mass Tolerance	Specifies the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value for the fragment ions and is separate from the mass tolerance specified for the parent (see “Editing the Acquisition Page” on page 261). Valid range: 0 through 500 Default: 5 Unit: mmu or ppm Note When using ion trap data, the application uses 300 mmu regardless of the value you enter here.
MS Order	Specifies that the confirming peaks come from the same scan (MS), are fragments from an adjacent scan (MS2), or come from the Source CID (MS–In Source CID).
Isotopic Pattern	Specifies either the Identify or Confirm option for an isotopic pattern match. To identify a compound, the application searches the specified RT window for a match. To confirm a compound, the application searches the entire raw data file.
Fit Threshold	To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage. Default: 90%

Table 59. Target Screening Settings pane parameters (Sheet 3 of 5)

Parameter	Description
Allowed Mass Deviation	<p>Specifies the allowed mass deviation in the spectrum data.</p> <p>The TraceFinder isotopic pattern algorithm considers an isotope peak as found if its measured m/z is less than this amount away from its expected m/z. For best results, set this value to a number that causes up to 98 percent of all mass deviations to be smaller than the allowed mass deviation value.</p> <p>Valid range: 3 through 100 ppm Default: 3 ppm</p>
Allowed Intensity Deviation	<p>Specifies the allowed intensity deviation of the mass spectrometer, relative to the monoisotopic ion, as a percentage of the base peak height.</p> <p>The TraceFinder isotopic pattern algorithm considers an isotope peak as not found if its intensity relative to the monoisotopic ion's intensity is more than this deviation percentage from the theoretical relative intensity of the isotope ion. For best results, set this value to a number that causes up to 98% of all intensity deviations to be smaller than the allowed intensity deviation value.</p> <p>Default: 10%</p>
Use Internal Mass Calibration	Specifies that the application require an isotope's m/z to be closer to its theoretical value to avoid a score penalty.
Library Search	Specifies either the Identify or Confirm option for a library search. To identify a compound, the application searches the specified RT window for a match. To confirm a compound, the application searches the entire raw data file.
Library Search Type	NIST or Library Manager
General Library Settings	
MS Order	Specifies that the confirming peaks come from the same scan (MS), are fragments from an adjacent scan (MS2), or come from the Source CID (MS-In Source CID).
Use Isolation Width	Specifies that the application use the isolation width to determine if there is an MS/MS scan within the same peak RT window that includes the precursor fragments. Available only when you set the MS Order to MS2 .

Table 59. Target Screening Settings pane parameters (Sheet 4 of 5)

Parameter	Description
NIST Settings	
Search Type	<p>Normal: Uses a more extensive set of presearch screenings—a total of four different criteria.</p> <p>MS/MS: Searches for an MS/MS spectrum in a library of MS/MS spectra.</p> <p>In-source HiRes: Searches for an in-source/EI with an accurate ion m/z or an MS/MS spectrum in a library that contains in-source/EI accurate ion m/z or MS/MS spectra.</p>
Precursor Tolerance	<p>Specifies the precursor m/z tolerance range as either amu or ppm.</p> <p>Valid range: 0.015 through 100 000 Default: 1.60 Available only when you select MS/MS or In-source HiRes search types.</p>
Product Tolerance	<p>Specifies the mass spectral peak tolerance range as either amu or ppm.</p> <p>Valid range: 0.015 through 100 000 Default: 1.60 Available only when you select MS/MS or In-source HiRes search types.</p>
Ignore Precursor	<p>Ignores mass spectral peaks within the specified precursor tolerance range.</p> <p>Available only when you select MS/MS or In-source HiRes search types.</p>
Use Alt Peak Matching	<p>Specifies that the application use an alternate peak matching method for searching the mass spectra.</p> <p>Available only when you select MS/MS or In-source HiRes search types.</p>
Reverse Search	<p>Specifies that the NIST library search use the reverse search method. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).</p>
Presearch	<p>Specifies that the application use presearch screening before calculating the spectrum-by-spectrum match factor.</p>

Table 59. Target Screening Settings pane parameters (Sheet 5 of 5)

Parameter	Description
SI Threshold	Specifies the lower threshold value for the search index method used to search the NIST library. The application does not return results below this value. Valid range: 0 through 999 Default: 250
RSI Threshold	Specifies the lower threshold value for the reverse search index method used to search the NIST library. The application does not return results below this value. Valid range: 0 through 999 Default: 250
Probability Threshold	Threshold value for the match probability.
Library Manager Settings	
Spectrum Tolerance	Specifies the spectrum tolerance as either amu or ppm. Valid range: 0.1 through 1000.0 Default: 5.00 ppm
Score Threshold	Specifies that the application does not return results below this value. Valid range: 0 through 100 Default: 80.00
Ignore Precursor	Specifies that the application ignore mass spectral peaks within the specified precursor tolerance range.
Reverse Search	Specifies using the reverse search method for a Library Manager search. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).

Understanding the Identification and Confirmation Process

By default, the application uses the mass-to-charge ratio (m/z) for filtering compound peaks. In the Identification and Confirmation Settings area, you can select additional criteria to help increase confidence using either of the following:

- Compound identification for identifying a sample compound as a minimum requirement for a match to be displayed in the results.

To identify a compound, the application searches within the specified RT window (or the RT window override if specified in the method) and compares the measured m/z of the sample peak against the expected m/z of the target compound. When the sample peak's m/z is within the default ± 5 ppm tolerance of the target compound's m/z , the application considers that this target compound is identified.

- Compound confirmation for confirming a sample compound and to increase confidence in the match results.

To confirm a compound, the application searches the entire raw data file and compares the measured m/z of the sample peak against the expected m/z of the target compound. When the sample peak's m/z is within the tolerance of the target compound's m/z , the application considers that this target compound is confirmed.

The application processes identification and confirmation settings in a specific order. When a compound passes identification at each point in the order of processing, the application continues to the next automatic or selected identification or confirmation test.

Note When you select the Ignore if Not Defined option and the related data is not defined in the compound databases, the application skips that criteria test.

When a compound fails identification at a point in the processing, the application skips the testing of all remaining criteria, even when they are selected, and the flags for those criteria are blank.

The application processes identification and confirmation settings in the following order:

1. m/z and Retention Time

The application automatically identifies the mass to charge ratio for all compounds. When you select the Retention Time settings, the compound must pass this criteria first. When a compound fails the m/z or the Retention Time identification test, the application does not perform identification or confirmation testing for any other selected criteria lower in the processing order.

For additional information about the m/z and Retention Time parameters, see [Mass to Charge \(\$m/z\$ \)](#) and [“Retention Time”](#) on page 281.

2. Threshold

The application automatically identifies the default area threshold (5000) for the compound after the compound passes the m/z and Retention Time criteria. When you specify a Threshold Override, the application uses the specified threshold value instead.

When a compound fails the Threshold identification test, the application does not perform the selected Fragment Ions or Library Search testing for identification or confirmation.

For additional information about the Threshold parameter, see [Threshold](#).

3. Isotopic Pattern

For additional information about the Isotopic Pattern parameter, see [“Isotopic Pattern”](#) on [page 282](#).

4. Fragment Ions

For additional information about the Fragment Ions parameter, see [“Fragment Ions”](#) on [page 281](#).

5. Library Search

For additional information about the Library Search parameter, see [“Library Search”](#) on [page 283](#).

Mass to Charge (m/z)

The application automatically uses the m/z and mass tolerance values to identify each compound, using the mass tolerance value you specified on the Acquisition page. See [“Editing the Acquisition Page”](#) on [page 261](#).

The application compares the measured m/z of the sample peak against the expected m/z of the target compound. When the measured m/z is within the mass tolerance of the expected m/z , the application considers that this target compound is found and the m/z criteria passes.

On the Target Screening page in Data Review, the MZ column in the Compounds table indicates whether this criteria passes or fails. The Flag column indicates whether the target compound is identified, fully confirmed, or both. For details, see [“Compounds Pane”](#) on [page 569](#).

The Compounds table also displays the m/z Expected, m/z Measured, and m/z Delta values for each compound.

Threshold

To identify each sample compound, the application automatically uses the area and threshold values defined in the selected compound database.

In the Identification and Confirmation Settings pane, you can specify a threshold override to use instead of the area threshold defined in the compound database.

The application compares the area of the sample peak against the defined area thresholds. When the sample peak's area is greater than or equal to the corresponding area threshold from the compound database or the override area threshold, the target compound is identified.

On the Target Screening page in Data Review, the Flag column in the Compounds table indicates whether this criteria passes or fails. The Flag column indicates whether the target compound is identified, fully confirmed, or both. For details, see “[Compounds Pane](#)” on [page 569](#).

The Compounds table also displays Measured Area column displays the area value in green to indicate that the peak's area is greater than or equal to the area threshold; otherwise, this column displays the area value in red.

Retention Time

The application uses the expected retention time and retention time window values defined in the selected compound database to identify or confirm each sample compound.

In the Identification and Confirmation Settings pane, you can set an override value to use for the retention time window instead of using the retention time window that is specified in the compound database.

When the compound database defines an expected retention time for a compound, it uses the following process to identify or confirm the compound.

- Identify: the application searches within the specified retention time window (or the retention time window override) and compares the measured m/z of the sample peak against the expected m/z of the target compound. When the measured m/z is within the mass tolerance of the expected m/z , this target compound is identified.
- Confirm: the application searches the entire raw data file and compares the measured m/z of the sample peak against the expected m/z of the target compound. When the measured m/z is within the specified mass tolerance of the expected m/z , the target compound is confirmed.

When the compound database does not define an expected retention time for a compound, the application cannot identify or confirm the compound. If you select the Ignore if Not Defined option, the application does not perform testing for the retention time and the RT flag is blank on the Target Screening page in Data Review.

On the Target Screening page in Data Review, the RT column in the Compounds table indicates whether this criteria passes or fails. The RT column indicates whether the target compound is identified, fully confirmed, or both. For details, see “[Compounds Pane](#)” on [page 569](#). The Compounds table also displays the RT Expected, RT Measured, and RT Delta values for each compound.

Fragment Ions

To use fragment ions for identification or confirmation, the application requires the following conditions:

- The selected compound databases contain the charged mass for each defined fragment ion of interest for the compounds in the target list.

- The HCD (higher energy collision-induced dissociation), source CID (source collision-induced dissociation), or AIF (all ions fragmentation) ion spectra exist at a time point within the compound's elution time range.

When no fragment is defined in a compound database for a target compound, the following apply:

- When the Ignore if Not Defined option is selected in the method, the application does not perform filtering for the Fragment Ions. In the Data Review view, the FI column is blank.
- When the Ignore if Not Defined option is not selected in the method, the application considers that this target compound is not identified. The Fragment Ions filter fails.

The application uses the number of fragment masses defined in the compound database when it processes a sample for fragment ions. The value you specify for Min. # of Fragments cannot be greater than the number of fragments defined in the compound database.

For example, if a compound has three fragment ion masses defined in a compound database, any of the following scenarios can occur:

- You enter "2" in the Min. # of Fragments box of the method, and the application finds at least two out of the three defined fragment ions. The Fragment Ions filter passes.
- You enter "4" in the Min. # of Fragments box of the method, and the application finds only the three defined fragment ions. The Fragment Ions filter fails.
- You enter "2" in the Min. # of Fragments box of the method, but the application finds only one of the three defined fragment ions. The Fragment Ions filter fails.

The application repeats the following process for each of the fragment ions:

1. When the mass of the parent (plus or minus half of the isolation window value from the acquired raw data file) is not within the mass range of the extracted ion chromatogram shown in the Chromatogram pane of the Data Review view, the application considers the fragment ion as not found and the application fails the Fragment Ions filter; otherwise, the application continues.
2. The application inspects the processed fragment ion scan closest to the target compound's expected retention time and locates the MS/MS spectrum closest to the compound's apex. Within this spectrum, the application finds the intensity for the tallest fragment whose mass is within the mass tolerance of an entered fragment ion mass. When this intensity is not found or when it is less than the intensity threshold defined in the method, the application determines that the entered fragment ion is not found; otherwise, it determines that the fragment ion is found.

Isotopic Pattern

You can choose to either identify or confirm the isotopic patterns for all compounds in a batch. The application calculates an isotopic pattern score (as a percentage value), using the target compound's formula.

For the isotopic pattern filter, enter the isotopic pattern parameters, including a fit threshold value, in the processing method. To identify or confirm the presence of a compound, the resulting score from isotopic pattern matching must be higher than the fit threshold.

To identify or confirm an isotopic pattern, the application must detect the compound for at least one of its defined adduct ions. The application identifies the elemental composition to match using the formula that is associated with the most intense adduct peak. The application then generates an isotopic pattern score (as a percentage value) for the match between the measured and expected isotopic patterns of the calculated elemental composition.

- For profile data, the application calculates the measured isotopic pattern using the average of all scans (within the allowed intensity deviation of the spectrum closest to the compound's apex retention time). In the Data Review view, the application displays both the expected and measured spectra.
- For centroid data, the application calculates the measured isotopic pattern using the apex scan. In the Data Review view, the application displays the expected spectra.

A high isotopic pattern score (approaching 100 percent) occurs when the measured isotope patterns, the expected isotope patterns, and the intensities are almost identical using the scoring parameters specified in the processing method. When the patterns are not similar, the score is closer to 0 percent. When the score is greater than or equal to the specified fit threshold and the number of isotopes matched is not 1 out of 1, this filter passes.

When you view results in the Data Review view, the IP column displays a green or red flag to indicate whether the compound passed or failed based on the criteria specified in the method.

Library Search

For a target screening analysis, you can select the Library Search criterion for either identification or confirmation in the processing method. The application identifies or confirms the sample compound by searching the selected library and returning the library entry with the highest score (as a percentage value) for the fragment ion spectrum in that library that matches the compound's ion spectrum.

For this criterion, you enter a score threshold value in the processing method. The resulting score from a library search match must be higher than your entered threshold value, and the library entry must match a compound's name, a compound's formula, or both to identify or confirm the presence of the compound.

The application uses the following logic to determine when a match is successful:

- When a formula is available in the library entry and the formula matches the target compound formula:
 - A library score that is higher than or equal to the score threshold meets the criteria.
 - A library score that is lower than the score threshold fails to meet the criteria.

- When a formula is available in the library entry and the name in the library entry matches the target compound name but the formula does not match the target compound formula (or it is not available):
 - A library score that is higher than or equal to the score threshold meets the criteria.
 - A library score that is lower than the score threshold fails to meet the criteria.
- When neither the formula nor the library entry name match the target compound, the criteria fails and the Lib Match Name, Library Score, and Library Match Rank columns display N/A in black text.

Note When the compound is identified, but no MS/MS scan has been performed, the Lib Match Name, Library Score, and Library Match Rank columns display N/A in red text.

- When an MS/MS scan has been performed and both the library entry and the formula match the target compound:
 - A library score that is higher than or equal to the score threshold meets the criteria. The Lib Match Name, Library Score, and Library Match Rank columns display their values in green text.
 - A library score that is lower than the score threshold fails to meet the criteria. The Lib Match Name, Library Score, and Library Match Rank columns display their values in red text.

To use a library search for identification or confirmation, the application requires that the data meet these conditions:

- The raw data file contains HCD (higher energy collision-induced dissociation), source CID (source collision-induced dissociation), or AIF (all ions fragmentation) ion spectra.
- The spectra exist at a time point within the compound's elution time range.

The application performs either a forward library search or a reverse library search. A forward search compares the mass spectrum of an unknown compound to a mass spectral library entry, whereas a reverse search compares a library entry to an unknown compound.

When a parent-selected MS/MS spectrum does not exist, the application performs a reverse library search because the compound scan contains a mixture of fragments from all co-eluting parents. A forward search with such a mixture biases the results toward the strongest parent because its fragments would be dominant, and a forward search also takes more time because the application must search every spectrum in the library.

When a parent-selected MS/MS spectrum exists, the application performs a forward library search because the scan usually contains fragments of only one or two parents, so matching this spectrum against the library is faster and more accurate. When you select the Use Reverse Library Searching Only check box in the processing method, the application performs only a reverse library search.

When you use profile data, the application uses the averaged spectrum of the unknown peak as the input spectrum for the library search. This averaged spectrum is based on the average of all scans within 10 percent of the spectrum closest to the peak's apex retention time. When you use centroid data, the application uses the apex scan as the input spectrum for the library search.

When the application locates a match, it generates a score percentage for the matching library entry. This library search can result in multiple matches with different scores.

After searching based on the m/z in the input spectrum, the application performs another search for only the matches from the first library search, but this time based on the name, and then the formula, of the target compound. If at least one match is found, the application displays the highest scoring match from the second search for data review. If no match is found from the second search, the application displays the highest scoring match from the first search.

Editing the Peak Detection Page

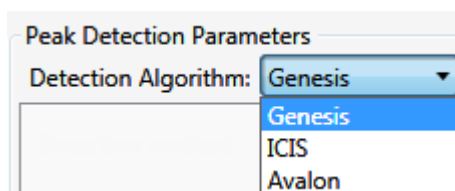
Use the features on the Peak Detection page to specify any of the following peak detection algorithms: Genesis, ICIS, or Avalon.

❖ To specify peak detection parameters

1. Click **Peak Detection** in the Method View navigation pane.

The Peak Detection page for the method opens.

2. In the Peak Detection Parameters area, select one of the detection algorithms: **Genesis**, **ICIS**, or **Avalon**.



- The Genesis peak detection algorithm provides backward compatibility with Xcalibur 1.0 studies. For detailed descriptions of the Genesis method parameters, see [Genesis Detection Method](#).
 - The ICIS peak detection algorithm is designed for MS data and has superior peak detection efficiency at low MS signal levels. For detailed descriptions of the ICIS method parameters, see “[ICIS Detection Method](#)” on [page 290](#).
 - The Avalon peak detection algorithm is designed for integrating UV/Vis and analog chromatograms. For detailed descriptions of the Avalon method parameters, see “[Avalon Detection Method](#)” on [page 293](#).
3. Specify the parameters for the selected detection algorithm.

Genesis Detection Method

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

Figure 86. Genesis peak detection

The screenshot shows the 'Peak Detection Parameters' dialog box. At the top, the 'Detection Algorithm' is set to 'Genesis'. Below this, the 'Detection method' is set to 'Nearest RT'. The 'Smoothing' parameter is set to 1, and the 'S/N threshold' is set to 2.00. There are two checkboxes: 'Enable valley detection' (unchecked) and 'Constrain peak width' (unchecked). Under 'Enable valley detection', the 'Expected width (sec)' is set to 0.00. Under 'Constrain peak width', the 'Peak height (%)' is set to 5.00, and the 'Tailing factor' is set to 1.00. Other parameters include 'Peak S/N cutoff' (200.00), 'Valley rise (%)' (2.00), 'Valley S/N' (1.10), and '# background scans' (5). The 'Report noise as' parameter is set to 'Peak To Peak'.

Table 60. Genesis peak detection parameters (Sheet 1 of 3)

Parameter	Description
Detection Algorithm	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.

Table 60. Genesis peak detection parameters (Sheet 2 of 3)

Parameter	Description
Smoothing	<p>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.</p> <p>Valid values: Any odd integer from 1 through 15 points Default: 1</p>
S/N threshold	<p>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.</p> <p>Valid range: 0.0 through 999.0</p>
Enable Valley Detection	<p>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.</p>
Expected Width	<p>The expected peak width parameter (in seconds). This parameter controls the minimum width that a peak is expected to have if you enable valley detection.</p> <p>With valley detection enabled, any valley points nearer than the <i>expected width</i>/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width.</p> <p>Valid range: 0.0 through 999.0</p>
Constrain Peak Width	<p>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 threshold and a tailing factor. Selecting the Constrain Peak Width check box activates the Peak Height (%) and Tailing Factor options.</p>
Peak Height (%)	<p>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.</p> <p>Valid range: 0.0 through 100.0%</p>

Table 60. Genesis peak detection parameters (Sheet 3 of 3)

Parameter	Description
Tailing Factor	<p>A factor that controls how the 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.</p> <p>Valid range: 0.5 through 9.0</p>
Peak S/N Cutoff	<p>The peak edge is set to values below this signal-to-noise ratio.</p> <p>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.</p> <p>When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the application defines the right and left edges of the peak when the S/N reaches a value less than 200.</p> <p>Valid range: 50.0 through 10000.0</p>
Valley Rise (%)	<p>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.</p> <p>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.</p> <p>When the trace exceeds rise percentage, the application applies valley detection peak integration criteria. This test is applied to both the left and right edges of the peak.</p> <p>Valid range: 0.1 through 500.0</p>
Valley S/N	<p>Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher.</p> <p>Valid range: 1.0 through 100.0 Default: 2.0</p>
# Background Scans	<p>Number of background scans performed by the application.</p>
Report Noise As	<p>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.</p>

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 87. ICIS peak detection

The screenshot shows a 'Peak Detection Parameters' dialog box. At the top, 'Detection Algorithm' is set to 'ICIS'. Below this, several parameters are listed with their current values and controls (spinners or checkboxes):

- Detection method: Nearest RT
- Smoothing: 1
- Area noise factor: 5
- Peak noise factor: 10
- Baseline window: 40
- Constrain peak width
- Peak height (%): 5.00
- Tailing factor: 1.00
- Noise method: Incos
- Min peak width: 3
- Multiplet resolution: 10
- Area tail extension: 5
- Area scan window: 0
- RMS

Table 61. ICIS peak detection parameters (Sheet 1 of 3)

Parameter	Description
Detection Algorithm	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. Valid values: Any odd integer from 1 through 15 points Default: 1

Table 61. ICIS peak detection parameters (Sheet 2 of 3)

Parameter	Description
Area Noise Factor	<p>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.</p> <p>Valid range: 1 through 500 Default: 5</p>
Peak Noise Factor	<p>The noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 1 through 1000 Default: 10</p>
Baseline Window	<p>The application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 1 through 500 Default: 40</p>
Constrain Peak Width	<p>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 activates the Peak Height (%) and Tailing Factor options.</p>
Peak Height (%)	<p>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.</p> <p>Valid range: 0.0 through 100.0%</p>
Tailing Factor	<p>A factor that controls how the 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.</p> <p>Valid range: 0.5 through 9.0</p>

Table 61. ICIS peak detection parameters (Sheet 3 of 3)

Parameter	Description
Noise Method	<p>The options are INCOS or Repetitive.</p> <p>INCOS: Uses a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value.</p> <p>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.</p>
Min Peak Width	<p>The minimum number of scans required in a peak. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 0 through 100 scans Default: 3</p>
Multiplet Resolution	<p>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.</p> <p>Valid range: 1 through 500 scans Default: 10</p>
Area Tail Extension	<p>The number of scans past the peak endpoint to use in averaging the intensity. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 0 through 100 scans Default: 5</p>
Area Scan Window	<p>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.</p> <p>Valid range: 0 through 100 scans Default: 0</p>
RMS	<p>Specifies that the 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.</p>

Avalon Detection Method

The Avalon peak detection algorithm is designed for UV data. The Avalon peak detection algorithm also supports negative peaks. You can edit the Event values from the [Avalon Event List](#).

Figure 88. Avalon peak detection

Peak Detection Parameters

Detection Algorithm: Avalon

Detection method: Nearest RT

Smoothing: 1

Time	Event	Value
Initial	Start Threshold	10000.000
Initial	End Threshold	10000.000
Initial	Area Threshold	10000.000
Initial	P-P Threshold	1.000
Initial	Bunch Factor	1.000
Initial	Negative Peaks	Off

Autocalc initial events Edit

Table 62. Avalon peak detection parameters

Parameter	Description
Detection Algorithm	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. Valid values: 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.
Autocalc Initial Events	Automatically calculates the events in the Event list.
Edit	Opens the Avalon Event List dialog box where you can edit the Time/Event/Value parameters. See “Avalon Event List.”

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](#).

Figure 89. Avalon Event List dialog box

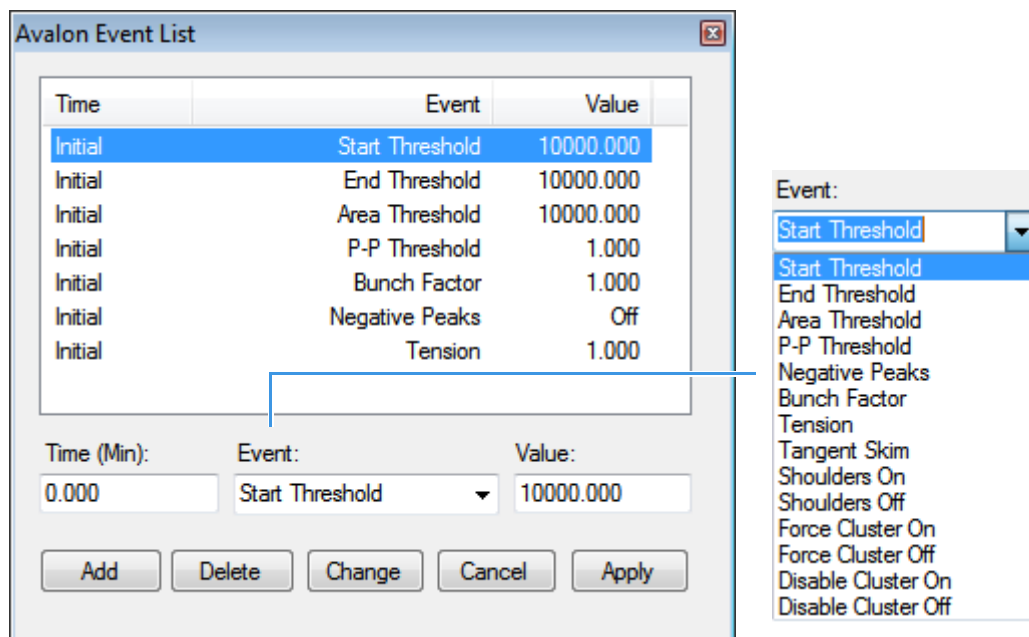


Table 63. Avalon Event List dialog box parameters

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.”
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 90. Event types

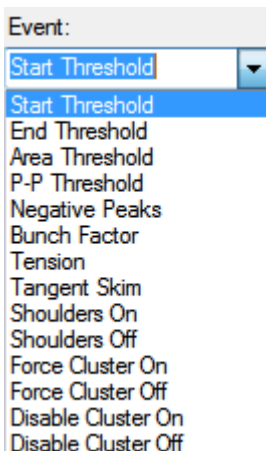


Table 64. Event type descriptions (Sheet 1 of 2)

Event type	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. Valid range: 0 through 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. Valid range: 0 through 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. Valid range: 0 through 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. Valid range: 0.1 through 99.99
Negative Peaks	Permits detection of a negative going peak. Automatically resets after finding a negative peak. Valid values: On or Off

Table 64. Event type descriptions (Sheet 2 of 2)

Event type	Description
Bunch Factor	<p>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.</p> <p>Valid range: 0 through 999</p>
Tension	<p>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.</p> <p>Valid range: 0 through 999.99 minutes</p>
Tangent Skim	<p>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.</p> <p>Valid range: 0 through 1</p>
Shoulders On	<p>Allows peak shoulders to be detected (peaks which are separated by an inflection rather than a valley) Sets a threshold for the derivative.</p>
Shoulders Off	<p>Disables peak shoulder detection.</p> <p>Valid range: 0 through 50</p>
Force Cluster On	<p>Force the following peaks to be treated as a cluster (single peak).</p>
Force Cluster Off	<p>End the forced clustering of peaks.</p>
Disable Cluster On	<p>Prevent any peaks from being clustered.</p>
Disable Cluster Off	<p>Permit clusters to occur again.</p>

Editing the Reports Page

Use the Reports page to specify the reports and report output formats that you want to create for the method. See [Reports Page](#).

Follow these procedures:

- [To open the Reports page](#)
- [To configure the compounds in the reports](#)
- [To specify output formats](#)

❖ To open the Reports page

Click **Reports** in the Method View navigation pane.

The Reports page for the method opens (see [Reports page](#)), displaying only the reports that are configured in the Configuration Console. To configure the reports that are available, see “[Specifying the Reports](#)” on [page 71](#).

❖ To configure the compounds in the reports

In the Target Screening Report Settings pane, select one of the following options:

- **Include All Compounds:** Generates reports that include all compounds from the screening library, whether or not they are found in the samples.
- **Include Only Found Compounds:** Generates reports that include only the compounds from the screening library that are found in the samples.

❖ To specify output formats

1. To edit the Report Title, double-click the name and type a new title.

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

2. To specify the type of report output to create for each report (hard copy, PDF, CSV, or Excel), select the check box in the appropriate column.
3. To duplicate an output type for all reports, click the cell to select it, and then right-click and choose **Copy Down** from the shortcut menu.

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

By default, all report types are cleared.

Reports Page

Use the features on the Reports page to specify the reports and report output formats that you want to create with the method.

Figure 91. Reports page




Report	Print	Create PDF	Create CSV	Create Excel	Exists
▶ Batch Report	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	
Target Screening High Density Sa...	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	
Target Screening Summary Report	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	

Table 65. Reports page parameters

Parameter	Description
Report list columns	
Report	The name of a report.
Print	Sends reports to the default printer.
Create PDF	Saves reports as PDF files.
Create CSV	Saves reports as CSV files.
Create Excel	Saves reports as Excel files.
Exists	Identifies the report template in the C:\TraceFinderData\3.3\Templates\ReportTemplates folder.

Saving a Master Method to a New Name

You can save any method to a new name, or you can use the current method data to overwrite an existing method. The new method contains all the data of the original method.

❖ To save a method to a new name

1. From the main menu, choose **File > Save As**.

The Save Master Method As dialog box opens, displaying all quantitation, target screening, and unknown screening methods.

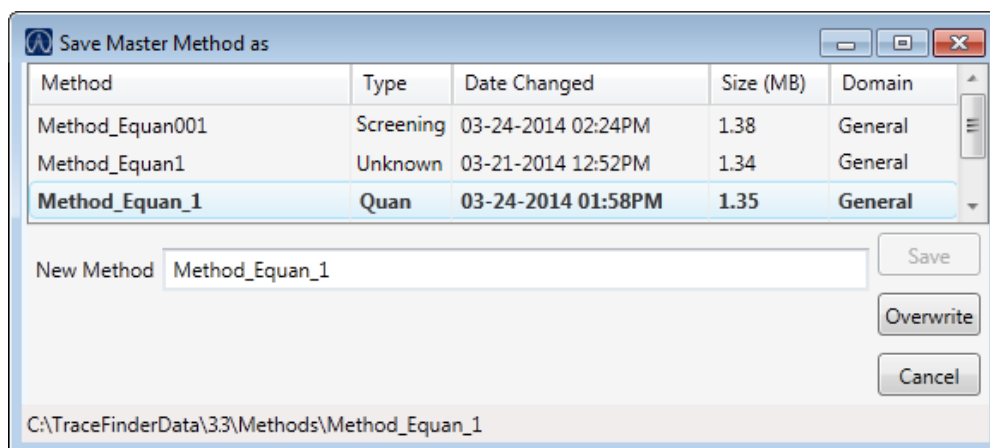


Table 66. Save Master Method As dialog box parameters

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method to display: Quan, Screening, or Unknown Only.
Date Changed	Date the method was last updated.
Size	Size of the method in megabytes.
Domain	TraceFinder domain for which the method was created.
New Method	Name of the new method to create.
<i>Path</i>	Path to the selected method in the Methods folder.

2. Do one of the following:
 - In the New Method box, type a name for the new method.
The application enables the Save button.
 - In the Method column, select a method to overwrite.
The application enables the Overwrite button.

3. Click **Save** or **Overwrite**.

The application saves all the method data using the specified name and opens the Acquisition page of the new method.

Using the Method Development Mode for Unknown Screening Methods

This chapter includes method development tasks for creating and editing an unknown screening method. (See [Method Development navigation pane](#).) When user security is activated, you must have Method Development Unknown Screening Access permission to use these features.

Contents

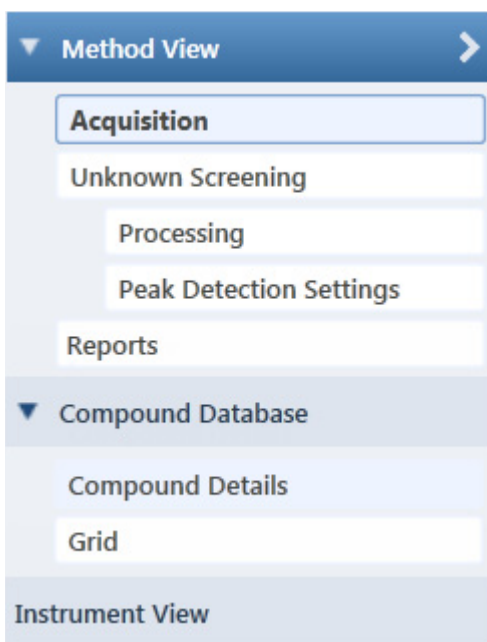
- [Opening a Master Method](#)
- [Starting a New Unknown Screening Master Method](#)
- [Editing a Master Method](#)

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 your application.

An unknown screening master method contains a list of compounds and the settings for detecting, processing, and reporting those compounds.

When you create a master method, the application uses the method to determine how the application 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 and how the reporting functionality defines the output for your data and results.

The 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.

Figure 92. Method Development navigation pane**Table 67.** Method Development navigation pane commands

Command	Description
Method View	Displays the Method View for the master method.
Acquisition	Displays the Acquisition page of the Method View. See “Editing the Acquisition Page” on page 307.
Unknown Screening	
Processing	Displays the Processing page of the Method View. See “Editing the Processing Pages” on page 311.
Peak Detection Settings	Displays the Peak Detection Settings page of the Method View. See “Editing the Peak Detection Settings Page” on page 334.
Reports	Displays the Reports page of the Method View. See “Editing the Reports Page” on page 345.
Compound Database	See “Working with the Compound Database” on page 74.
Instrument View	See “Working with Instrument Methods” on page 108.

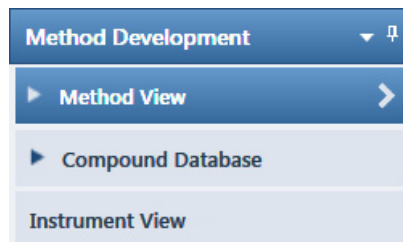
Opening a Master Method

Use the TraceFinder application to open an unknown screening master method that was created and saved in the current application.

❖ To open an unknown screening method in the Method Development mode

1. Click **Method Development** in the navigation pane.

The Method Development navigation pane opens.



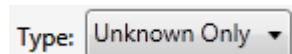
For descriptions of all the features in this navigation pane, see “[Starting a New Unknown Screening Master Method](#)” on [page 305](#).

2. Choose **File > Open > Master Method** from the main menu.

Tip You can also open one of your most recently used master method files. Choose **Files > Recent Files > Method**.

The Open Master Method dialog box opens, displaying all available methods. See [Open Master Method dialog box](#).

3. Select **Unknown Only** in the Type list.



The method list displays all unknown screening methods.

4. Select an unknown screening master method and click **Open**.

The Acquisition page for the selected method opens. For detailed descriptions of all the features on the Acquisition page, see “[Acquisition Page for an Unknown Screening Method](#)” on [page 309](#).

7 Using the Method Development Mode for Unknown Screening Methods

Opening a Master Method

Figure 93. Open Master Method dialog box

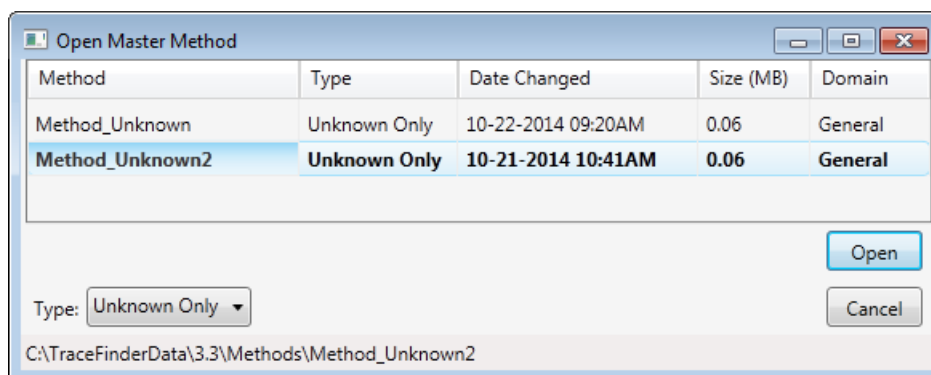


Table 68. Open Master Method dialog box parameters

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan, Screening, or Unknown Only.
Date Changed	Date the method was last updated.
Size	Size of the method in megabytes.
Domain	TraceFinder domain for which the method was created.
Type	Type of method to display: Quan, Screening, Unknown Only, or Any.
<i>Path</i>	Path to the selected method in the TraceFinderData\3.3\Methods folder.

Starting a New Unknown Screening Master Method

The following procedure includes the basic parameters you must define to create and save an unknown screening master method. For a detailed description of how to modify all parameters in a master method, see [“Editing a Master Method”](#) on page 307.

❖ To create a new method

1. Choose **File > New > Master Method** from the main menu.

The Create Master Method dialog box opens.

IMPORTANT The Unknown Screening Method - Only feature is available only when you select the Allow Unknown Screening option in the application configuration console. See [“Processing Options”](#) on page 62.

2. Select the **Unknown Screening Method – Only** option and click **OK**.

<input type="radio"/> Unknown Screening method - Only	Create an unknown screening method. This method will not have quan or target screening elements.
---	---

The Method View for an unknown screening method includes the Acquisition, Processing, Peak Detection Settings, and Reports pages.

The Acquisition page for the method opens.

Method View - Unnamed*

Calibration file last used:

Lab Name:

Assay type:

Injection Volume:

Mass Precision:

Ion range calc method:

Instrument Method:

3. From the Instrument Method list, select an instrument method.
4. Click **Processing** in the Method View navigation pane.

The Processing page for the method opens. See [Processing page for an unknown screening method](#).



This animation shows how to create a new unknown screening method. To view the animation, click and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.

7 Using the Method Development Mode for Unknown Screening Methods

Starting a New Unknown Screening Master Method

Figure 94. Processing page for an unknown screening method

Method View Auto Reprocess (Quan Only)

Calibration file last used:

Peak Settings

Autocalc defaults from rawfiles

1000000.00	Absolute MS Signal Threshold
0.00	Min Peak Width
0.00	Max Peak Width
0.00	RT Shift (minutes)
30.00	RT Window (seconds)

Use RT Limits

Search from minutes to minutes

ppm Mass tolerance

Alignment and Gap Filling

All Peaks Top Peaks

Top Peaks

Search Options

Search Types

- Database Search
- Library Search
- Elemental Composition
- ChemSpider Search

Highest Point Analysis

Estimate amount using closest ISTD

Exhaustive Search Simple Search

Number of top matches

Library Settings

Library Selection

	Enabled	Database Name	Database Type
1	<input type="checkbox"/>	mainlib	NIST
2	<input type="checkbox"/>	New Library	NIST
3	<input type="checkbox"/>	NISTDEMO	NIST
4	<input type="checkbox"/>	nist_msms	NIST
5	<input type="checkbox"/>	HRAM_Spectral_Library_Cc	LibraryManager

General Library Settings

MS Order

Use Isolation Width

NIST Settings

Search Type

Precursor tolerance ppm

Product tolerance ppm

Ignore Precursor Use alt peak matching

Reverse Search

Presearch

SI Threshold

RSI Threshold

Probability Threshold

Library Manager Settings

Spectrum Tolerance ppm

Score Threshold

Ignore Precursor Reverse Search

Editing a Master Method

You can open an unknown screening master method to specify acquisition instructions and the settings for processing, peak detection, and reports.

See the instructions for the following tasks:

- [Editing the Acquisition Page](#)
- [Editing the Processing Pages](#)
- [Editing the Peak Detection Settings Page](#)
- [Editing the Reports Page](#)

Editing the Acquisition Page

The Acquisition page defines basic information used to acquire samples. For detailed descriptions of all the features, see “[Acquisition Page for an Unknown Screening Method](#)” on [page 309](#).

Follow these procedures:

- [To open the Acquisition page](#)
- [To specify acquisition information for a master method](#)
- [To edit an instrument method](#)

❖ To open the Acquisition page

Click **Acquisition** in the Method View navigation pane.


The Acquisition page for the method opens. See “[Acquisition Page for an Unknown Screening Method](#)” on [page 309](#).

❖ To specify acquisition information for a master method

1. In the Lab Name box, type the name to be displayed at 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 for the method.
3. From the Injection Volume box, select an injection volume (between **0.1** and **2000** μL) that the method uses for sample injection.

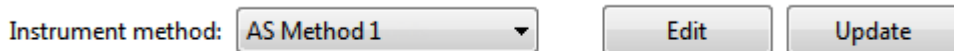
Use the Up/Down arrows, , to change the volume in increments/decrements of 1 μL , or use the keyboard to enter non-integer injection volumes.

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

4. From the Mass Precision box, select a precision value (between **2** and **6** inclusive) for the number of decimal places to use in reports and in peak and spectrum displays.

❖ **To edit an instrument method**

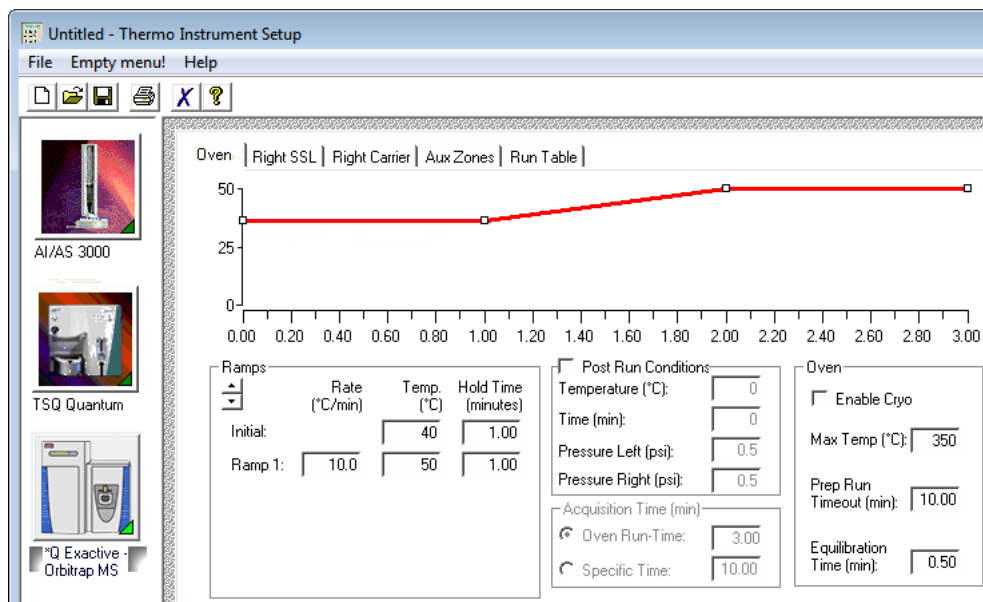
1. From the Instrument Method list on the Acquisition page, select an instrument method.



2. To edit the selected instrument method, click **Edit**.

The Thermo Instrument Setup window opens. This example of an instrument setup shows multiple configured instruments. (See [Thermo Instrument Setup window](#).)

Figure 95. Thermo Instrument Setup window

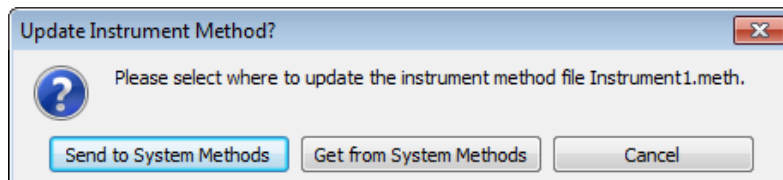


3. Edit the values on the instrument page for your instrument.
4. From the main menu in the Thermo Instrument Setup window, choose **File > Save** and then choose **File > Exit**.

The application returns you to the Acquisition page. See [“Acquisition Page for an Unknown Screening Method”](#) on page 309.

- 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.



- Choose one of the following options:
 - **Send to System Methods:** Overwrites the instrument method in the C:\TraceFinderData\3.3\Methods folder with the current instrument method.
 - **Get from System Method:** Overwrites the current instrument method with the instrument method in the C:\TraceFinderData\3.3\Methods folder.
 - **Cancel:** Makes no changes to the instrument method in the current master method.

Acquisition Page for an Unknown Screening Method

Use the features on the Acquisition page to define basic information about the method.

Figure 96. Acquisition page for an unknown screening method

Table 69. Acquisition page parameters (Sheet 1 of 2)

Parameter	Description
Lab Name	Specifies the laboratory name to be displayed at the top of each printed, saved, or exported report. Default: Default Laboratory To specify this default laboratory name, see “Specifying Application Defaults” on page 37.

Table 69. Acquisition page parameters (Sheet 2 of 2)

Parameter	Description
Assay Type	Specifies 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).
Injection Volume	<p>Specifies the system uses the injection volume (in μL) for sample injection. For a more detailed explanation, refer to the documentation for the autosampler.</p> <p>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.</p> <p>Valid range: 0.1 through 2000 μL</p>
Mass Precision	<p>Specifies the number of decimal places used in reports and in peak and spectrum displays.</p> <p>Valid range: Integers from 2 to 6, inclusive.</p>
Instrument Method	Specifies the instrument method used for acquiring samples.
Edit	Opens the Thermo Instrument Setup window where you can edit the instrument method.
Update	<p>Specifies one of the following:</p> <p>Send to System Methods: Overwrites the system method in the C:\TraceFinderData\3.3\Methods folder with the current instrument method.</p> <p>Get from System Methods: Overwrites the current instrument method with the system method in the C:\TraceFinderData\3.3\Methods folder.</p>

Editing the Processing Pages

The Unknown Screening – Processing pages define basic information about the method.

❖ To open the Processing pages

Click **Processing** in the Method View navigation pane.

The Processing pages include settings for peaks and settings for library, database, element, and ChemSpider searches.

See the following topics:

- [Editing the Peak Settings](#)
- [Editing the Library Settings](#)
- [Editing the Database Settings](#)
- [Editing the Element Settings](#)
- [Editing the ChemSpider Settings](#)

IMPORTANT After the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages in the method and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Editing the Peak Settings

Use the features on the Peak Settings page to define how the method detects and identifies peaks.

Follow these procedures:

- [To open the Peak Settings page](#)
- [To calculate default peak detection values from a raw data file](#)
- [To specify the peak detection settings](#)
- [To specify the search options](#)

❖ **To open the Peak Settings page**

Click **Processing** in the Method View navigation pane.

By default, the Peak Settings page opens. See “[Peak Settings Page](#)” on [page 314](#) or “[Peak Settings page parameters](#)” on [page 315](#).

❖ **To calculate default peak detection values from a raw data file**

For the Autocalc Defaults from Rawfiles box, click and select a raw data file.

The application populates the parameters in the Peak Detection Settings area with the values from the raw data file. (To reset the default values in the method, click .)

❖ **To specify the peak detection settings**

1. In the Absolute MS Signal Threshold box, type the number of counts for the application to detect an ion.

The application calculates the MS signal threshold (noise level) from the raw data file and sets this value to reflect a signal-to-noise level of 20.

Valid range: This value depends on the instrument. The minimum value is 0, and the maximum value is never larger than the maximum intensity component in the sample.
Default: Calculated from the raw data file

2. In the Min Peak Width box, type a value for the minimum acceptable peak width for the chromatographic peak.
3. In the Max Peak Width box, type a value for the maximum acceptable peak width for the chromatographic peak.
4. In the RT Shift box, type a value for the maximum allowable peak alignment correction for the chromatographic peak.

The application applies this value only when you enable batch processing.

5. In the RT Window box, type a value for the maximum viewable window around the identified chromatographic peak.
6. To create one peak list for the batch regardless of threshold settings, select the **Alignment and Gap Filling** check box.

The application processes the batch as a group instead of as individual samples. When the application finds a peak in one sample but not in another, this option adds the missing peak to all sample lists and displays N/A or the found peak information in the results. This option is similar to the Show All Compounds option in a quantitation or a target screening method. The application displays the results for the batch in a color-coded heat map grid. See “[Heat Map Pane](#)” on [page 645](#).

IMPORTANT To perform alignment, each sample in the batch must include the same scan filters used by the first sample. Samples 2-*n* can have additional filters as long as they also include all filters specified in the first sample.

When you clear this option, the application creates a unique peak list for each sample based on the method peak settings, similar to clearing the Show All Compounds option in a target screening method.

❖ To specify the search options

1. In the Search Types area, select the check box for the type of search that you want to perform:

- Database Search
- Library Search
- Elemental Composition
- ChemSpider Search

You can select as many search types as you want.

2. To perform the search only on the sample that has the highest peak response in the batch, select the **Highest Point Analysis** check box.

When you select this option, the application performs the search only on the sample in the batch that has the highest peak response.

When you clear this option, the application uses all search criteria on a per-peak basis.

For example, in a batch with samples 1, 2, and 3 with responses of 10, 1000, and 50, respectively, the application performs the search only on the peak from sample 2 with the greatest peak response. Because the mass and retention time for the peak are the same in each sample, the application identifies the same chemical. When you use this option with the Top Peaks option, the application uses the responses across the batch to filter the results and treats the entire batch of sample data as it would when returning the top *n* responses for a single sample.

3. Select one of the following options:
 - **Simple Search:** When the application identifies a peak by one of the identification points, it lists only that compound name in Data Review.
 - **Exhaustive Search:** The application lists all identified peaks from each search criterion and displays them as hierarchical entries under the top hit in Data Review.
4. To specify the number of matching peaks to display for each search type, enter a value for **Number of Top Matches**.

Peak Settings Page

Use the features on the Peak Settings page to define how the method detects and identifies peaks.

Figure 97. Peak Settings page

The screenshot shows the 'Peak Settings' dialog box. It is divided into two main sections: 'Peak Detection Settings' and 'Search Options'.

Peak Detection Settings

- Autocalc defaults from rawfiles
- Absolute MS Signal Threshold: 1000000.00
- Min Peak Width: 0.00
- Max Peak Width: 0.00
- RT Shift (minutes): 0.00
- RT Window (seconds): 30.00
- Use RT Limits
 - Search from: 0.00 minutes
 - to: 0.00 minutes
- Mass tolerance: 5.00 ppm
- Alignment and Gap Filling
 - All Peaks
 - Top Peaks
 - Top Peaks: 50

Search Options

- Search Types**
 - Database Search
 - Library Search
 - Elemental Composition
 - ChemSpider Search
- Highest Point Analysis
- Estimate amount using closest ISTD
 - Exhaustive Search
 - Simple Search
- Number of top matches: 0

Table 70. Peak Settings page parameters (Sheet 1 of 3)

Command	Description
Peak Detection Settings	
Autocalc Defaults from Rawfiles	Populates the parameters in the Peak Detection Settings area with the values from the selected raw data file.
Absolute MS Signal Threshold	<p>Specifies the number of counts that the application uses to detect an ion. The application calculates the MS signal threshold (noise level) from the raw data file and sets this value to reflect a signal-to-noise level of 20.</p> <p>Valid range: This value depends on the instrument. The minimum value is 0, and the maximum value is never larger than the maximum intensity component in the sample.</p> <p>Default: Calculated from the raw data file</p>
Min Peak Width	<p>Specifies the minimum allowable peak width for chromatographic peak detection.</p> <p>Default: 0.50</p>
Max Peak Width	<p>Specifies the maximum allowable peak width for chromatographic peak detection.</p> <p>Default: 1.00</p>
RT Shift (minutes)	<p>Specifies the maximum allowable peak alignment for chromatographic peak detection.</p> <p>Default: 1.0</p>
RT Window (seconds)	<p>Specifies the maximum viewable window around the identified chromatographic peak.</p> <p>Default: 30.00</p>
Use RT Limits	<p>Specifies a lower and upper limit for searches.</p> <p>Valid range: 0.00 through 999.99 minutes Default: 0.00 minutes for lower limit; 999.00 minutes for upper limit</p>
Mass Tolerance	<p>Specifies the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value.</p> <p>Valid range: 0 through 500 Default: 5.00 Unit: mmu or ppm</p> <p>Note When using ion trap data, the application uses 300 mmu regardless of the value you enter here.</p>

Table 70. Peak Settings page parameters (Sheet 2 of 3)

Command	Description
Alignment and Gap Filling	<p>Specifies that the application create a single peak list for the whole batch whether or not a peak was found in a raw data file.</p> <p>Note To perform alignment, each sample in the batch must include the same scan filters used by the first sample. Samples 2-<i>n</i> can have additional filters as long as they also include all filters specified in the first sample.</p> <p>When you clear this option, each data file has its own unique peak list based on the unknown peak settings.</p>
All Peaks / Top Peaks	Specifies that the application display results for the top <i>n</i> peaks or for all peaks.
(number of) Top Peaks	<p>Specifies the maximum number of peaks to identify. Available only when you select the previous Top Peaks option.</p> <p>Default: 50</p>
Search Options	
Search Types	<p>Database Search: To specify the unknown database search parameters, see “Editing the Database Settings” on page 323.</p> <p>Library Search: To specify the unknown library search parameters, see “Editing the Element Settings” on page 327.</p> <p>Elemental Composition: To specify the unknown elemental search parameters, see “Editing the Element Settings” on page 327.</p> <p>ChemSpider Search: To specify the ChemSpider search parameters, see “Editing the ChemSpider Settings” on page 331.</p>
Highest Point Analysis	<p>Specifies that the application perform the search only on the sample that has the highest peak response of all samples in the batch, working in conjunction with the Alignment and Gap Filling option.</p> <p>For example, in a batch with samples 1, 2, and 3 with responses of 10, 1000, and 50, respectively, the application performs the search only on the peak from sample 2 with the greatest peak response. Because the mass and retention time for the peak are the same in each sample, the application identifies the same chemical. When you use this option with the Top Peaks option, the application uses the responses across the batch to filter the results and treats the entire batch of sample data as it would when returning the top <i>n</i> responses for a single sample.</p> <p>When you clear this option, the application uses single-sample logic.</p>

Table 70. Peak Settings page parameters (Sheet 3 of 3)

Command	Description
Exhaustive Search / Simple Search	<p>Simple Search (Default): When the application identifies a peak by one of the identification points, it lists only that compound name in Data Review.</p> <p>Exhaustive Search: The application lists all identified peaks from each search criterion and displays them as hierarchical entries under the top hit entry in Data Review.</p>
Number of Top Matches	<p>Specifies the maximum number of matches returned from a library search that you want to display in the Cross Sample Peak List in Data Review and in reports.</p> <p>Valid range: 1 through 99 Default: 3</p>

Editing the Library Settings

Use the Library Settings page to specify the settings for library searches. The application uses these settings only when you select the Library Search option as a search type. See [“To specify the compound databases to use”](#) on [page 324](#).

To find the identity of an unknown compound, the application searches the MS/MS spectrum against a mass spectral library using the library search parameters specified in the method. The application displays the results in Data Review. The application uses the MS/MS scan closest to the apex of the detected peak or from the associated data-dependent scan for the extracted mass chromatogram and submits it for a library search.

When the application finds a library match and the formula is present in the library record, the application reports the formula in Data Review.

When the application does not find a library match, or when the match does not have an associated formula, the application does the following:

- Performs a reverse search of the mass spectrum against the library.
- Returns the top n hits, where n is the value of the Number of Top Matches parameter.
- Displays each match as a separate row in Data Review.
- Shows the score for each match in Data Review (except matches with a score of zero).

Follow these procedures:

- [To open the Library Settings page](#)
- [To specify the libraries to use](#)
- [To specify the general library settings](#)
- [To specify the NIST settings](#)
- [To specify the Library Manager settings](#)

❖ **To open the Library Settings page**

Click the **Library Settings** tab.

The Library Settings page opens. See “[Library Settings Page](#)” on [page 320](#) or “[Library Settings page parameters](#)” on [page 321](#).

❖ **To specify the libraries to use**

In the Library Selection area, select the **Enabled** check box for each library that you want to use for unknown screening searches.

The Database Name list displays the libraries located in the following folders:

C:\Program Files (x86)\NISTMS\MSSEARCH

C:\TraceFinderData\New Libraries

❖ **To specify the general library settings**

1. To specify the source for the confirming peaks, select one of the following:

- **MS:** Confirming peaks come from the same scan.
- **MS2:** Confirming peaks are fragments from an adjacent scan.
- **MS–In Source CID:** Confirming peaks come from the Source CID.

2. (Optional only when you select MS2) To use the isolation width when no precursor match is found, select the **Use Isolation Width** check box.

The application uses the isolation width to determine if there is an MS/MS scan within the same peak RT window that includes the precursor fragments.

❖ **To specify the NIST settings**

1. To specify the type of search to perform, select one of the following:

- **Normal:** Uses a more extensive set of presearch screenings—a total of four different criteria.

When you select this option, skip to [step 6](#).

- **MS/MS:** Searches for an MS/MS spectrum in a library of MS/MS spectra.
- **In-source HiRes:** Searches for an in-source/EI with an accurate ion m/z or an MS/MS spectrum in a library that contains in-source/EI accurate ion m/z or MS/MS spectra.

2. Select a value for Precursor Tolerance, and then select the units of measure.

3. Select a value for Product Tolerance, and then select the units of measure.

4. To ignore mass spectral peaks within the specified precursor tolerance range, select the **Ignore Precursor** check box.

Note This option is available only when you select MS/MS as the NIST search type.

5. To use alternate peak matching, select the **Use Alt Peak Matching** check box.

Note This option is available only when you select MS/MS as the NIST search type.

6. To specify that the application use the reverse search method, select the **Reverse Search** check box.

A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).

7. For libraries created before 2014, set the Presearch option to **Off**.

8. Select a threshold value for SI Threshold.

The application uses this lower threshold value for the search index method used to search the NIST library. The application does not return results below this value.

9. Select a threshold value for RSI Threshold.

The application uses this lower threshold value for the reverse search index method used to search the NIST library. The application does not return results below this value.

10. Select a threshold value for Probability Threshold.

The application uses this lower threshold value for the match probability.

❖ To specify the Library Manager settings

1. Select a value for Spectrum Tolerance.
2. Select the units of measure for spectrum tolerance.
3. Select a threshold value for Score Threshold.

The application uses this lower threshold value for the Library Score in Data Review. The application does not return results below this value. See [“Peak Identifications Pane” on page 652](#).

4. To ignore mass spectral peaks within the specified precursor tolerance range, select the **Ignore Precursor** check box.

5. To specify that the application use the reverse search method, select the **Reverse Search** check box.

A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).

Library Settings Page

Use the Library Settings page to specify the parameters for library searches. The application uses these settings only when you select the Library Search option as a search type.

Figure 98. Library Settings page

The screenshot shows the 'Library Settings' window. At the top is a 'Library Selection' table with columns for 'Enabled', 'Database Name', and 'Database Type'. Below the table are sections for 'General Library Settings', 'NIST Settings', and 'Library Manager Settings', each containing various input fields, checkboxes, and dropdown menus.

	Enabled	Database Name	Database Type
1	<input type="checkbox"/>	mainlib	NIST
2	<input type="checkbox"/>	New Library	NIST
3	<input type="checkbox"/>	NISTDEMO	NIST
4	<input type="checkbox"/>	nist_msms	NIST
5	<input type="checkbox"/>	HARAM_Spectral_Library_Combined_v1_0.db	LibraryManager

General Library Settings

MS Order: MS

Use Isolation Width

NIST Settings

Search Type: Normal

Precursor tolerance: 1.60 ppm

Product tolerance: 1.60 ppm

Ignore Precursor Use alt peak matching

Reverse Search

Presearch: Default

SI Threshold: 250

RSI Threshold: 250

Probability Threshold: 10.00

Library Manager Settings

Spectrum Tolerance: 5.00 ppm

Score Threshold: 80.00

Ignore Precursor Reverse Search

Table 71. Library Settings page parameters (Sheet 1 of 2)

Parameter	Description
Library Selection	
Enabled	The databases for unknown screening searches.
Library Name	Specifies all libraries that you configured in the Configuration Console. See “ Screening Libraries ” on page 59 .
Library Type	Specifies the library type as either NIST or LibraryManager.
General Library Settings	
MS Order	Specifies that the confirming peaks come from the same scan (MS), are fragments from an adjacent scan (MS2), or come from the Source CID (MS–In Source CID).
Use Isolation Width	Specifies that the application use the isolation width to determine if there is an MS/MS scan within the same peak RT window that includes the precursor fragments. Available only when you set the MS Order to MS2 .
NIST Settings	
Search Type	<p>Normal: Uses a more extensive set of presearch screenings—a total of four different criteria.</p> <p>MS/MS: Searches for an MS/MS spectrum in a library of MS/MS spectra.</p> <p>In-source HiRes: Searches for an in-source/EI with an accurate ion <i>m/z</i> or an MS/MS spectrum in a library that contains in-source/EI accurate ion <i>m/z</i> or MS/MS spectra.</p>
Precursor Tolerance	<p>Specifies the precursor <i>m/z</i> tolerance range as either amu or ppm.</p> <p>Valid range: 0.015 through 100 000 Default: 1.60 Available only when you select MS/MS or In-source HiRes search types.</p>
Product Tolerance	<p>Specifies the mass spectral peak tolerance range as either amu or ppm.</p> <p>Valid range: 0.015 through 100 000 Default: 1.60 Available only when you select MS/MS or In-source HiRes search types.</p>
Ignore Precursor	<p>Ignores mass spectral peaks within the specified precursor tolerance range.</p> <p>Available only when you select MS/MS or In-source HiRes search types.</p>

Table 71. Library Settings page parameters (Sheet 2 of 2)

Parameter	Description
Use Alt Peak Matching	Specifies that the application use an alternate peak matching method for searching the mass spectra. Available only when you select MS/MS or In-source HiRes search types.
Reverse Search	Specifies that the NIST library search use the reverse search method. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
Presearch	Specifies that the application use presearch screening before calculating the spectrum-by-spectrum match factor.
SI Threshold	Specifies the lower threshold value for the search index method used to search the NIST library. The application does not return results below this value. Valid range: 0 through 999 Default: 250
RSI Threshold	Specifies the lower threshold value for the reverse search index method used to search the NIST library. The application does not return results below this value. Valid range: 0 through 999 Default: 250
Probability Threshold	Threshold value for the match probability.
Library Manager Settings	
Spectrum Tolerance	Specifies the spectrum tolerance as either amu or ppm. Valid range: 0.1 through 1000.0 Default: 5.00 ppm
Score Threshold	Specifies that the application does not return results below this value. Valid range: 0 through 100 Default: 80.00
Ignore Precursor	Specifies that the application ignore mass spectral peaks within the specified precursor tolerance range.
Reverse Search	Specifies using the reverse search method for a Library Manager search. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).

Editing the Database Settings

Use the Database Settings page to specify the compound databases and the settings for database searches. The application uses these settings only when you select the Database Search option as a search type. See [“To specify the compound databases to use” on page 324](#). The application compares the specified compound databases with found peaks from the mass analyzer peak detector.

When a found peak is within the mass range of a compound in a specified database, the application scores it as a match and adds the labeled peak result to the Data Review results grid for unknown screening analysis.

If the application finds a conflict of information, then the application uses the next level of identification to compare the fragments of any associated data-dependent scan. The application chooses the peak with the most matching fragments as the name of the peak.

If there are no fragments available, then the application labels the compound database entry with the mass that is closest to the mass of the extracted mass analyzer peak.

Follow these procedures:

- [To open the Database Settings page](#)
- [To specify the database matching settings](#)
- [To specify the fragments settings](#)
- [To specify the isotopes settings](#)
- [To specify the compound databases to use](#)

❖ To open the Database Settings page

Click the **Database Settings** tab.

The Database Settings page opens. See [“Database Settings Page” on page 325](#).

❖ To specify the database matching settings

1. In the CDB RT Window box, type a value (in seconds) for the database retention time window.
2. Specify the number of millimass units or parts per million for the $m/z \pm$ tolerance value.
3. Select the units of measure for mass tolerance.

The application applies this mass tolerance to the extracted chromatograms.

❖ To specify the fragments settings

1. In the Intensity Threshold box, type a value for the minimum intensity value for fragments.

Fragments with intensity values less than this value are ignored.

2. Specify the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value for fragments.

3. Select the units of measure that you want to use for mass tolerance for fragments.

The application applies this mass tolerance to the fragment chromatograms.

4. To specify the source for the fragment peaks, select one of the following:

- **MS:** Fragment peaks come from the same scan.
- **MS2:** Fragment peaks are fragments from an adjacent scan.
- **MS–In Source CID:** Fragment peaks come from the Source CID.

❖ **To specify the isotopes settings**

1. In the Allowed Mass Deviation box, type a value (in parts per million) to specify the allowed mass deviation in the spectrum data.

The isotopic pattern algorithm considers an isotope peak as found if its measured m/z is less than this deviation amount away from its expected m/z . For best results, set this value to a number that causes up to 98 percent of all mass deviations to be smaller than the allowed mass deviation value.

2. In the Allowed Intensity Deviation box, type a value to specify the allowed intensity deviation of the mass spectrometer relative to the monoisotopic ion, as a percentage of the base peak height.

The isotopic pattern algorithm considers an isotope peak as not found if its intensity relative to the monoisotopic ion's intensity is more than this deviation percentage from the theoretical relative intensity of the isotope ion. For best results, set this value to a number that causes up to 98 percent of all intensity deviations to be smaller than the allowed intensity deviation value.

3. To specify that isotopic pattern calculations use internal mass calibration, select the **Use Internal Mass Calibration** check box.

Otherwise, to use external mass calibration, clear the check box.

When selected, the application applies a requirement that an isotope's m/z must be closer to its theoretical value to avoid a score penalty.

For more information, see [“Isotopic Pattern Score Calculations”](#) on [page 725](#).

❖ **To specify the compound databases to use**

1. Select the **Selected** check box for each compound database that you want to use for the database search.
2. (Optional) To edit a database, click **open** and do the following:

- a. Edit the database.

See [“Editing Compounds in the Database”](#) on [page 84](#).

- b. When you finish editing the database, click **Processing** in the Method View navigation pane to return to the Processing page.

Database Settings Page

Use the Database Settings page to specify the compound databases and settings for database searches. The application uses these settings only when you select the Database Search option as a search type.

Figure 99. Database Settings page

The screenshot shows the 'Database Settings' window with the following parameters:

- CDB Matching:** CDB RT Window (seconds) = 30.00; Mass Tolerance = 5.00 ppm.
- Fragments:** Intensity Threshold = 10,000; Mass tolerance = 5.00 ppm; MS Order = MS.
- Isotopes:** Allowed Mass Deviation (ppm) = 5; Allowed Intensity Deviation (%) = 10; Use Internal Mass Calibration = .
- Database List:**


	Selected	Database Name	
1	<input checked="" type="checkbox"/>	DefaultGC	open
2	<input checked="" type="checkbox"/>	DefaultLC	open

Table 72. Database Settings page parameters (Sheet 1 of 2)

Parameter	Description
CDB Matching	
CDB RT Window (seconds)	Specifies the database retention time window in seconds. Default: 30.00
Mass Tolerance	Specifies the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value for CDB matching and for calculating isotopic patterns. Default: 5.00 Valid range: 0.1 through 999 Unit: mmu or ppm <ul style="list-style-type: none"> mmu (millimass units): mmu is a static calculation to the extracted mass. (Default) 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.

IMPORTANT If you set this mass tolerance value greater than the value for [Allowed Mass Deviation](#), the application might not be able to generate the isotopic patterns.

Table 72. Database Settings page parameters (Sheet 2 of 2)

Parameter	Description
Fragments	
Intensity Threshold	Fragments with intensity values less than this are ignored. Default: 10 000
Mass Tolerance	Specifies the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value for calculating fragments. Default: 5.00 Valid range: 0.1 through 999 Unit: mmu or ppm <ul style="list-style-type: none"> • mmu (millimass units): mmu is a static calculation to the extracted mass. • (Default) 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.
MS Order	Specifies that the confirming peaks come from the same scan (MS), are fragments from an adjacent scan (MS2), or come from the Source CID (MS–In Source CID).
Isotopes	
Allowed Mass Deviation	Specifies the allowed mass deviation in the spectrum data. Valid range: 3 through 100 ppm Default: 5 ppm
IMPORTANT If you set this mass deviation value less than the value for Mass Tolerance , the application might not be able to generate the isotopic patterns.	
Allowed Intensity Deviation	Specifies the allowed intensity deviation of the mass spectrometer relative to the monoisotopic ion, as a percentage of the base peak height. Valid range: 1 through 100% Default: 10%
Use Internal Mass Calibration	Specifies that isotopic pattern calculations use internal mass calibration.
Database List	
Selected	Specifies that the application use the compound database for a database search.
Database Name	Specifies the name of the database.
Refresh 	Updates the database list.
Open	Opens the compound database in the Method Development mode.

Editing the Element Settings

Use the Element Settings page to specify settings to use for elemental composition searches. The application uses these settings only when you select the Elemental Composition option as a search type. See [“To specify the compound databases to use”](#) on page 324.

Follow these procedures:

- [To open the Element Settings page](#)
- [To specify the scoring settings](#)
- [To specify the elemental composition settings](#)
- [To select elements to use in the elemental formula](#)

❖ To open the Element Settings page

Click the **Element Settings** tab.

The Element Settings page opens. See [“Element Settings Page”](#) on page 330.

❖ To specify the scoring settings

1. In the Allowed Mass Deviation box, type a value (in parts per million) to specify the allowed mass deviation in the spectrum data.

The isotopic pattern algorithm considers an isotope peak as found if its measured m/z is less than this deviation amount away from its expected m/z . For best results, set this value to a number that causes up to 98 percent of all mass deviations to be smaller than the allowed mass deviation value.

2. In the Allowed Intensity Deviation box, type a value to specify the allowed intensity deviation of the mass spectrometer relative to the monoisotopic ion, as a percentage of the base peak height.

The isotopic pattern algorithm considers an isotope peak as not found if its intensity relative to the monoisotopic ion's intensity is more than this deviation percentage from the theoretical relative intensity of the isotope ion. For best results, set this value to a number that causes up to 98 percent of all intensity deviations to be smaller than the allowed intensity deviation value.

3. To specify that isotopic pattern calculations use internal mass calibration, select the **Use Internal Mass Calibration** check box.

Otherwise, to use external mass calibration, clear the check box.

When using internal mass calibration, the application applies a requirement that an isotope's m/z must be closer to its theoretical value to avoid a score penalty.

For more information, see [“Isotopic Pattern Score Calculations”](#) on page 725.

❖ **To specify the elemental composition settings**

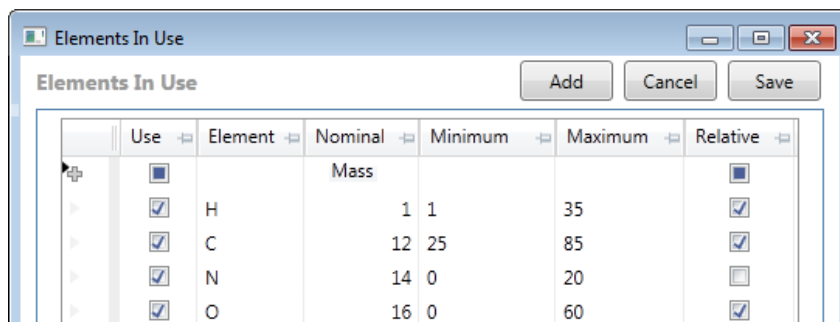
1. From the Electron Rule list, select one of the following rules to use in the formula calculation: **Do Not Use**, **Even Electrons**, or **Odd Electrons**.
2. In the RDB Equiv Low and the RDB Equiv High boxes, type values for double bonds and ring equivalents—a measure of the number of unsaturated bonds in a compound—to limit the calculated formulas to only those that make sense.
The RDB Equiv Low value must be smaller than the RDB Equiv High value.

❖ **To select elements to use in the elemental formula**

1. Click **View Elements**.

The Elements In Use dialog box opens. By default, all elements are selected for use.

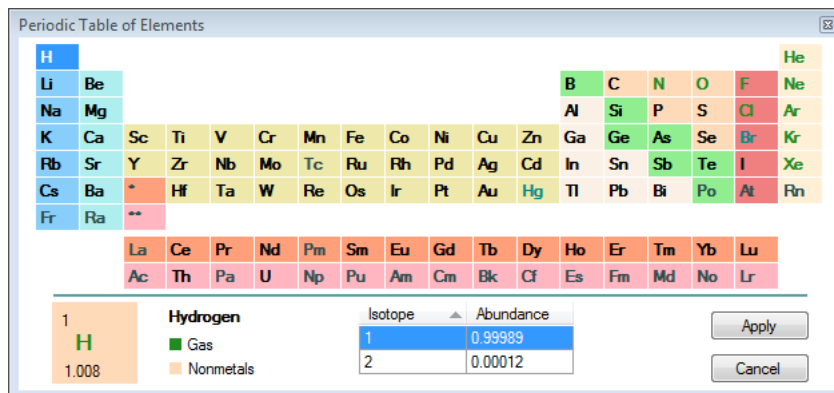
Figure 100. Element in Use dialog box



2. To activate an element in the list, select the corresponding **Use** check box.
3. To deactivate an element in the list, clear the corresponding **Use** check box.
4. To add an element to the list, do the following:
 - a. Click **Add**.

The Periodic Table of Elements opens. See [Periodic Table of Elements](#).

Figure 101. Periodic Table of Elements



- b. Select an element and click **Apply**.

Tip If the element you select displays several isotopes, for best results, select the most abundant one before you click **Apply**.

Isotope	Abundance
1	0.99989
2	0.00012

The periodic table closes, and the application adds the selected element to the Elements In Use dialog box.

The values in the Element column and the Nominal Mass column are read-only. You can edit the values in the Minimum, Maximum, and Relative columns.

IMPORTANT Add candidates only for the neutral molecule, not for adducts.

5. In the Relative column, do one of the following:
- To specify the maximum or minimum value as an absolute number of atoms, clear the check box.
 - To specify the maximum or minimum value as a relative percentage by weight, select the check box.

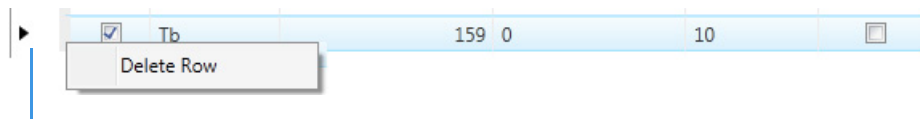
Default: Selected for H, C, and O; cleared for all other elements

6. In the Minimum and Maximum columns, specify a minimum value and a maximum value to define the calculated element.

You can type each of these values as either an absolute number of atoms (0 through 1000) or as a relative percentage by weight (0 through 100%), depending on the setting in the Relative column.

The value you enter for the Minimum column must be smaller than the value for the Maximum column.

7. To remove elements from use in the elemental formula, do the following:
- Select the element row by clicking in the row selector area marked by the arrow icon.
 - Right-click and choose **Delete Row** from the shortcut menu (or press the DELETE key).



Click here to select the row, right-click, and select **Delete Row**.

- Click **Yes** in the confirmation dialog box to remove the selected rows from the table.

Tip To select noncontiguous rows, hold down the CTRL key when you select them. To select contiguous rows, select the first row in the group, hold down the SHIFT key, and then select the last row in the group. Or, drag your pointer across the group of rows.

Tip You can also deactivate an element from use in the elemental formula without removing it from the table by clearing the element's Use check box.

Element Settings Page

Use the Element Settings page to specify settings to use for elemental composition searches.

Figure 102. Element Settings page

Table 73. Element Settings page parameters (Sheet 1 of 2)

Parameter	Description
Scoring Settings	
Allowed Mass Deviation (ppm)	Specifies the allowed mass deviation in the spectrum data. Valid range: 3 through 100 ppm Default: 5 ppm
Allowed Intensity Deviation (%)	Specifies the allowed intensity deviation of the mass spectrometer relative to the monoisotopic ion, as a percentage of the base peak height. Valid range: 1 through 100% Default: 10%
Use Internal Mass Calibration	Specifies that isotopic pattern calculations use internal mass calibration.

Table 73. Element Settings page parameters (Sheet 2 of 2)

Parameter	Description
Elemental Composition	
Electron Rule	Specifies whether to use a rule in the formula calculation. Valid values: Do Not Use, Even Electrons, Odd Electrons Default: Even Electrons
RDB Equiv Low	Specifies the lower limit value for double bonds and ring equivalents—a measure of the number of unsaturated bonds in a compound—to limit the calculated formulas to only those that make sense. The RDB Equiv Low value must be smaller than the RDB Equiv High value. Valid range: -1.5 through 99.9 Default: -1.5
RDB Equiv High	Specifies the upper limit value for double bonds and ring equivalents—a measure of the number of unsaturated bonds in a compound—to limit the calculated formulas to only those that make sense. Valid range: 0 through 100 Default: 100.00
View Elements	Opens the Elements in Use dialog box where you can specify the elements to use in the elemental formula.

Editing the ChemSpider Settings

Use the ChemSpider Settings page to specify settings to use for ChemSpider searches. The application uses these settings only when you select the ChemSpider Search option as a search type. See [“To specify the compound databases to use” on page 324](#).

ChemSpider is an online search engine that provides access to millions of chemical structures in databases. The ChemSpider search engine aggregates and indexes chemical structures and their associated information into a single, searchable repository.

IMPORTANT You must have an Internet connection to access the ChemSpider databases.

The application sends suggested elemental compositions to the ChemSpider search engine and retrieves compound names that match the searched elemental compositions. The application uses the active databases that you select and ranks the results according to the number of databases that return found references for each matched compound. The higher the number of databases with found references, the higher the ranking for that match. To speed processing, the application stores the results in a local cache. The cache maintains the age of each result from the time that the entry is saved. During a search, the application deletes any cached entry older than the time period specified in the Cached Entries Expire After list and replaces it with newer information.

Each time you update the list of active databases, the application clears the entire cache and starts over with new information from the next search. Unknown screening searches that use the ChemSpider search engine might take longer until the application populates the cache with results again. When you change the list of active databases, the ranking of the results might also change accordingly.

Follow these procedures:

- [To open the ChemSpider Settings page](#)
- [To update the list of available databases](#)
- [To make databases active](#)
- [To specify an expiration time for cached entries](#)

❖ **To open the ChemSpider Settings page**

Click the **ChemSpider Settings** tab.

The ChemSpider Settings page opens. See [ChemSpider Settings Page](#).

❖ **To update the list of available databases**

Click **Refresh**.


The application updates the list of available databases with the most current list from the ChemSpider website.

IMPORTANT Each time you access the ChemSpider Settings page, the application automatically compares the list of available databases with the most current list from the ChemSpider website. The Refresh button becomes available only when there is a difference between the two lists.

❖ **To make databases active**

1. From the Available Databases list, select the ChemSpider databases that you want to search.

Note Use the CTRL or SHIFT keys to select multiple databases.

2. Click  to move the selected databases to the Active Databases list.

The application searches all active ChemSpider databases for matching compound formulas.

IMPORTANT Whenever you change the list of active databases, the application deletes all previous results stored in the cache and starts over with new information from the next search. This might increase the time required to complete the search.

IMPORTANT If a database in the Active Databases box is no longer available on the website, the application automatically removes that database name.

❖ To specify an expiration time for cached entries

Select one of the following time periods from the Cached Entries Expire After list:

- ThreeMonths
- SixMonths
- OneYear
- Never

During a search, the application deletes any cached entry older than this value and replaces it with newer information.

ChemSpider Settings Page

Use the ChemSpider Settings page to specify settings to use for ChemSpider searches.

Figure 103. ChemSpider Settings page

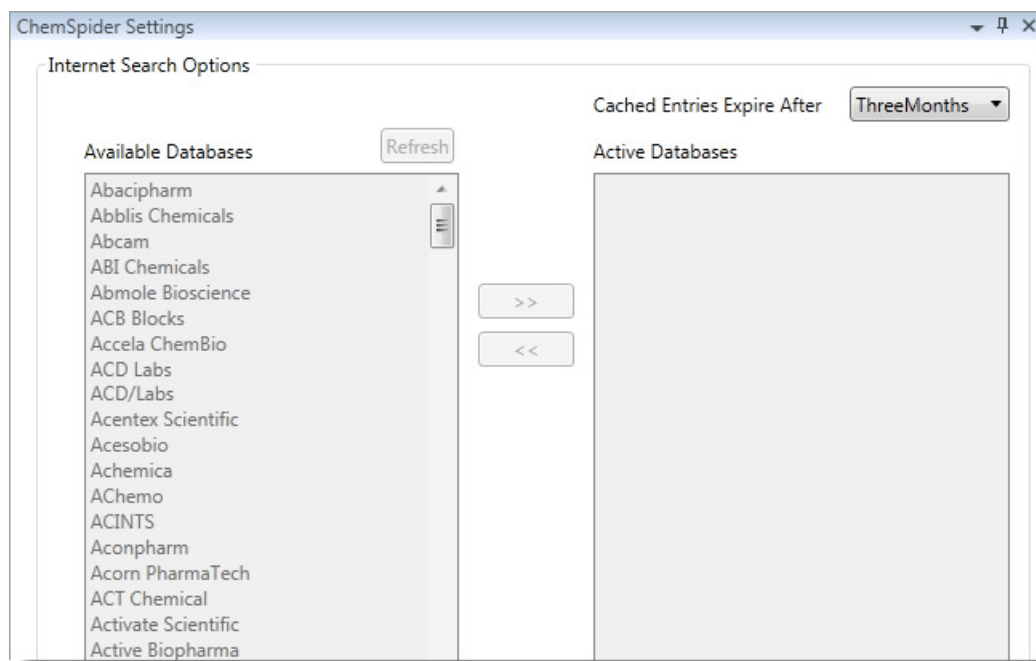


Table 74. ChemSpider Settings page parameters

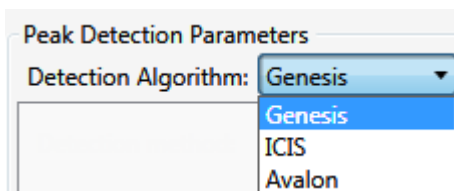
Parameter	Description
Available Databases	Lists the most current databases from the ChemSpider website.
Refresh	Updates the list of available databases with the most current list from the ChemSpider website.
Cached Entries Expire After	During a search, the application deletes any cached entry older than the specified value and replaces it with newer information.
Active Databases	Lists the ChemSpider databases that you can search.

Editing the Peak Detection Settings Page

Use the features on the Peak Detection page to specify any of the following peak detection algorithms: Genesis, ICIS, or Avalon.

❖ To specify peak detection parameters

1. Click **Peak Detection** in the Method View navigation pane.
2. In the Peak Detection Parameters area, select one of the detection algorithms: **Genesis**, **ICIS**, or **Avalon**.



- The Genesis peak detection algorithm provides backward compatibility with Xcalibur 1.0 studies. For detailed descriptions of the Genesis method parameters, see [Genesis Detection Method](#).
 - The ICIS peak detection algorithm is designed for MS data and has highly efficient peak detection at low MS signal levels. For detailed descriptions of the ICIS method parameters, see [“ICIS Detection Method”](#) on [page 338](#).
 - The Avalon peak detection algorithm is designed for integrating UV/Vis and analog chromatograms. For detailed descriptions of the Avalon method parameters, see [“Avalon Detection Method”](#) on [page 341](#).
3. Specify the parameters for the selected detection algorithm.

Genesis Detection Method

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

Figure 104. Genesis peak detection

The screenshot shows the 'Peak Detection Parameters' dialog box. The 'Detection Algorithm' is set to 'Genesis'. The 'Detection method' is set to 'Nearest RT'. Other parameters include Smoothing (1), S/N threshold (2.00), Expected width (sec) (0.00), Peak height (%) (5.00), Tailing factor (1.00), Peak S/N cutoff (200.00), Valley rise (%) (2.00), Valley S/N (1.10), # background scans (5), and Report noise as (Peak To Peak).

Table 75. Genesis peak detection parameters (Sheet 1 of 3)

Parameter	Description
Detection Algorithm	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. Valid values: Any odd integer from 1 through 15 points Default: 1

Table 75. Genesis peak detection parameters (Sheet 2 of 3)

Parameter	Description
S/N threshold	<p>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.</p> <p>Valid range: 0.0 through 999.0</p>
Enable Valley Detection	<p>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.</p>
Expected Width (sec)	<p>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.</p> <p>With valley detection enabled, any valley points nearer than the <i>expected width</i>/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width.</p> <p>Valid range: 0.0 through 999.0</p>
Constrain Peak Width	<p>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 threshold and a tailing factor. Selecting the Constrain Peak Width check box activates the Peak Height (%) and Tailing Factor options.</p>
Peak Height (%)	<p>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.</p> <p>Valid range: 0.0 through 100.0%</p>
Tailing Factor	<p>A factor that controls how the 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.</p> <p>Valid range: 0.5 through 9.0</p>

Table 75. Genesis peak detection parameters (Sheet 3 of 3)

Parameter	Description
Peak S/N Cutoff	<p>The peak edge is set to values below this signal-to-noise ratio.</p> <p>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.</p> <p>When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the application defines the right and left edges of the peak when the S/N reaches a value less than 200.</p> <p>Valid range: 50.0 through 10000.0</p>
Valley Rise (%)	<p>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.</p> <p>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.</p> <p>When the trace exceeds rise percentage, the application applies valley detection peak integration criteria. This test is applied to both the left and right edges of the peak.</p> <p>Valid range: 0.1 through 500.0</p>
Valley S/N	<p>Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher.</p> <p>Valid range: 1.0 through 100.0 Default: 2.0</p>
# Background Scans	Number of background scans performed by the application.
Report Noise As	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or peak-to-peak resolution threshold. Options are RMS or Peak To Peak.

ICIS Detection Method

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

Figure 105. ICIS peak detection

The screenshot shows a 'Peak Detection Parameters' dialog box. At the top, 'Detection Algorithm' is set to 'ICIS'. Below this, 'Detection method' is set to 'Nearest RT'. The 'Smoothing' parameter is set to 1. 'Area noise factor' is 5, 'Peak noise factor' is 10, and 'Baseline window' is 40. There is an unchecked checkbox for 'Constrain peak width'. 'Peak height (%)' is 5.00 and 'Tailing factor' is 1.00. 'Noise method' is set to 'Incos'. 'Min peak width' is 3, 'Multiplet resolution' is 10, 'Area tail extension' is 5, and 'Area scan window' is 0. At the bottom, there is an unchecked checkbox for 'RMS'.

Table 76. ICIS peak detection parameters (Sheet 1 of 3)

Parameter	Description
Detection Algorithm	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. Valid values: Any odd integer from 1 through 15 points Default: 1

Table 76. ICIS peak detection parameters (Sheet 2 of 3)

Parameter	Description
Area Noise Factor	<p>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.</p> <p>Valid range: 1 through 500 Default: 5</p>
Peak Noise Factor	<p>The noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 1 through 1000 Default: 10</p>
Baseline Window	<p>The application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 1 through 500 Default: 40</p>
Constrain Peak Width	<p>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 activates the Peak Height (%) and Tailing Factor options.</p>
Peak Height (%)	<p>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.</p> <p>Valid range: 0.0 through 100.0%</p>
Tailing Factor	<p>A factor that controls how the 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.</p> <p>Valid range: 0.5 through 9.0</p>

Table 76. ICIS peak detection parameters (Sheet 3 of 3)

Parameter	Description
Noise Method	<p>The options are INCOS or Repetitive.</p> <p>INCOS: Uses a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value.</p> <p>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.</p>
Min Peak Width	<p>The minimum number of scans required in a peak. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 0 through 100 scans Default: 3</p>
Multiplet Resolution	<p>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.</p> <p>Valid range: 1 through 500 scans Default: 10</p>
Area Tail Extension	<p>The number of scans past the peak endpoint to use in averaging the intensity. The ICIS peak detection algorithm uses this value.</p> <p>Valid range: 0 through 100 scans Default: 5</p>
Area Scan Window	<p>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.</p> <p>Valid range: 0 through 100 scans Default: 0</p>
RMS	<p>Specifies that the 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.</p>

Avalon Detection Method

The Avalon peak detection algorithm is designed for UV data. The Avalon peak detection algorithm also supports negative peaks. You can edit the Event values from the [Avalon Event List](#).

Figure 106. Avalon peak detection

Peak Detection Parameters

Detection Algorithm: Avalon

Detection method: Nearest RT

Smoothing: 1

Time	Event	Value
Initial	Start Threshold	10000.000
Initial	End Threshold	10000.000
Initial	Area Threshold	10000.000
Initial	P-P Threshold	1.000
Initial	Bunch Factor	1.000
Initial	Negative Peaks	Off

Autocalc initial events Edit

Table 77. Avalon peak detection parameters

Parameter	Description
Detection Algorithm	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. Valid values: 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.
Autocalc Initial Events	Automatically calculates the events in the Event list.
Edit	Opens the Avalon Event List dialog box where you can edit the Time/Event/Value parameters. See “Avalon Event List.”

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](#).

Figure 107. Avalon Event List dialog box

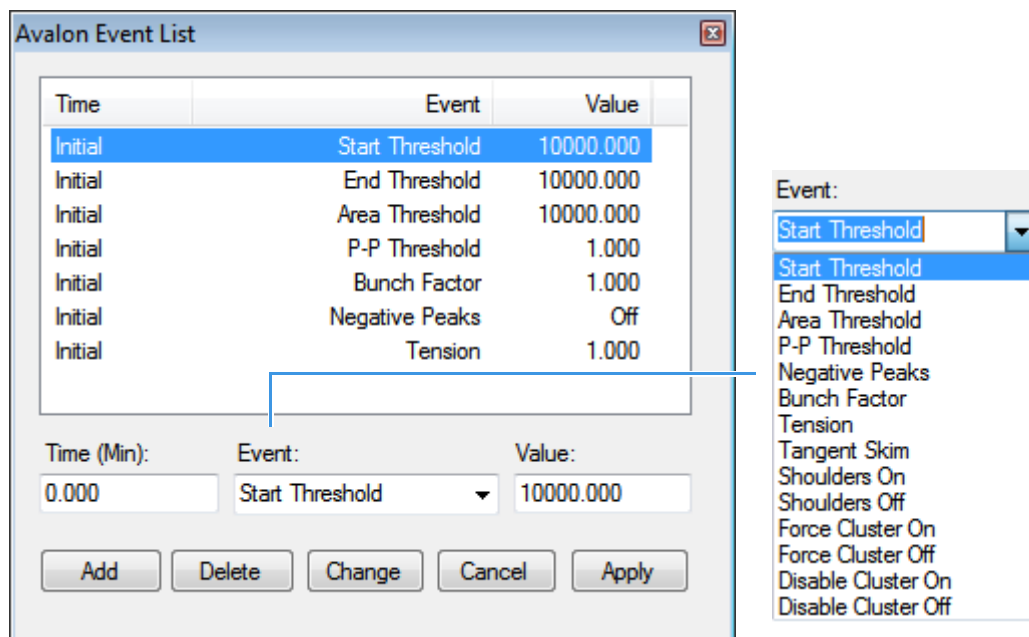
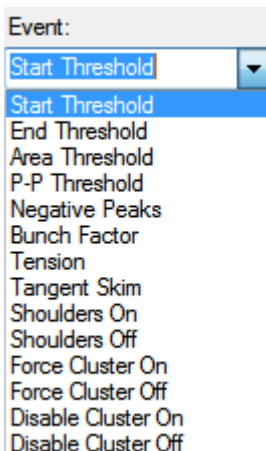


Table 78. Avalon Event List dialog box parameters

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.”
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 108. Event types**Table 79.** Event type descriptions (Sheet 1 of 2)

Event type	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. Valid range: 0 through 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. Valid range: 0 through 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. Valid range: 0 through 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. Valid range: 0.1 through 99.99
Negative Peaks	Permits detection of a negative going peak. Automatically resets after finding a negative peak. Valid values: On or Off

Table 79. Event type descriptions (Sheet 2 of 2)

Event type	Description
Bunch Factor	<p>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.</p> <p>Valid range: 0 through 999</p>
Tension	<p>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.</p> <p>Valid range: 0 through 999.99 minutes</p>
Tangent Skim	<p>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.</p> <p>Valid range: 0 through 1</p>
Shoulders On	<p>Allows peak shoulders to be detected (peaks which are separated by an inflection rather than a valley) Sets a threshold for the derivative.</p>
Shoulders Off	<p>Disables peak shoulder detection.</p> <p>Valid range: 0 through 50</p>
Force Cluster On	<p>Force the following peaks to be treated as a cluster (single peak).</p>
Force Cluster Off	<p>End the forced clustering of peaks.</p>
Disable Cluster On	<p>Prevent any peaks from being clustered.</p>
Disable Cluster Off	<p>Permit clusters to occur again.</p>

Editing the Reports Page

Use the Reports page to specify how you want to save or print your reports. For descriptions of the features on the Reports page, see [Reports Page](#).

See the instructions for the following tasks:

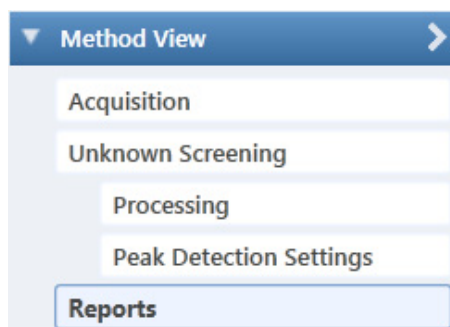
- [Specifying Report Formats](#)
- [Specifying Report Options](#)

Specifying Report Formats

For each report type, you can create a hard-copy printout, a PDF file, a CSV file, or an Excel file.

❖ To open the Reports page

Click **Reports** in the Method View navigation pane.

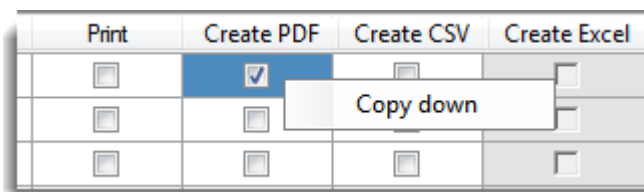


The Reports page opens with a list of all configured reports.

To configure which reports are available when you create a master method or which reports create a batch-level report, see [“Specifying the Reports”](#) on page 71.

❖ To specify reports and output formats

1. To specify the type of report output to create for each report, select the check box in the appropriate column.
2. To duplicate an output type for all reports, click the cell to select it, and 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 type options are cleared.

Reports Page

Use the features on the Reports page to specify how you want to save or print your reports.

Figure 109. Reports page

	Report	Print	Create PDF	Create CSV	Create Excel	Exists
	HeatMap Report(Unknown)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	Results Detail Long Report(Unknown)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	Unknown Screening High Density	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Table 80. Reports page parameters

Parameter	Description
Report list columns	
Report	The name of a report.
Print	Sends reports to the default printer.
Create PDF	Saves reports as PDF files.
Create CSV	Saves reports as CSV files.
Create Excel	Saves reports as Excel files.
Exists	Indicates that the report template is identified in the C:\TraceFinderData\3.3\Templates\ReportTemplates folder.

Specifying Report Options

Use the options on the Report Options page to choose the compounds to display in reports.

Figure 110. Reports Options page

Table 81. Report Options page parameters

Parameter	Description
Include All Compounds	Generates reports that include all compounds results, whether or not they are found in the samples.
Include Only Found Compounds	Generates reports that include only the compounds that are found in the samples.

Using the Acquisition Mode

This chapter describes the tasks associated with the Acquisition mode.

Contents

- [Working with Batches](#)
- [Real Time Status Pane](#)
- [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), you can define a batch template that supplies the basic structure of a batch.

IMPORTANT When user security is activated, you must have Acquisition Wizard – Template Editing permission to create a batch template.

Using a master method, you can create a batch and run the samples. A batch represents 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 Data Review or you can go directly to viewing and printing reports.

You can set up a calibration batch with known concentrations of the target compounds and compare the calibration values against samples in future batches.

You can also use the Quick Acquisition feature to quickly submit a single sample from any page in the Acquisition mode. See [Appendix A, “Using Quick Acquisition.”](#)

Working with Batches

See the instructions for the following tasks:

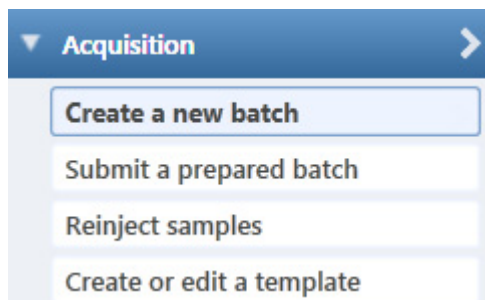
- [Opening and Navigating the Acquisition Mode](#)
- [Creating and Submitting Batches](#)

Opening and Navigating the Acquisition Mode

❖ To access the Acquisition mode

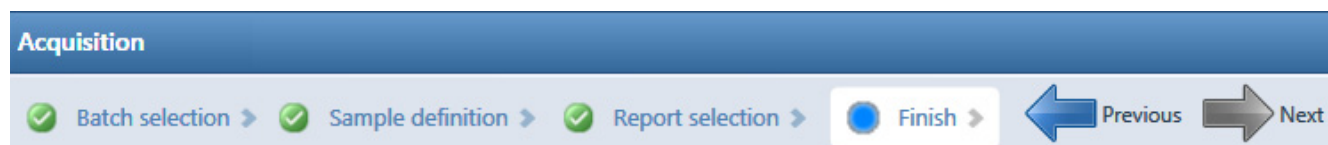
Click **Acquisition** in the navigation pane.

The navigation pane for the Acquisition mode opens.

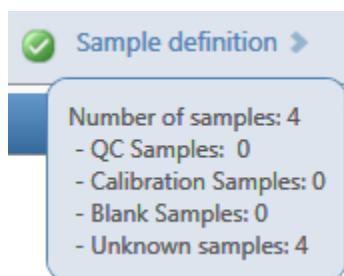
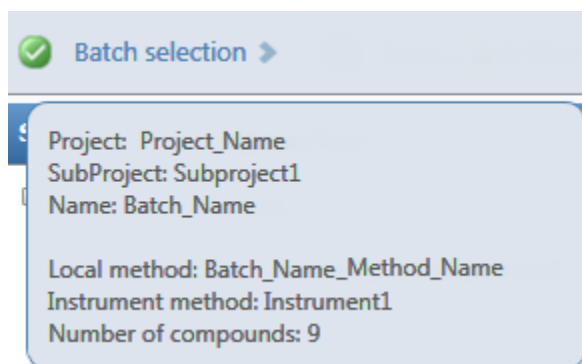


As you progress through the Acquisition mode using any of these methods for creating a batch, the task pane at the top of the view tracks your progress. As you complete each stage, you can hold your cursor over the view name in the task pane to display the parameters that you specified for the batch. See [Example task pane when you have completed the Acquisition mode](#).

Figure 111. Example task pane when you have completed the Acquisition mode



Hold your cursor over Batch Selection, Sample Definition, or Report Selection to view the parameters for your batch.



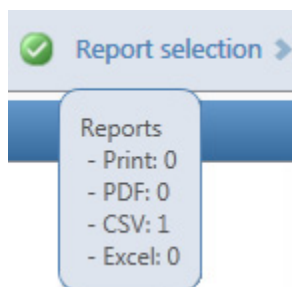
Categories in the Sample Definition list:

QC Samples: QC Std

Calibration Samples: Cal Std

Blank Samples: Matrix Blank

Unknown Samples: All other samples



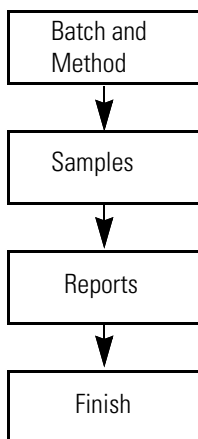
Creating and Submitting Batches

To create and submit a batch, the Acquisition mode uses a wizard-style interface to guide you through these major steps:

1. [Selecting a Batch](#)
2. [Defining a Sample List](#)
3. [Selecting and Reviewing Reports](#)
4. [Submitting a Batch](#)

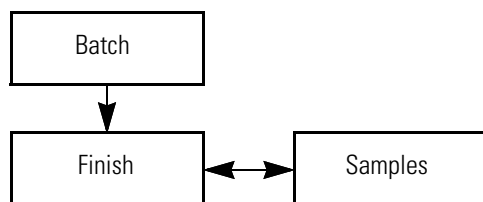
The Acquisition mode provides multiple techniques for creating either a batch or a batch template. Each batch creation technique has an associated workflow, as shown in the following flowcharts. Each workflow uses a different combination of Acquisition mode pages.

Workflow for Creating an Original Batch



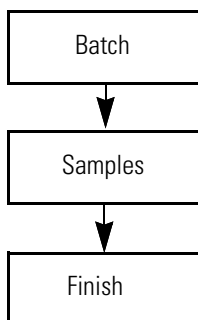
To create an original batch, start with any of these instructions: [“To start a new quantitation batch”](#) on [page 352](#), or [“To start a new target screening batch”](#) on [page 353](#), or [“To start a new unknown screening batch”](#) on [page 354](#).

Workflow for Acquiring a Prepared Batch



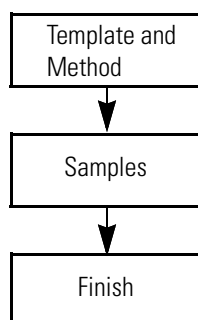
To acquire a prepared batch, start with the instructions [“To select a prepared batch”](#) on [page 355](#).

Workflow for Reinjecting a Previously Acquired Batch



To process a previously acquired batch, start with the instructions [“To reinject samples in a previously acquired batch”](#) on [page 356](#).

Workflow for Creating or Editing a Batch Template



IMPORTANT When user security is activated, you must have Acquisition Wizard – Template Editing permission to create a batch template.

To create a batch template, start with any of these instructions: [“To create a quantitation batch template”](#) on [page 357](#), [“To create a target screening batch template”](#) on [page 358](#), or [“To create an unknown screening batch template”](#) on [page 359](#).

Selecting a Batch

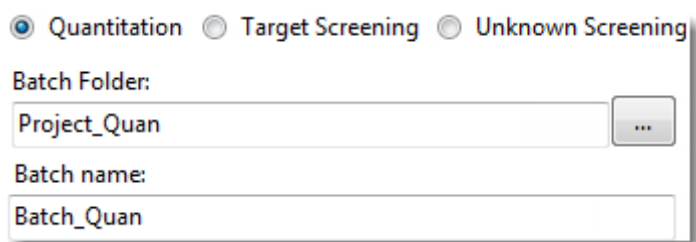
On the Batch Selection page of the Acquisition mode, you can create a new quantitative, target screening, or unknown screening batch in any of your current projects/subprojects. Or, you can submit a batch that you previously prepared and saved, reinject the samples in a batch that you previously acquired, or create a batch template to use for future batches.

Follow these procedures:

- [To start a new quantitation batch](#)
- [To start a new target screening batch](#)
- [To start a new unknown screening batch](#)
- [To start a new batch from a template](#)
- [To select a prepared batch](#)
- [To reinject samples in a previously acquired batch](#)
- [To create a quantitation batch template](#)
- [To create a target screening batch template](#)
- [To create an unknown screening batch template](#)

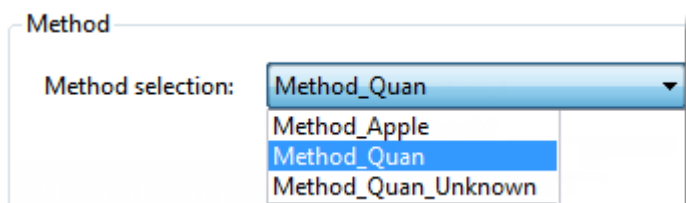
❖ To start a new quantitation batch

1. Click **Create a New Batch** in the navigation pane.
2. Select the **Quantitation** option.
3. Select the batch folder where you want to create the new batch.
4. Type a unique name for the new batch in the Batch Name box.



If the name you enter is not unique, a red warning flashes.

5. 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.

Method

Method selection:

Method Compound Data					
	RT	Compound	Compound type	Active	CAS No
▶	3.14	Propanenitrile	Target Compound	<input checked="" type="checkbox"/>	107120
	3.15	EDIFENPHOS-CE5-R20-T...	Target Compound	<input checked="" type="checkbox"/>	17109498

- To continue to the next page, click **Next**.

The Sample Definition page opens. See “[Defining a Sample List](#)” on [page 360](#).

❖ To start a new target screening batch

- Click **Create a New Batch** in the navigation pane.
- Select the **Target Screening** option.
- Select the batch folder where you want to create the new batch.
- Type a name for the new batch in the Batch Name box.

Quantitation Target Screening Unknown Screening

Batch Folder:

Batch name:

If the name you enter is not unique, a red warning flashes.

- Select a method from the Method Selection list.

The Method Compound Databases pane displays the compound databases in the method. The application uses these databases to identify the compounds in the samples. You cannot edit the compound database list from the Acquisition mode.

Method

Method selection:

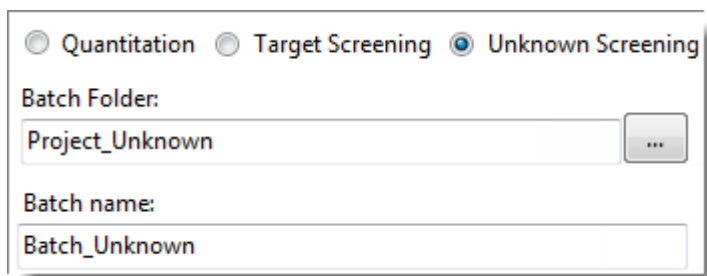
Method Compound Databases	
	Enabled Database File
▶	<input checked="" type="checkbox"/> Default Database
	<input checked="" type="checkbox"/> General_Database
	<input checked="" type="checkbox"/> General_Database2

- To continue to the next page, click **Next**.

The Sample Definition page opens. See “[Defining a Sample List](#)” on [page 360](#).

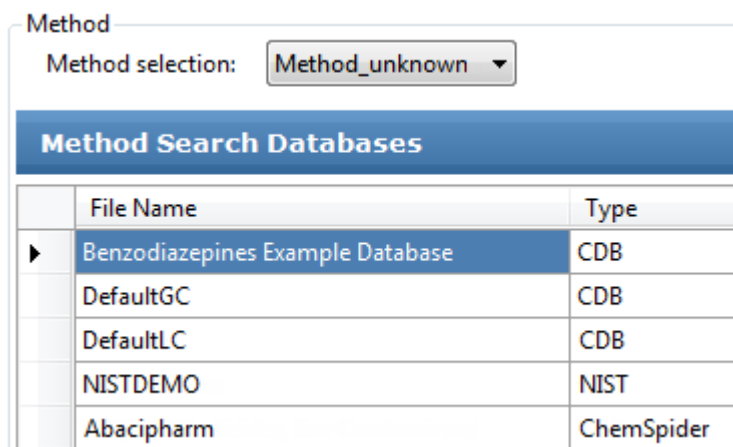
❖ **To start a new unknown screening batch**

1. Click **Create a New Batch** in the navigation pane.
2. Select the **Unknown Screening** option.
3. Select the batch folder where you want to create the new batch.
4. Type a name for the new batch in the Batch Name box.



5. Select a method from the Method Selection list.

The Method Search Databases pane displays the databases that you selected in the method. The application uses these databases to identify the compounds in the samples. You cannot edit the database list from the Acquisition mode.



File Name	Type
Benzodiazepines Example Database	CDB
DefaultGC	CDB
DefaultLC	CDB
NISTDEMO	NIST
Abacipharm	ChemSpider

6. To continue to the next page, click **Next**.

The Sample Definition page opens. See [“Defining a Sample List”](#) on [page 360](#).

❖ **To start a new batch from a template**


1. Click **Create a New Batch** in the navigation pane.
2. Select either the **Quantitation**, **Target Screening**, or **Unknown Screening** option.

The Available Templates pane displays only batch templates for the selected option.

3. In the Available Templates pane, select the template and method combination that you want to use.

Batch name: Template_Quan_1	
Available Templates	
Template name	Method
Template_Quan	Method_Quan

The system creates a batch name with the selected template name and appends the date and time stamp. You can change the batch name, the default batch folder, or the method associated with this template.

4. (Optional) Click  and select a different batch folder where you want to create the new batch.
5. (Optional) Select a different method to use for the new batch.

Method selection: Method_Quan

- Method_Quan
- Method_Apple
- Method_Quan
- Method_Quan_Unknown

6. To continue to the next page, click **Next**.

The Sample Definition page of the Acquisition mode opens. See [“Defining a Sample List”](#) on page 360.

❖ To select a prepared batch

1. Click **Submit a Prepared Batch** in the navigation pane.

The application displays all your unacquired, saved batches. The application stores all unacquired batches in the ...\\TraceFinderData\3.3\Projects\... folder.

2. Select the batch that you want to acquire.

Batch name	Folder	Last modified
Batch_Quan_1	Project_Quan	02-05-2015 11:00AM
Batch_Quan_1	Project_Quan	02-05-2015 10:59AM
Batch_Target_1	Project_Target	02-05-2015 11:00AM
Batch_Unknown_1	Project_Unknown	02-05-2015 11:01AM

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

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


- If the batch is unreadable, the application reports that the batch file is not valid and cannot be opened.
- If a sample in the batch is unreadable, the application cannot open the sample. The application creates a new sample with the same name and flags the sample. You must complete the missing information such as Sample Type, Level, and so forth, and then save the batch before you submit it for acquisition. Or, you can browse in a new raw data file to replace the corrupt file.

4. Do one of the following:

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


For detailed instructions, see “[Defining a Sample List](#)” on [page 360](#).

–or–

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

For detailed instructions, see “[Submitting a Batch](#)” on [page 379](#).

–or–

- To save the batch to be acquired later, click **Save**,  **Save**.

The application saves your batch in the following folder:

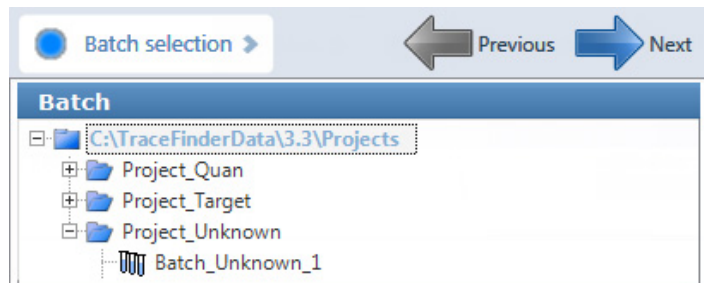
...\TraceFinderData\3.3\Projects\...

The application closes the Acquisition mode and returns you to the mode you were last using.

❖ **To reinject samples in a previously acquired batch**

1. Click **Reinject Samples** in the navigation pane.
2. On the Batch page, select the batch that you want to reacquire.

The Batch page displays all previously acquired quantitation, target screening, and unknown screening batches.



- To continue to the next page, click **Next**.

The Sample Definition page of the Acquisition mode opens. See “[Defining a Sample List](#)” on page 360.

- If the batch is unreadable, the application reports that the batch file is not valid and cannot be opened.
- If a sample in the batch is unreadable, the application creates a new sample with the same name and flags the sample. You must complete the missing information, such as Sample Type, Level, and so forth, and then save the batch before you submit it for acquisition. Or, you can browse in a new raw data file to replace the corrupt file.

❖ **To create a quantitation batch template**

- Click **Create or Edit a Template** in the navigation pane.

Note When user security is activated, you must have Acquisition Wizard – Template Editing permission to create a batch template.

- Select the **Quantitation** option.
- Click and select the folder where you want to create the new batch template.
- Type a name for the new batch template in the Template Name box.

- 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.

Method

Method selection:

Method Compound Data					
	RT	Compound	Compound type	Active	CAS No
▶	3.14	Propanenitrile	Target Compound	<input checked="" type="checkbox"/>	107120
	3.15	EDIFENPHOS-CE5-R20-T...	Target Compound	<input checked="" type="checkbox"/>	17109498

6. To continue to the next page, click **Next**.

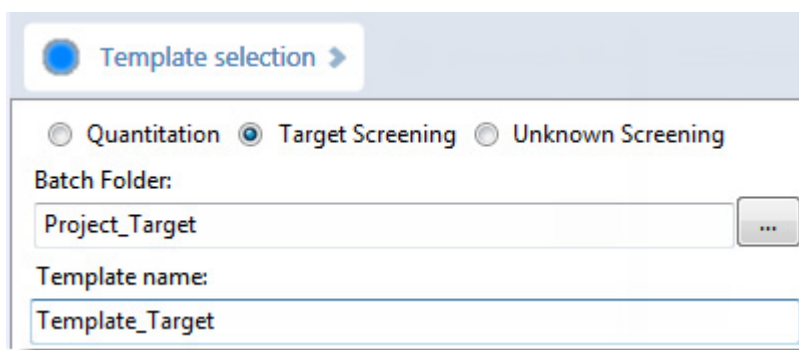
The Sample Definition page of the Acquisition mode opens. See “[Defining a Sample List](#)” on page 360.

❖ **To create a target screening batch template**

1. Click **Create or Edit a Template** in the navigation pane.

Note When user security is activated, you must have Acquisition Wizard – Template Editing permission to create a batch template.

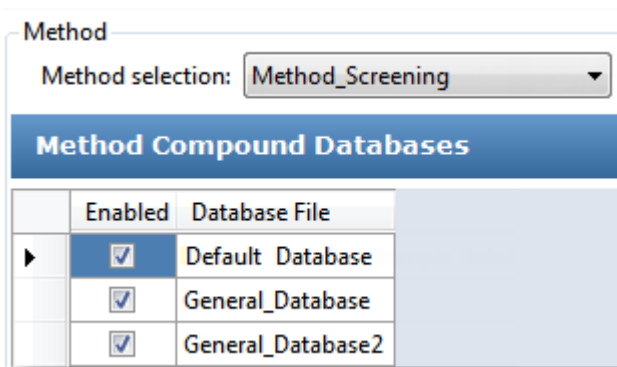
2. Select the **Target Screening** option.
3. Click and select the folder where you want to create the new batch template.
4. Type a name for the new batch template in the Template Name box.



The screenshot shows a dialog box titled "Template selection" with a blue header and a right-pointing arrow. Below the header are three radio buttons: "Quantitation", "Target Screening" (which is selected), and "Unknown Screening". Underneath are two text input fields. The first is labeled "Batch Folder:" and contains the text "Project_Target" with a small "..." button to its right. The second is labeled "Template name:" and contains the text "Template_Target".

5. Select a method from the Method Selection list.

The Method Compound Databases pane displays the screening databases available for the selected method.



The screenshot shows a pane titled "Method" with a "Method selection:" dropdown menu set to "Method_Screening". Below this is a section titled "Method Compound Databases" with a blue header. Underneath is a table with three columns: a selection column (with a right-pointing triangle), an "Enabled" column (with checkboxes), and a "Database File" column.

	Enabled	Database File
▶	<input checked="" type="checkbox"/>	Default Database
	<input checked="" type="checkbox"/>	General_Database
	<input checked="" type="checkbox"/>	General_Database2

6. Select the check box for each database that you want to use for screening.
7. To continue to the next page, click **Next**.

The Sample Definition page of the Acquisition mode opens. See “[Defining a Sample List](#).”

❖ **To create an unknown screening batch template**

1. Click **Create or Edit a Template** in the navigation pane.

Note When user security is activated, you must have Acquisition Wizard – Template Editing permission to create a batch template.

2. Select the **Unknown Screening** option.
3. Click and select the folder where you want to create the new batch template.
4. Type a name for the new batch template in the Template Name box.

The screenshot shows a dialog box titled "Template selection" with a right-pointing arrow. It contains three radio buttons: "Quantitation", "Target Screening", and "Unknown Screening", with "Unknown Screening" selected. Below the radio buttons are two text input fields. The first is labeled "Batch Folder:" and contains the text "Project_Unknown" followed by a "..." button. The second is labeled "Template name:" and contains the text "Template_Unknown".

5. Select a method from the Method Selection list.

The Method Compound Databases pane displays the unknown screening databases available for the selected method.

The screenshot shows a section titled "Method" with a "Method selection:" dropdown menu set to "Method_unknown". Below this is a table titled "Method Search Databases".

	File Name	Type
<input checked="" type="checkbox"/>	Benzodiazepines Example Database	CDB
<input type="checkbox"/>	DefaultGC	CDB
<input type="checkbox"/>	DefaultLC	CDB
<input type="checkbox"/>	NISTDEMO	NIST
<input type="checkbox"/>	Abacipharm	ChemSpider

6. Select the check box for each database that you want to use for unknown screening.
7. To continue to the next page, click **Next**.

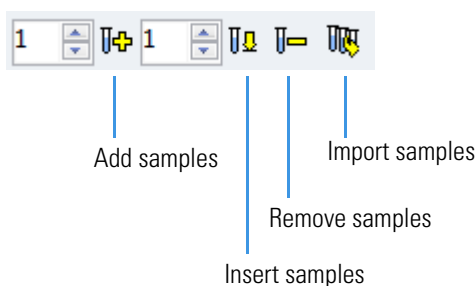
The Sample Definition page of the Acquisition mode opens. See [“Defining a Sample List.”](#)

Defining a Sample List

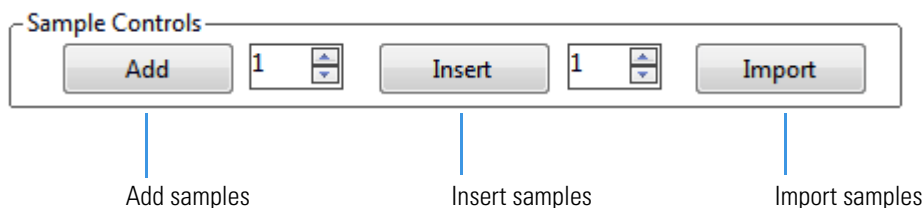
Use the Samples page on the Sample Definition page of the Acquisition mode, to create a list of samples for the batch. See “[Samples](#)” on [page 371](#). You can add samples, insert samples, import a sample list, or remove samples from the list. You can use the Reference Sample page to select a reference sample to use as a reference peak in the Data Review. See “[Reference Sample](#)” on [page 376](#).

To create the sample list, you can use either of two sets of function buttons (described in the following graphic) or you can use commands in the shortcut menu (see the Shortcut menu commands area of the “[Samples page parameters](#)” on [page 371](#)).

Icons in the toolbar



Buttons at the bottom of the sample definition page



As you enter sample values, you can use the Copy Down and Fill Down commands to quickly enter column values. For detailed instructions on using Copy Down and Fill Down to enter column values, see [Appendix C, “Using Copy Down and Fill Down.”](#)



Use any of the following procedures to create a sample list. When you finish defining the list of samples, click **Next**.

- When you create a batch from scratch and click Next, the Report Selection page opens. See “[Selecting and Reviewing Reports](#)” on [page 377](#).
- When you edit a prepared batch, reinject samples, create a batch from a template, or edit a batch template and then click Next, the Finish Selection page opens. See “[Submitting a Batch](#)” on [page 379](#).

Follow these 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
- To select a reference sample
- To add an auto sample type
- To specify different instrument methods for samples

❖ **To add samples to the list**

1. Select the number of sample rows to add and then click the **Add** icon,  or .
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 sample types			
Matrix Blank	Solvent	QC Std	Unknown
Cal Std			




For a detailed description of each sample type, see “Sample Types” on page 404.

4. For each Cal Std or QC Std sample, select a level from the Level list.
The master method defines the sample levels. If there are no levels to select in the Level list, ask a user with Method Development permission to edit the method and specify the levels. Then return to the Acquisition mode, and begin the batch again. The application does not save a batch when you leave the Acquisition mode.
If you have Method Development permission, do the following:
 - a. Return to the Method Development mode.
 - b. Open the method.
 - c. Click the **Compounds** tab.
 - d. Click the **Calibration Levels** tab.
 - e. Add the levels.
 - f. Save the method.

For detailed instructions, see “Calibration Levels” on page 207.

5. (Optional) To assign samples to a group, do the following:
 - a. For each sample, type a group name in the Groups column.
Repeat this for each sample that you want to include in a group.
 - b. Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
	Benzo26473	groupB, groupA
	Benzo25557	groupB
	Benzo26154	groupB, groupA

In unknown screening analysis, the application uses only the first group listed for the Maximum Fold analysis and in the Group Averages pane.

For information about Group Averages, see [“Group Averages Pane”](#) on page 656. For information about Maximum Fold analysis, see [“Cross Sample Peak List Pane”](#) on page 643.

- For quantitation experiments, after creating groups, you can choose one of the samples as a threshold sample for the group and then compare all of the samples in the Comparative View in Data Review.

For information about specifying a threshold sample for a group of samples, see [“Threshold Samples Page”](#) on page 446. For information about viewing grouped samples in Data Review, see [“Comparative View”](#) on page 468.

- For unknown screening experiments, you can create a control group (specify the group name as Control) to use for group averages in Data Review.

For information about Group Averages, see [“Group Averages Pane”](#) on page 656.

6. For each sample, type a vial position in the Vial Position column.

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

7. For each sample, type a volume in the Injection Volume column.

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

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


Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name, while the other columns scroll right and left.

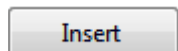
For instructions to automatically copy or fill values in these columns, see [Appendix C, “Using Copy Down and Fill Down.”](#)

❖ **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 then click the **Insert** icon,  or



The application inserts the Unknown samples above the selected sample.

	Status	Filename	Sample type	Groups
1		cal_std_5	Cal Std	
2		Unknown2	Unknown	
3		Unknown1	Unknown	
4		cal_std_10	Cal Std	

Inserted samples

3. For each sample, type a file name in the Filename column.

Each file name must be unique.

4. For each sample, select a sample type from the Sample Type list.

Available sample types

Matrix Blank	Solvent	QC Std	Unknown
Cal Std			

5. For each Cal Std or QC Std sample, click the Level cell and select a level from the list.

The master method defines the sample levels. If there are no levels to select from the Level list, ask a user with Method Development permission to edit the method and specify the levels. Then return to the Acquisition mode, and begin the batch again. The application does not save a batch when you leave the Acquisition mode.

If you have Method Development permission, follow the instructions in [step 4](#) of the procedure “[To add samples to the list](#)” on [page 361](#).

6. (Optional) To assign samples to a group, do the following:
 - a. For each sample, type the group name in the Groups column.
Repeat this for each sample that you want to include in a group.
 - b. Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
●	Benzo26473	groupB, groupA
●	Benzo25557	groupB
●	Benzo26154	groupB, groupA

In unknown screening analysis, the application uses only the first group listed for the Maximum Fold analysis and in the Group Averages pane.

For information about Group Averages, see [“Group Averages Pane”](#) on page 656. For information about Maximum Fold analysis, see [“Cross Sample Peak List Pane”](#) on page 643.

- For quantitation experiments, after creating groups, you can choose one of the samples as a threshold sample for the group and then compare all of the samples in the Comparative View in the Analysis mode.

For information about specifying a threshold sample for a group of samples, see [“Threshold Samples Page”](#) on page 446.

For information about viewing grouped samples in Data Review, see [“Comparative View”](#) on page 468.

- For unknown screening experiments, you can create a control group (specify the group name as Control) to use for group averages in Data Review.

For information about group averages, see [“Group Averages Pane”](#) on page 656.

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

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

8. For each sample, type a volume in the Injection Volume column.

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

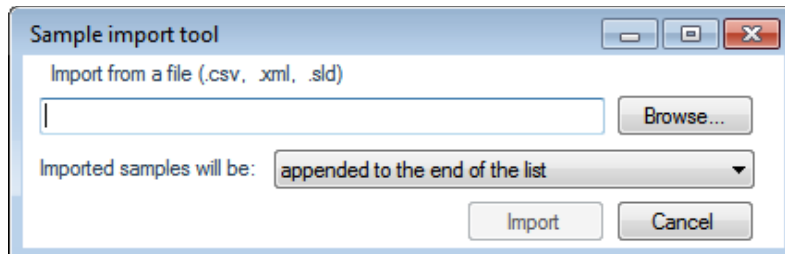
9. (Optional) Type or edit the values for the remaining columns.

Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name, while the other columns scroll right and left.

❖ **To import samples into the list**

1. Click **Import**, .

The Sample Import Tool dialog box opens.



Use this dialog box to import a sample list from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file with the sample definitions that you want to import.

Note The .csv, .xml, or .sld data format must match the TraceFinder data 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 application adds the specified samples to the sample list.

When you import samples from an Xcalibur sequence file (.sld), the application makes the following column name substitutions.

Xcalibur column	TraceFinder column
Position	Vial position
Inj Vol	Injection volume
Dil Factor	Conversion Factor

When you import samples from an Xcalibur sequence file (.sld), the application makes the following sample type substitutions.

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	QC Std
Std Bracket	Cal Std

For each imported sample, the application uses the Instrument Method specified in the local method.

5. For each Cal Std or QC Std sample, click the Level cell and select a level from the list.

The master method defines the sample levels. If there are no levels to select from the Level list, ask a user with Method Development permission to edit the method and specify the levels. Then return to the Acquisition mode, and begin the batch again. The application does not save a batch when you leave the Acquisition mode.

If you have Method Development permission, follow the instructions in [step 4](#) of the procedure “[To add samples to the list](#)” on [page 361](#).

For detailed instructions about defining calibration levels, see “[Calibration Levels](#)” on [page 207](#).

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 0.1 μL ; the maximum injection volume value allowed is 5000 μL .

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

Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name, 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 that 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 to reinject.
2. Right-click and choose **Reinject Selected Samples** from the shortcut menu.

The 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 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).

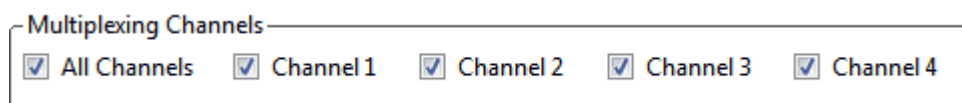
	cal_std_50_INJ001	Cal Std	10
	cal_std_50	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

When you submit this batch, the application acquires only the reinjection samples.

❖ To select channels for the batch

Note These features are available only when you have activated multiplexing in the Configuration console. See “Multiplexing” on page 61.

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 console. See “Multiplexing” on page 61.

Clearing 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 is not available.

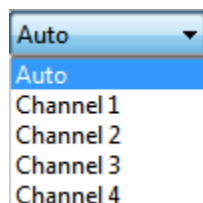
❖ To assign a specific channel to a sample

1. Scroll to the Channel column.

Note The Channel column is available only when you have activated multiplexing in the Configuration console. See “Multiplexing” on page 61.

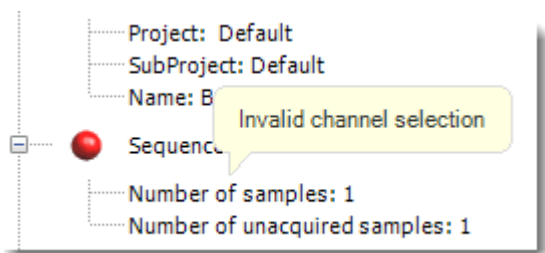
All samples default to Auto.

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 application flags the sample sequence 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.

❖ **To select a reference sample**

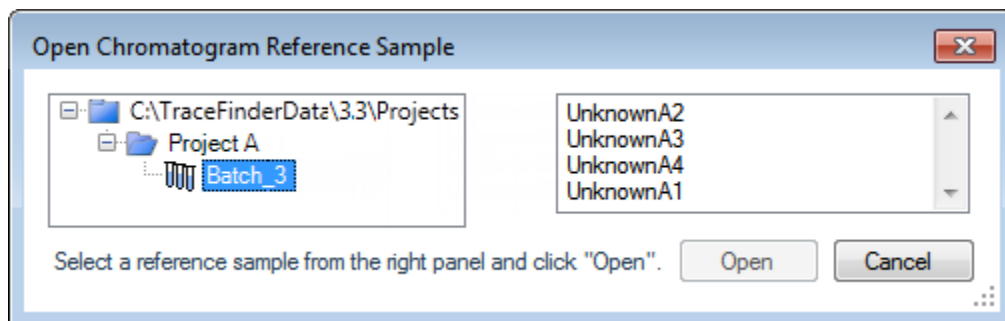
1. Click the **Reference Sample** tab.

The Reference Sample page on the Sample Definition page opens. See [“Reference Sample”](#) on page 376.

You can select one reference sample to use as a reference peak in the Data Review.

2. Right-click the Reference Sample page and choose **Add Reference Sample** from the shortcut menu.

The Open Chromatogram Reference Sample dialog box opens.



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

3. Select a batch from the list.

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

4. Select a sample from the list of processed samples on the right.

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

5. Click **Open**.

The application adds the reference sample to the Reference Sample page.

6. (Optional) Enter values for Sample ID, Sample Name, Comment, and Barcode Actual.
7. (Optional) Change the Vial Position for the sample.

The application uses the peak in this sample as a reference peak in Data Review. See “Reference Peak” on page 513.

❖ To add an auto sample type

1. Click the **Auto Samples** tab.

The Auto Samples page opens. See “Auto Samples” on page 375.

2. Right-click and choose **Add Auto Sample** from the shortcut menu, or click the **Add New Auto Sample** icon, .

The application adds a Solvent sample to the sample list.

You can add, insert, or remove samples from this list as you would any sample list.

3. To change the sample type to a Matrix Blank, click the Sample Type column and select **Matrix Blank** from the list.
4. In the Injection Volume column for the sample, type a volume.

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


5. In the Number of Injections column, type the number of injections available in the designated Solvent or Matrix Blank vial.

After auto sample injections have occurred, you can return to this page to view the number of Injections Used in each vial.

6. In the Vial Position column, type the vial position for the Solvent or Matrix Blank sample.

❖ To specify different instrument methods for samples

Note By default, the Instrument Method column is not displayed on the Sample Definition page. See [Instrument method column](#).

1. Display the Instrument Method column in the sample list:
 - a. Right-click the sample list and choose **Modify Columns** from the shortcut menu.
The Modify Columns dialog box opens.
 - b. In the Available Columns pane, select **Instrument Method**.
 - c. Click  to move the Instrument Method column to the Displayed Columns pane.
 - d. Click **OK**.

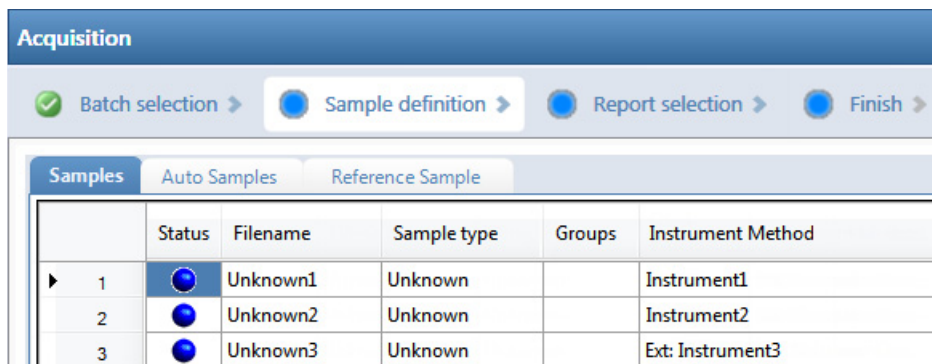
The application displays the Instrument Method column, defaulting to the instrument method specified in the master method.

2. Click the Instrument Method column and select an instrument method from the list.

This list contains all the available instrument methods. The application prefixes instrument methods from external sources with “Ext:”.

You can specify a different instrument method for each sample.

Figure 112. Instrument method column



Acquisition					
Batch selection > Sample definition > Report selection > Finish >					
Samples					
	Status	Filename	Sample type	Groups	Instrument Method
▶ 1		Unknown1	Unknown		Instrument1
2		Unknown2	Unknown		Instrument2
3		Unknown3	Unknown		Ext: Instrument3

When you submit the batch, the application saves a copy of the selected instrument methods to the following folders:

External instrument methods:

...\\TraceFinderData\\3.3\\Projects\\...\\batch\\Methods\\method\\ExternalMethods

Local instrument methods:

...\\TraceFinderData\\3.3\\Projects\\...\\batch\\Methods\\method

Samples

Use the features on the Samples page to create a list of samples for the batch.

Figure 113. Samples page on the Sample Definition page

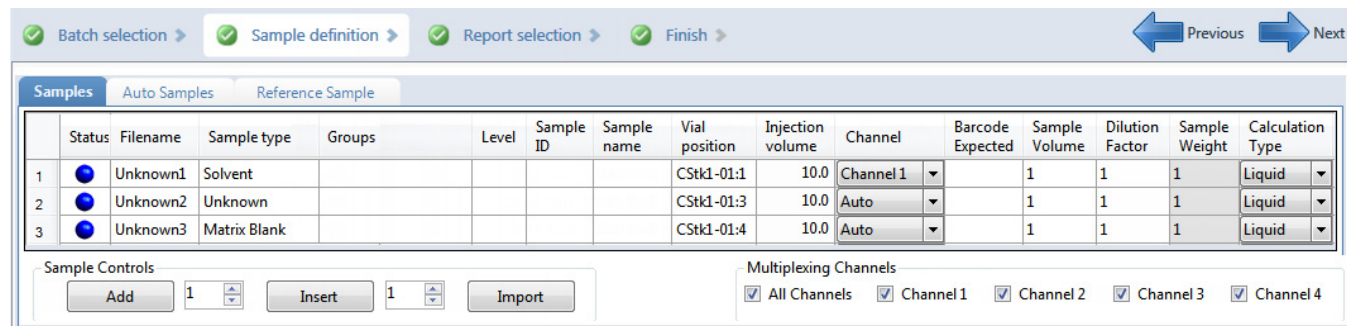


Table 82. Samples page parameters (Sheet 1 of 2)





Parameter	Definition
Previous	Returns you to the previous Acquisition page.
Next	Takes you to the next Acquisition page.
Status color codes	<ul style="list-style-type: none">  Sample is not acquired.  Sample is acquired but not processed.  Sample is acquired and processed.  Sample is currently acquiring.
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 to import samples from a CSV, an XML, or an SLD file.
Multiplexing Channels	These features are available only when you have activated multiplexing in the Configuration console. See “Multiplexing” on page 61.
All Channels	Uses all configured channels to acquire this batch.
Channel 1- <i>n</i>	Uses only the selected channels to acquire this batch.
Shortcut menu commands	
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.

Table 82. Samples page parameters (Sheet 2 of 2)

Parameter	Definition
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 365.
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 C, “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 C, “Using Copy Down and Fill Down.”
Modify Columns	Opens the Modify Columns dialog box. See Column Display .
Enable/Disable Sample Weight Calculation	Displays or hides the Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information to a text editor or spreadsheet application. 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 a text editor or spreadsheet application. You cannot paste this data back into the Acquisition mode sample list.
Paste	Pastes a single column of copied data from a text editor or spreadsheet application, into the selected column.
Undo Last Paste	Removes the last pasted item in the Acquisition mode sample list.
Export to CSV File	Opens the Save As dialog box where you can save the current sample list to a CSV file.
Edit Instrument Method	<p>Opens the Instrument Setup window where you can edit the parameters of the instrument method.</p> <ul style="list-style-type: none"> • When you edit an external method, the application updates the method in the ...\\Xcalibur\\methods folder. • When you edit an internal method, the application updates the method in the ...\\TraceFinderData\\3.3\\Projects\\<i>project\\subproject\\batch</i>\\Methods\\<i>method</i> folder. <p>For detailed information about editing instrument methods, see “Working with Instrument Methods” on page 108.</p>

Column Display

The Samples page contains many columns of information. You can scroll to see all the columns, and you can customize which ones to display and their display order.

❖ To scroll the sample list

Use the horizontal scroll bar at the bottom of the sample list to view all the information.

When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening) Level, Sample ID, and Sample Name, while the other columns scroll right and left.

❖ To customize the column display

1. Right-click the sample list and choose **Modify Columns** from the shortcut menu.

The Modify Columns dialog box opens. See [“Modify Columns dialog box.”](#)

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

These columns appear after the Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

- a. In the Displayed Columns pane, select a column name.
- b. Use **Up** or **Down** to move the selected column up or down in the list.

The first column in the list represents the leftmost column in the Samples page sample list, and the last column in the list represents the rightmost column in the Samples page sample list.

Note The following columns are fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

- a. In the Displayed Columns pane, select the column width.

5	Sample ID	100
▶ 6	Sample name	100
7	Vial position	100

- b. Type a new value for the width.

5. Repeat [step 4](#) for all columns whose widths you want to change, and click **OK**.

The columns in the sample list immediately reflect your changes.

Figure 114. Modify Columns dialog box

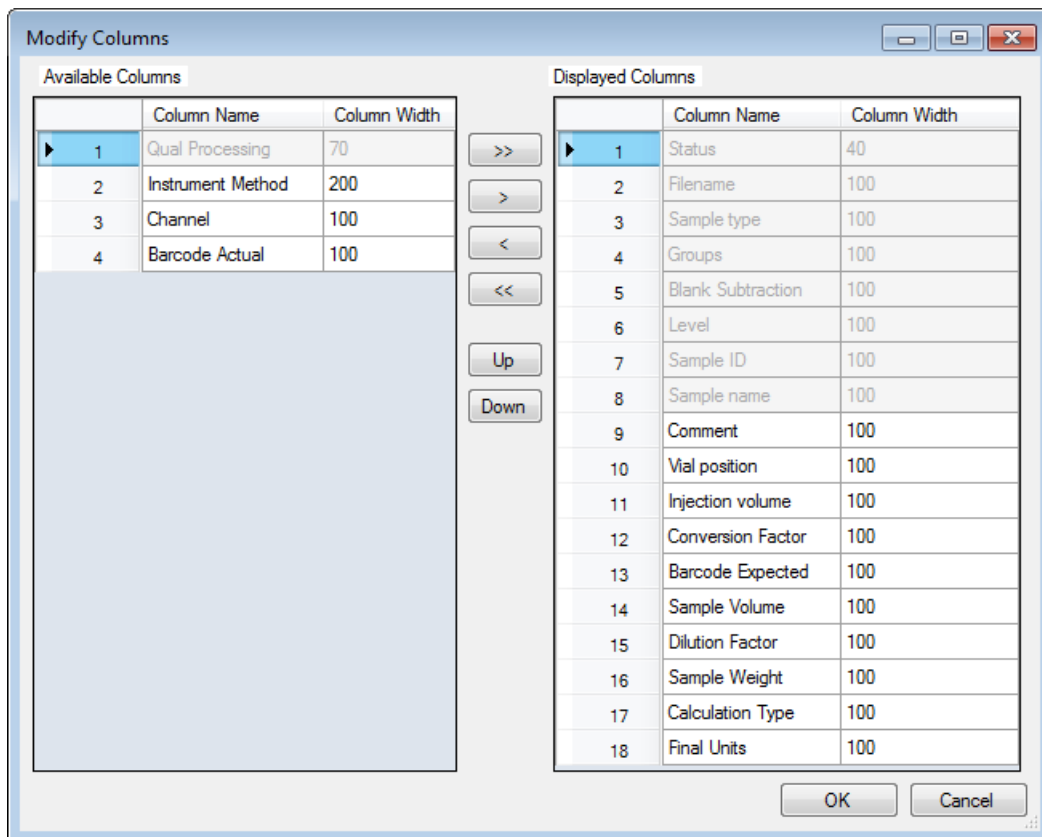








Table 83. Button descriptions for the Modify Columns dialog box

Button	Description
	Moves all columns to the Displayed Columns pane.
	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name.	
	Moves the selected column to the Available Columns pane.
	Moves all columns except fixed columns.
	Moves the selected column name in the Displayed Columns pane one row up in the column order.
	Moves the selected column name in the Displayed Columns pane one row down in the column order.

Auto Samples

Use the features on the Auto Samples Sample page to identify the Solvent or Matrix Blank samples to use for any Auto Sample or Auto Sample and Reinject failure actions as specified on the Intelligent Sequencing page of the method. See [“Editing the Intelligent Sequencing Page”](#) on page 228.

Each sample type that you specify for a failure action on the Intelligent Sequencing page must be defined in the samples list on the Auto Samples page.

Figure 115. Auto Samples page on the Sample Definition page

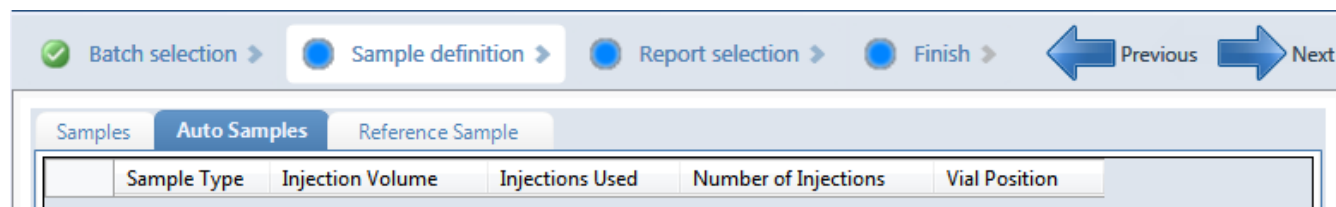


Table 84. Auto Samples page parameters

Column	Description
Sample Type	The sample type for the auto sample injection as specified on the Intelligent Sequencing page of the method—either Solvent or Matrix Blank. Default: Solvent
Injection Volume	The injection volume used for the sample acquisition as specified on the Samples page. Valid range: 0.1 through 5000 µL
Injections Used	The number of times a vial has been used. The count is cumulative across all batches.
Number of Injections	The number of injections available in the designated Solvent or Matrix Blank vial.
Vial Position	Vial position for this sample type as specified on the Samples page.

Reference Sample

Use the features on the Reference Sample page to select a sample to use as a reference peak in Data Review.

Figure 116. Reference Sample page on the Sample Definition page

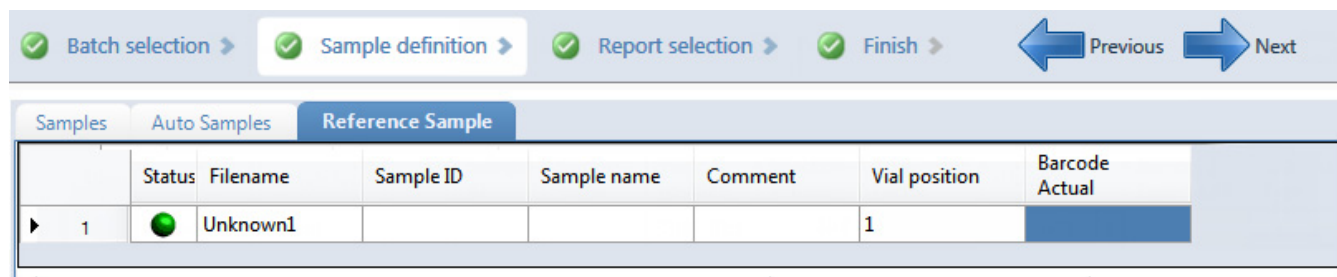






Table 85. Reference Sample page parameters

Parameter	Description
Status	<ul style="list-style-type: none">  Sample is not acquired.  Sample is acquired but not processed.  Sample is acquired and processed.  Sample is currently acquiring.
Filename	Name of the raw data file that contains the sample data.
Sample ID	A user-defined, alphanumeric string that identifies a sample.
Sample Name	A user-defined name that identifies a sample.
Vial Position	The tray vial number used for an autosampler acquisition.
Barcode Actual	A user-entered barcode for the vial.
Shortcut menu commands	
Add Reference Sample	Opens the Open Chromatogram Reference Sample dialog box where you can select a reference sample.
Delete Selected	Deletes the reference sample.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information to a text editor or spreadsheet application. You cannot paste this data back into the reference 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 a text editor or spreadsheet application. You cannot paste this data back into the reference sample list.
Paste	Pastes a single column of copied data from a text editor or spreadsheet application, into the selected column.
Export to CSV File	Opens the Save As dialog box where you can save the current sample list to a CSV file.

Selecting and Reviewing Reports

On the Report Selection page, you can specify the types of reports that you want to create. See [Report Selection](#). In addition to the report type, you can specify a report description for each of your reports.

For each report that you generate, you can create a hard-copy printout, a PDF file, a CSV file, or an Excel file.

Use any of the following procedures to create a reports list. When you finish specifying your report options, click **Next** to go to the Finish page and submit your batch. See “[Submitting a Batch](#)” on [page 379](#).

The application writes the resulting output files for your reports to the following folder:

```
...\TraceFinderData\3.3\Projects\...\batch\Reports
```

Follow these procedures:

- [To edit a report title](#)
- [To specify a report in print format or as a PDF, a CSV, or an Excel file](#)

❖ To edit a report title

Select the Report Title column and edit the default title.

The default report title is the same as the report name.

❖ To specify a report in print format or as a PDF, a CSV, or an Excel file

1. For each type of report that you want to create, select the corresponding check box in the Print, Create PDF, Create CSV, or Create Excel column.
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. This action applies only to report types that make this output format available.

Report Selection

Use the features on the Report Selection page to specify the types of reports that you want to create.

Figure 117. Report Selection page

Report Name	Report Title	Print	Create PDF	Create CSV	Create Excel
Batch Report	Batch Report	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Blank Report	Blank Report	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Calibration Report	Calibration Report	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Check Standard Report	Check Standard Report	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Table 86. Report Selection page parameters

Parameter	Description
Report Name	The name of a report.
Report Title	User-editable description to be used on a report.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files.
Create CSV	Reports to be exported as CSV files.
Create Excel	Reports to be exported as Excel files.
Shortcut menu: Copy Down	Copies the selected or cleared state to all subsequent reports in the column.

Submitting a Batch

In the Finish page 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 page” on page 387.

Note If you are working with a batch template, the only available function is Save.

Follow these procedures:

- To specify startup or shutdown methods
- To automatically update the timed SRM information
- To specify a calibration batch
- To specify device states
- To save a batch for later acquisition or processing
- To start acquisition or processing
- To view the output files

❖ To specify startup or shutdown methods

1. Select a method from the System Startup Method list.

The application runs this method before running the batch. No autosampler injection takes place. This feature is not available for all instruments.

2. Select a method from the System Shutdown Method list.

The application runs this method after running the batch. This feature is not available for all instruments.

System startup method:

AS Method 1 ▼

System shutdown method:

AS Method 3 ▼

❖ To automatically update the timed SRM information

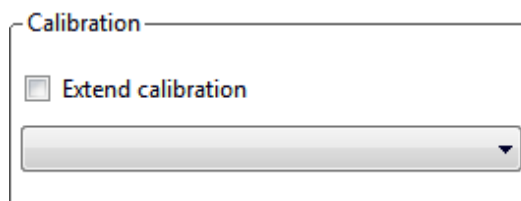
Select the **Auto TSRM Update** check box.

Auto TSRM Update

When you submit the batch, the application updates the TSQ method with mass transitions, collision energy, and other appropriate data for TSRM functionality.

❖ **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 calibration (.calx) file.

2. 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.

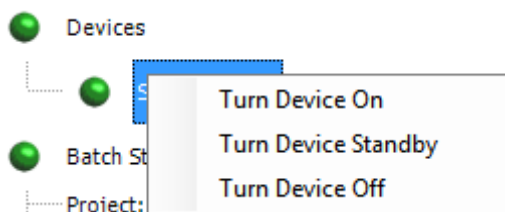






Table 87. Instrument states (Sheet 1 of 2)

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.

Table 87. Instrument states (Sheet 2 of 2)

Instrument state	Description
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 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 or processing**

From the Finish page, click **Save**,  **Save**.

The application saves your batch as a prepared file.

❖ **To start acquisition or processing**

1. Click **Submit**,  **Submit**.

The Submit Options dialog box opens. For detailed descriptions of the parameters, see “Submit Options dialog box” on page 384.

2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.
 - When all submitted samples have been previously acquired, this option is (by default) not selected.
 - When one or more submitted samples have not been acquired, this option is (by default) selected.

Tip You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

3. To process the submitted samples, select the **Process Data** check box.

The application displays options for each type of method that the batch uses: Quantitation, Target Screening, Unknown Screening, or a combination of methods.

4. For each method type, select the check box for the options that you want to use.

Peak Detect: Performs peak detection for all method types. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

Quantitate: Performs quantitation for quantitation methods.

Identify: Performs identification for unknown screening methods.

Identify and Confirm: Performs both identification and confirmation for target screening methods.

With RT Alignment: Performs retention time alignment for unknown screening methods. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.

5. (Optional) Select the **Create Reports** check box.

6. (Optional with multiplexing activated) 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 activated) 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.

Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.

- a. Select the **Use** check box for the device that you want to use for this acquisition.
- b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

This is usually the autosampler.

- c. Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

When you clear this check box, individual instruments can start at different times and then must wait for the last instrument to be ready.

- d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.

9. To start the selected processes, click **OK**.

The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Acquisition mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT When your batch uses unknown screening features, after the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages for the unknown screening features ([“Editing the Processing Pages”](#) on [page 311](#)) and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Figure 118. Submit Options dialog box

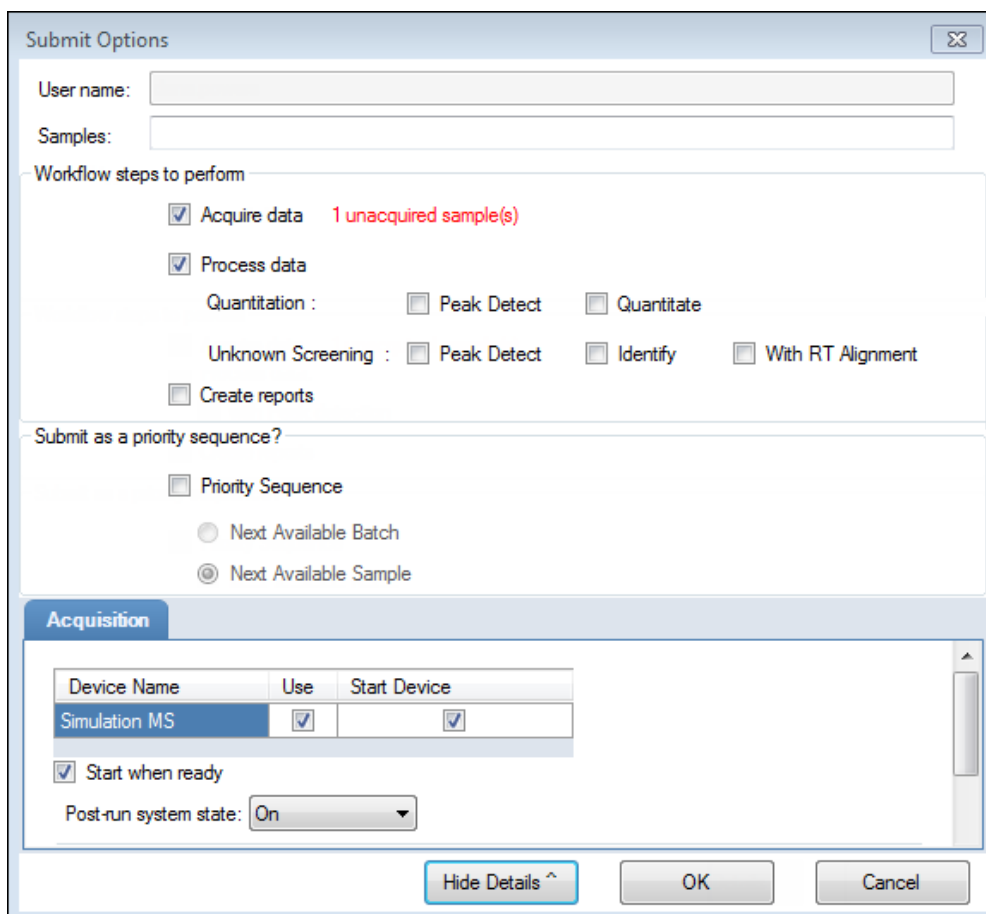


Table 88. Submit Options dialog box parameters (Sheet 1 of 3)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Method Types	Lists the types of methods (quantitation, target screening, or unknown screening) used in the submitted batches.
Workflow Steps to Perform	
Acquire Data	Submits the current batch to acquisition. <ul style="list-style-type: none"> When all submitted samples have been previously acquired, this option is (by default) not selected. When one or more samples in the batch have not been acquired, this option is (by default) selected.

Table 88. Submit Options dialog box parameters (Sheet 2 of 3)

Parameter	Description
Process Data	<p>Processes the data for the current batch using any of the following options:</p> <p>Peak Detect: Performs peak detection for all method types. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.</p> <p>Quantitate: Performs quantitation for quantitation methods.</p> <p>Identify: Performs identification for unknown screening methods.</p> <p>Identify and Confirm: Performs both identification and confirmation for target screening methods.</p> <p>With RT Alignment: Performs retention time alignment for unknown screening methods. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.</p>
Create Reports	Creates reports for the current batch.
Submit as a Priority Sequence?	
Priority Sequence	<p>With multiplexing activated, places the batch immediately after the currently acquiring batch.</p> <p>Without multiplexing activated, specifies one of the following priority options to place the batch in the queue:</p> <p>Next Available Batch: Places the batch immediately after the currently acquiring batch.</p> <p>Next Available Sample: Places the batch immediately after the currently acquiring sample.</p> <p>Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.</p>
Acquisition pane	
Device Name	<p>Lists all configured instruments.</p> <p>If the instrument that 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.</p> <p>Available only when you select the Acquire Data check box.</p>

Table 88. Submit Options dialog box parameters (Sheet 3 of 3)

Parameter	Description
Use	Specifies the instruments used for this acquisition. Available only when you select the Acquire Data check box.
Start Device	Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler. Available only when you select the Acquire Data check box.
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.
Post-run System State	Specifies the system state after it acquires the last batch: On (default), Standby, or Off.
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.

❖ **To view the output files**

Locate the files to view from the following directories:

The application writes saved batches to the project folder:

...\\TraceFinderData\\3.3\\Projects\\...

For each acquired sample, the application writes an RSX file to the batch Data folder:

...\\TraceFinderData\\3.3\\Projects\\...\\Data

The application saves method information to the batch Methods folder:

...\\TraceFinderData\\3.3\\Projects\\...\\Methods

The application writes the reports to the batch Reports folder:

...\\TraceFinderData\\3.3\\Projects\\...*batch*\\Reports

Finish

Use the features on the Finish page to save the batch to be acquired later or acquire and process data and optionally create reports.

Figure 119. Finish page

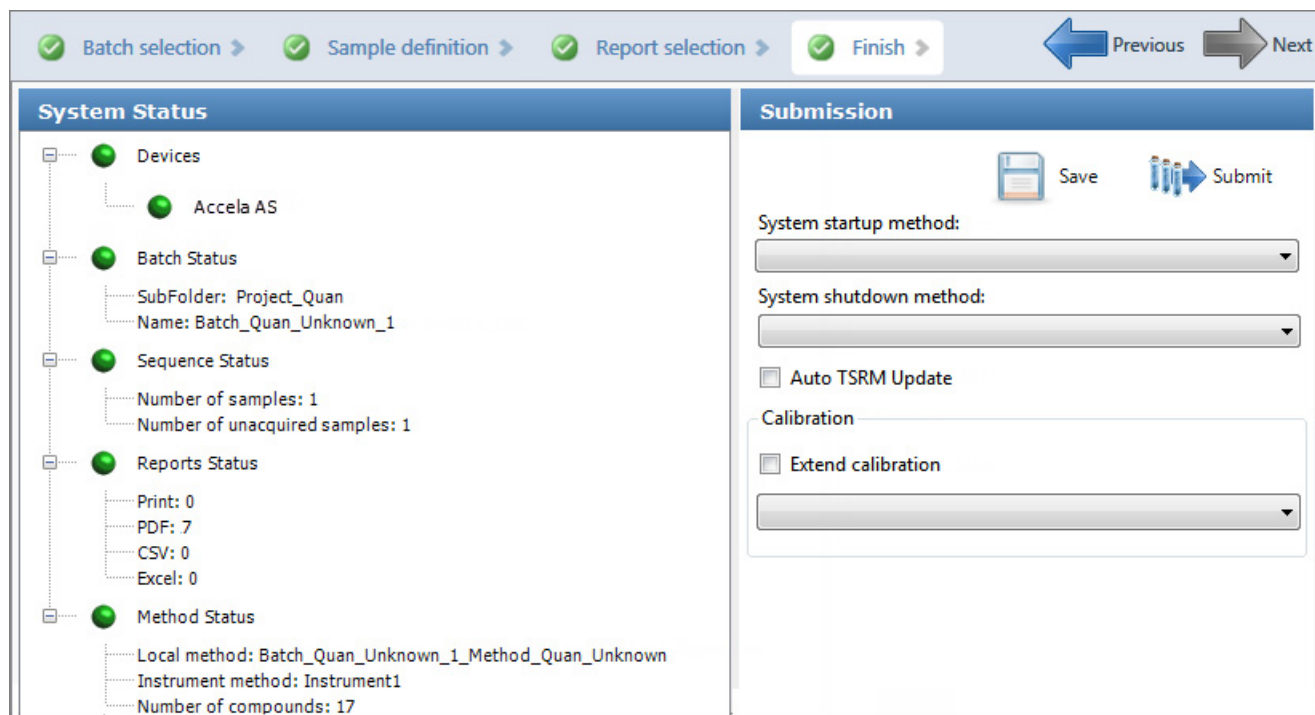


Table 89. Finish page parameters

Parameter	Description
System Status	The System Status pane displays the following: <ul style="list-style-type: none"> • Devices used for the acquisition • Project, subproject, and name of the batch • Number of acquired and unacquired samples in the batch • Number of reports to be printed and saved as PDF, CSV, or Excel files • Local method and instrument method used for the batch • Number of compounds in the method
System Startup Method	The instrument methods that run before and after the batch. No autosampler injection
System Shutdown Method	takes place. These features are not available for all instruments.
Auto TSRM Update	Updates the TSQ method with mass transitions, collision energy, and other appropriate data for TSRM functionality.
Calibration	<ul style="list-style-type: none"> • 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 prepared batch.
Submit	Opens the Submit Options dialog box.

Real Time Status Pane

You can access the Real Time Status pane from any mode in the application.

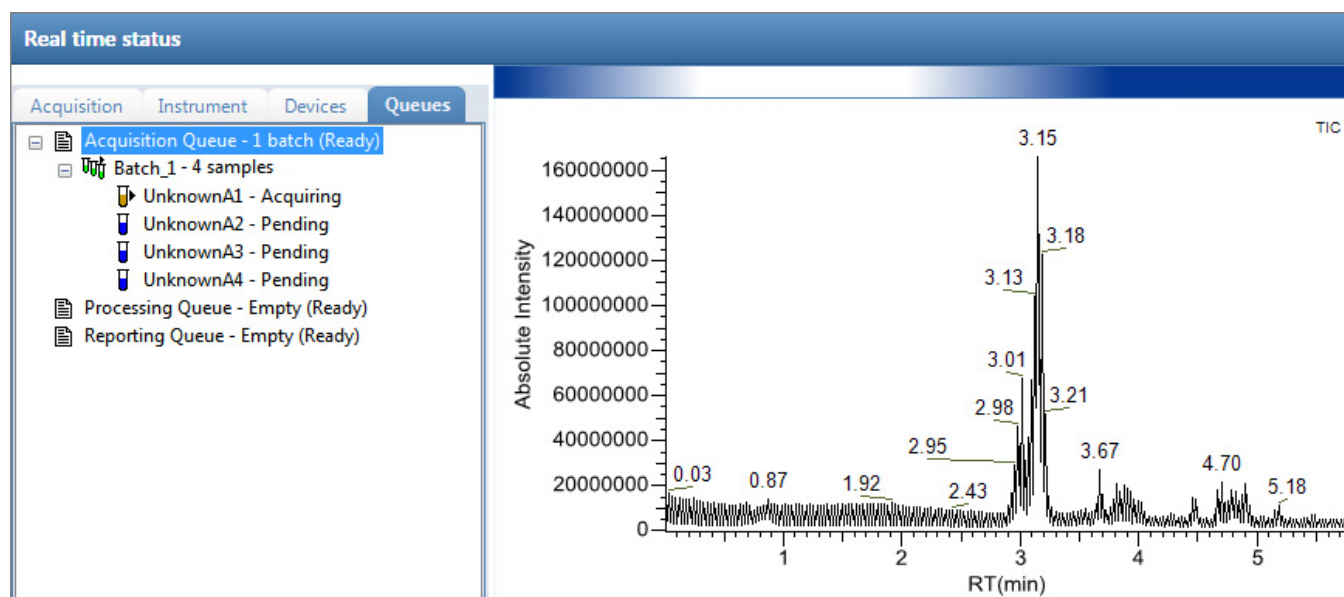
❖ **To access the Real Time Status Pane from any mode**

Click **Real Time Status** in the upper right corner of the TraceFinder window.

Real time status

The Real Time Status pane opens at the bottom of the current view.

Figure 120. Real Time Status pane



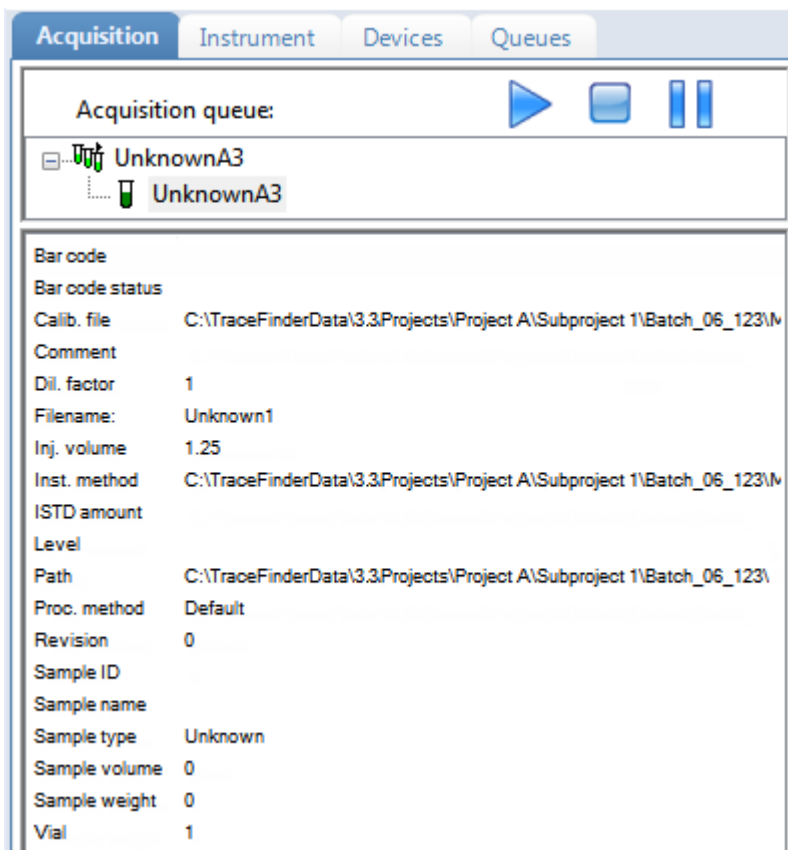
The Real Time Status pane has four pages of information and a real-time trace pane:

- [Acquisition Page](#)
- [Instrument Page](#)
- [Devices Page](#)
- [Queues Page](#)
- [Real-Time Trace Display](#)

Acquisition Page

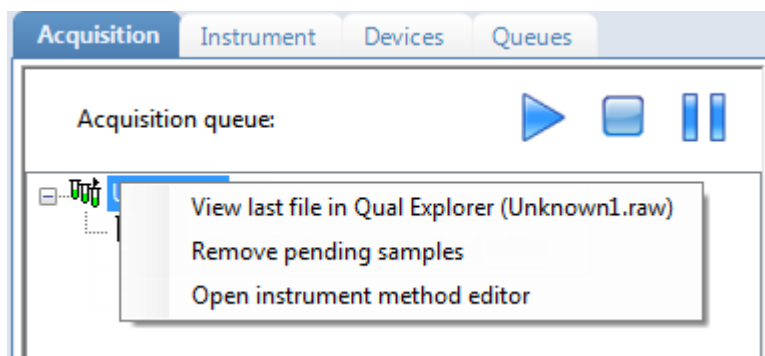
Use the Acquisition page to monitor the progress as the application acquires the samples.

Use the Start, Stop, or Pause, icons to control batches in the Acquisition queue.



❖ To display the last acquired raw data file in a qualitative browser

On the Acquisition page of the real-time status pane, right-click and choose **View Last File in Qual Explorer** from the shortcut menu.



The last acquired file opens in either the FreeStyle or Qual Browser application.

❖ **To open the Instrument Setup window**

Right-click anywhere in the Acquisition page and choose **Open Instrument Method Editor** from the shortcut menu.

The Thermo Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see “Working with Instrument Methods” on page 108.

Note Changes you make and save to the instrument method do not affect the currently running batch.

Instrument Page

Use the Instrument page to monitor the currently acquiring sample.

Device Name	Status
Accela AS	Ready for Run

When you run single sample submission, this displays the sample name instead of the batch name.

❖ **To view the last acquired file in a qualitative browser**

Right-click anywhere in the top pane of the Instrument page and choose **View Last File in Qual Explorer** from the shortcut menu.

The last acquired file opens in either the FreeStyle or Qual Browser application.

❖ To open the Instrument Setup window

Right-click anywhere in the top pane of the Instrument page and choose **Open Instrument Method Editor** from the shortcut menu.

The Thermo Instrument Setup window opens, displaying the currently running instrument method.

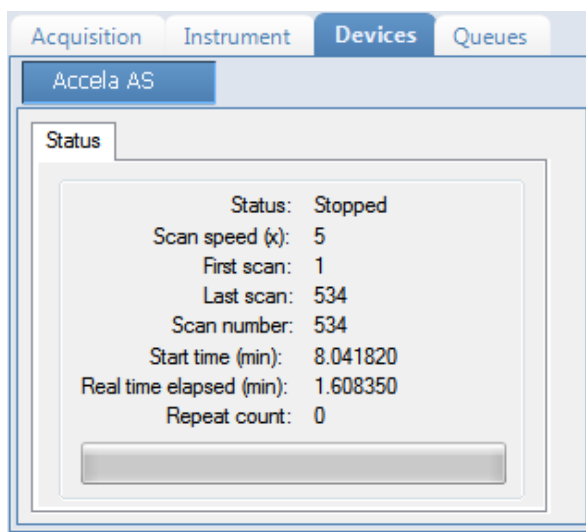
For detailed information about editing instrument methods, see “[Working with Instrument Methods](#)” on [page 108](#).

Note Changes you make and save to the instrument method do not affect the currently running batch.

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.

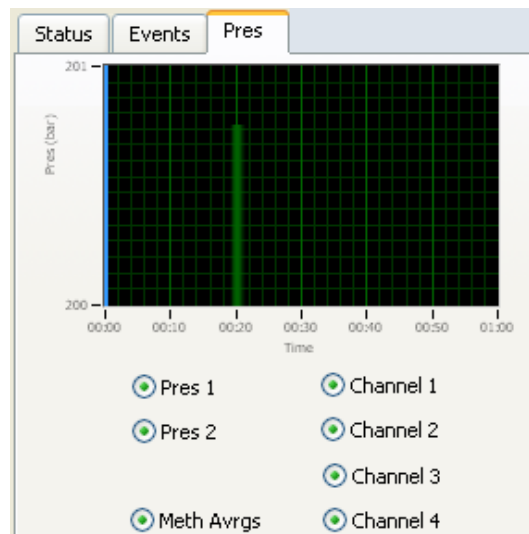
Accela Autosampler Feedback



Aria Multiplexing Feedback

The screenshot shows the 'Aria MX' interface with the 'Devices' tab selected. It displays the status of various components: Autosampler 1 (READY), Channel 1 (READY, 40 bar), Channel 3 (READY), and Detector (NOT READY). There are buttons for 'Hold Autosampler' and 'Direct Control'. A sub-panel shows 'Autosampler 1' with 'READY' in green, 'Channel 1' with 'READY' in green and '40 bar', 'Channel 3' with 'READY' in green, and 'Detector' with 'NOT READY' in yellow. At the bottom, there is a '1' button and an 'Inline' button.

Time	Ch	Msg
11:40:38.48	1	Chan Status NOT READY
11:40:36.48	1	(Channel1\Pump1) Std Pump 1
11:35:38.76		Detector NOT READY
11:35:36.30	1	Chan Status READY
11:33:24.39		System Init



Follow these procedures:

- To pause the autosampler
- To control the channels
- To open the Instrument Setup window
- To view the pressure trace
- To access the Aria multiplexing controls
- To view the last acquired file in a qualitative browser

❖ **To pause the autosampler**

1. Click **Hold Autosampler**.

The autosampler finishes the current autosampler step and then pauses. The autosampler and LC pumps continue to run.

2. To restart the autosampler, click **Hold Autosampler** again.

❖ **To control the channels**

Right-click the channel name and choose a command from the shortcut menu.

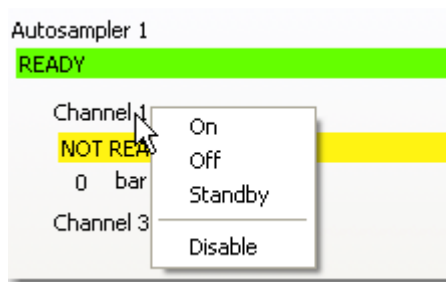


Table 90. Autosampler shortcut menu commands

Command	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	<p>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.</p> <p>Enable: Allows the channel to receive samples.</p> <p>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.</p>

❖ **To open the Instrument Setup window**

Right-click in the header of the Devices page and choose **Open Instrument Method Editor** from the shortcut menu.

The Thermo Instrument Setup window opens, displaying the currently running instrument method.

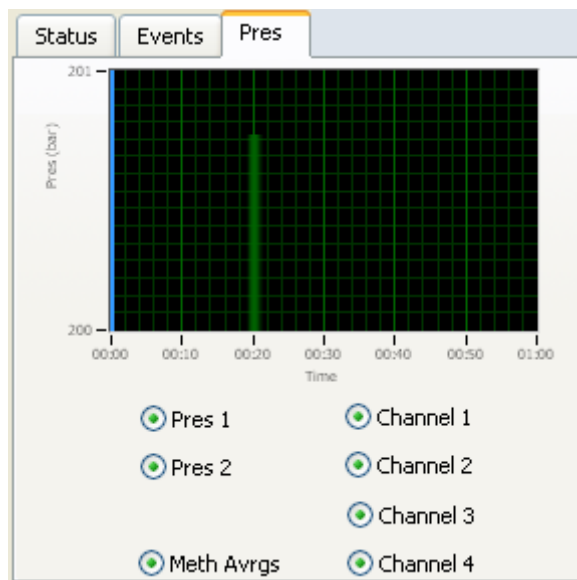
For detailed information about editing instrument methods, see [“Working with Instrument Methods”](#) on page 108.

Note Changes you make and save to the instrument method do not affect the currently running batch.

❖ **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.

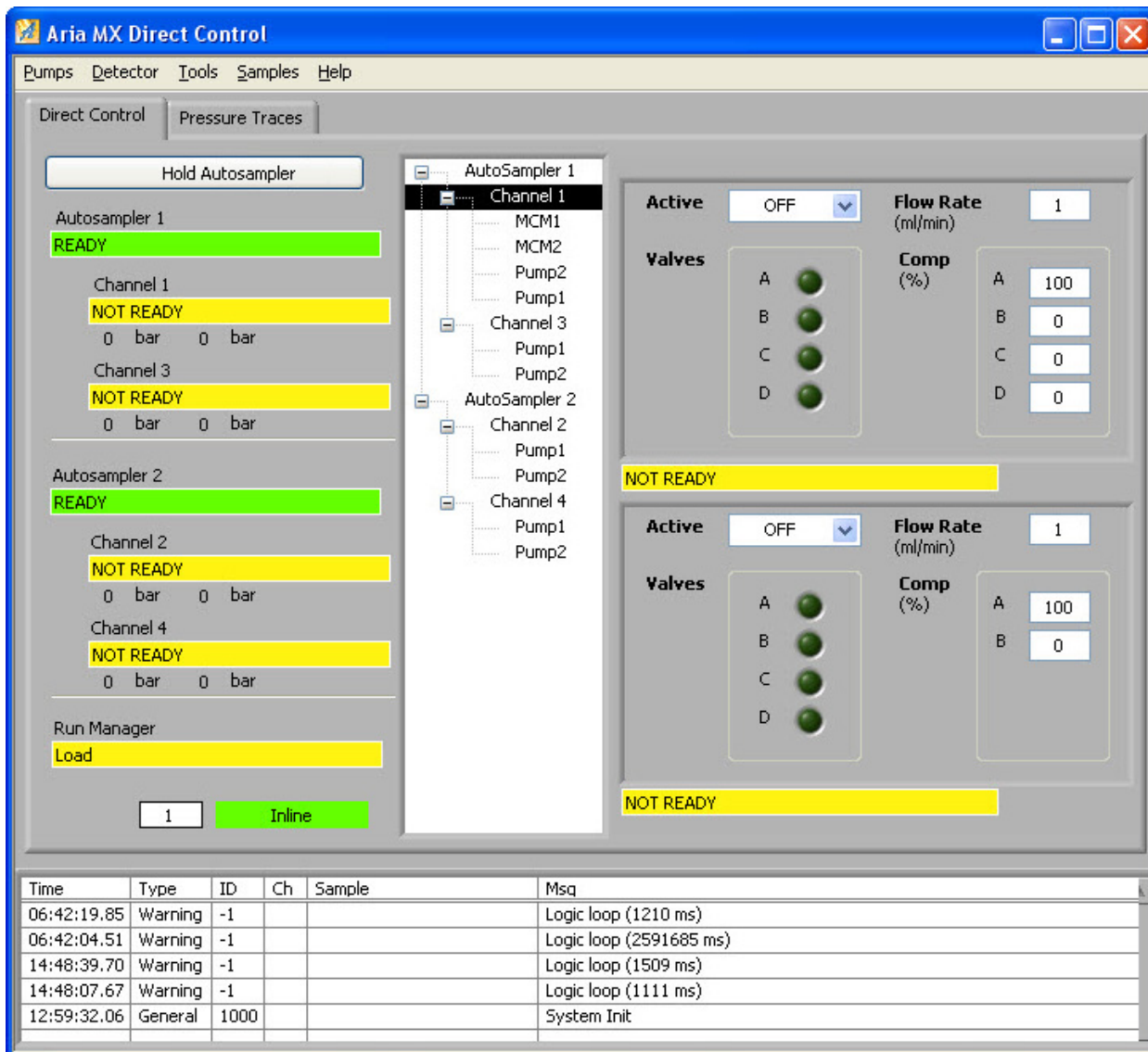


2. To view the pressure for a specific pump, select the **Pres 1** or **Pres 2** option.
By default, the pressure for all pumps are displayed.
3. To view the pressure for a specific channel, select the corresponding channel number.
By default, the pressure for all channels is displayed.

❖ **To access the Aria multiplexing controls**

Click **Direct Control**.

The Aria MX Direct Control window opens.



For detailed descriptions of the features in this window, refer to the *Transcend Systems with Xcalibur Software User Guide*.

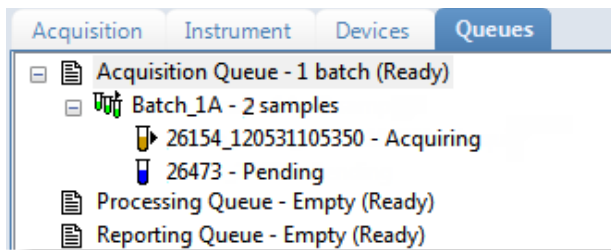
❖ **To view the last acquired file in a qualitative browser**

Right-click in the header of the Devices page and choose **View Last File in Qual Explorer** from the shortcut menu.

The last acquired file opens in either the FreeStyle™ or Qual Browser application.

Queues Page

Use the Queues page to monitor and control the Acquisition, Processing, and Reporting queues.



- **Queue-Level Commands:** Pause or remove batches in any of the queues.
- **Batch-Level Commands:** Pause or remove entire batches or samples within batches from any of the queues.
- **Additional Commands:** Open the FreeStyle application or the Instrument Setup window.

Queue-Level Commands

Use the queue-level commands to pause or remove batches in any of the queues on the Queues page. See “Queue-Level Shortcut Menu” on page 398.

Follow these 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

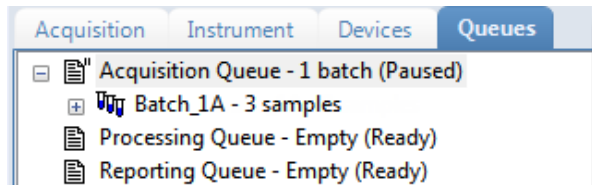
❖ To pause all batches in a queue

1. Select a queue (Acquisition, Processing, or Reporting).

Note When multiplexing is activated, you can have as many as four samples 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.

Queue-Level Shortcut Menu

Use the commands in the shortcut menu to pause or remove batches in any of the queues on the Queues page.

Figure 121. Queue-level shortcut menu

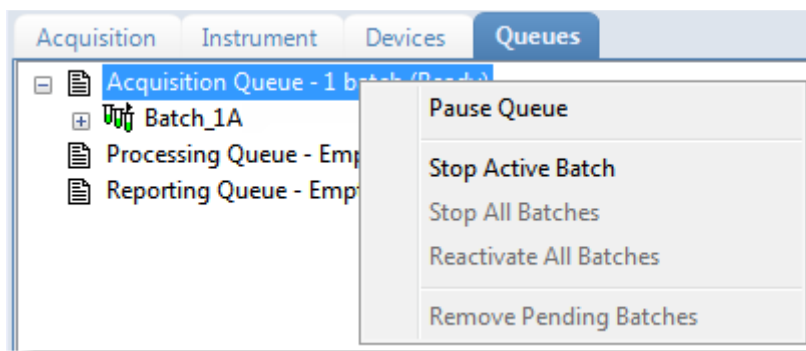


Table 91. Queue-level shortcut menu commands

Command	Description
Pause Queue	After the current sample completes, the application pauses the specified queue. Only the selected queue is affected.
Resume Queue	Returns the paused queue to active status.
Stop Active Batch	Removes all pending samples from the specified queue. The active sample is not affected.
Stop All Batches	Removes all pending samples and batches from the specified queue. The active sample is not affected.
Reactivate All Batches	Returns all paused batches to active status.
Remove Pending Batches	Removes all pending batches from the specified queue. The active batch is not affected.

Batch-Level Commands

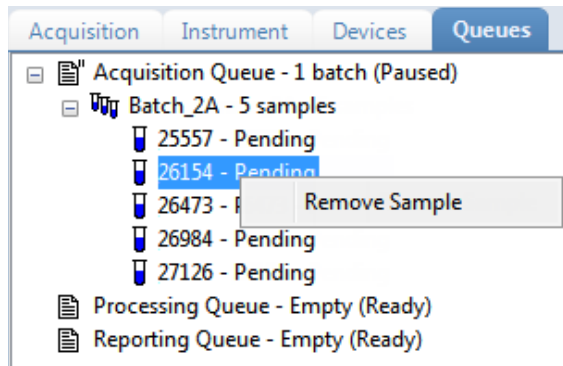
Use the batch-level commands to pause or remove entire batches or samples within batches from any of the queues on the Queues page. See “[Batch-level shortcut menu](#)” on [page 400](#).

Follow these procedures:

- [To remove a single pending sample from a batch](#)
- [To remove all pending samples from a batch](#)
- [To stop a batch](#)
- [To remove a pending batch](#)

❖ **To remove a single pending sample from a batch**

1. Select a pending sample.
2. Right-click the sample 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.

❖ **To remove all pending samples from a batch**

1. Select a batch in any of the queues (Acquisition, Processing, or Reporting).

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 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.

Figure 122. Batch-level shortcut menu

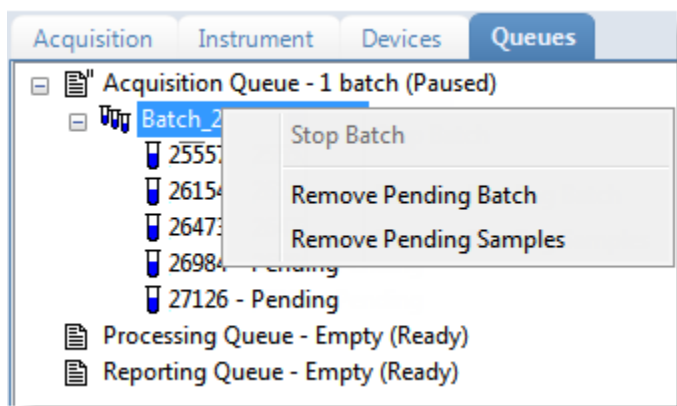


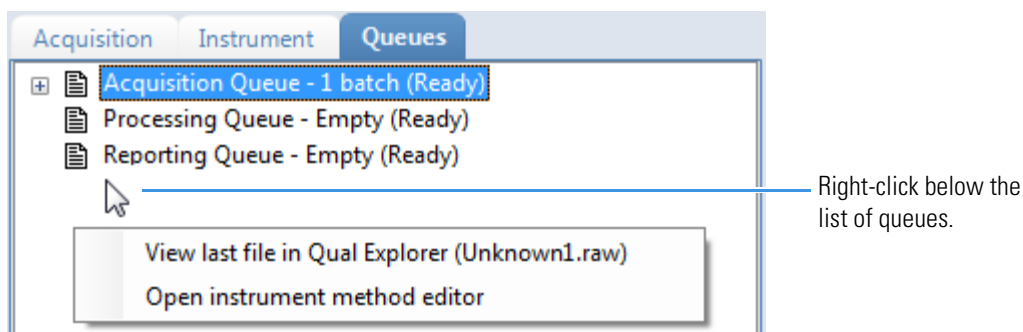
Table 92. Batch-level shortcut menu commands

Command	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.

Additional Commands

You can open the FreeStyle application or the Instrument Setup window using additional commands that you access from the Queues page.

To access the shortcut menu with these commands, you must click in the white space below the list of queues. If you click on the name of or to the right of the queues, the application displays queue-, batch-, or sample-level shortcut menus.



❖ To view the last acquired file in a qualitative browser

Right-click below the queues list on the Queues page and choose **View Last File in Qual Explorer** from the shortcut menu.

The last acquired file opens in either the FreeStyle or Qual Browser application.

❖ To open the Instrument Setup window

Right-click below the queues list on the Queues page and choose **Open Instrument Method Editor** from the shortcut menu.

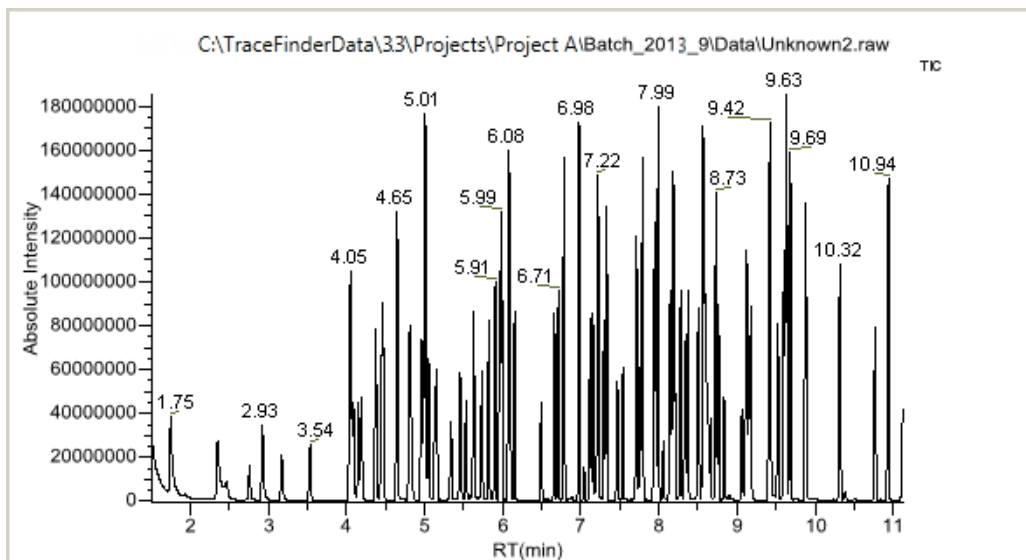
The Thermo Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see [“Working with Instrument Methods”](#) on [page 108](#).

Note Changes you make and save to the instrument method do not affect the currently running batch.

Real-Time Trace Display

As each sample acquires, the real-time chromatogram pane shows the retention time and intensity of the TIC trace.

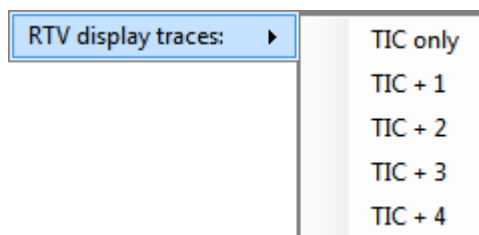


By default, the Real Time Status pane shows only the TIC trace as each sample acquires. To observe specific traces, such as the internal standard, use the RTV Display Traces function to display multiple traces.

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 Status Pane](#)” on [page 388](#).

❖ To display multiple traces

Right-click the chromatogram pane and choose the number of traces to display.

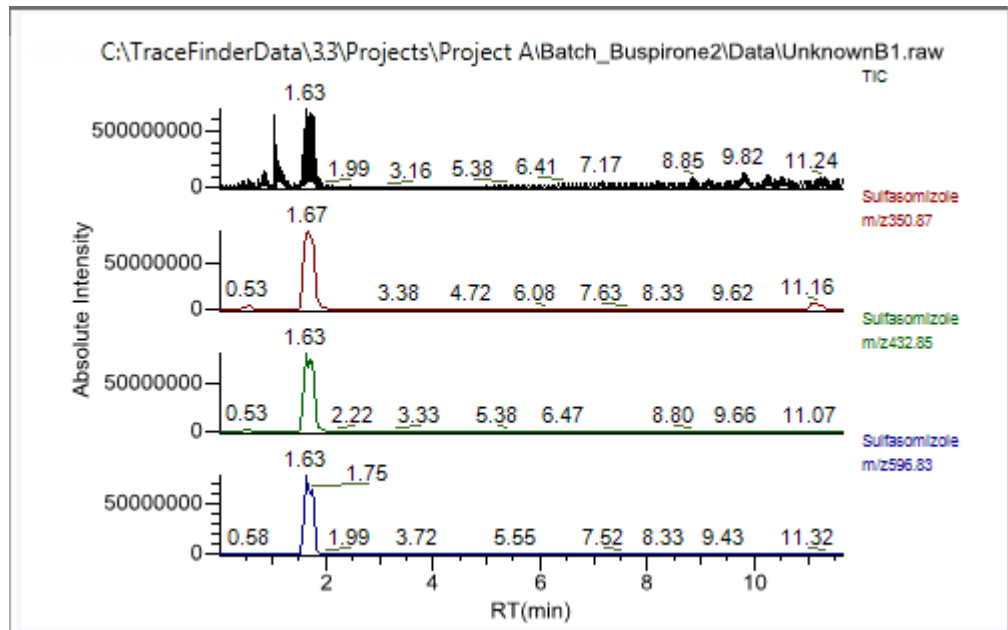


The chromatogram pane displays real-time chromatograms for the selected number of traces.

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. See [Real-time trace display with multiple traces](#).

Figure 123. Real-time trace display with multiple traces



Sample Types

The TraceFinder application uses the following sample types in all sample definitions and reports.

Table 93. 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 application can generate a calibration curve for each compound.
QC Std	(Quality 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 QC Std sample, it compares the measured quantity with the expected value and an acceptability range. The quantitative analysis of a QC Std sample is classified as <i>passed</i> if the difference between the observed and expected quantities is within the user-defined tolerance. A QC Std sample is classified as <i>failed</i> 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.

Using the Analysis Mode for Quantitation Batches

This chapter includes instructions about using the features of the Analysis mode to do the following:

- Create quantitation batches.
- Submit quantitation batches for acquisition, processing, or report generation.
- Review quantitation batches, batch data, reports, and local methods.

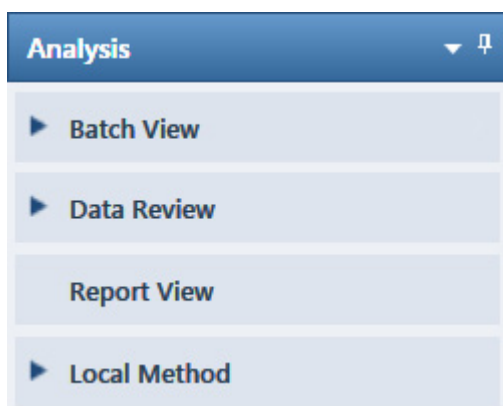
Contents

- [Working in the Batch View](#)
- [Working in Data Review](#)
- [Working in the Report View](#)
- [Working in the Local Method View](#)

❖ To access the Analysis mode

Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.



Working in the Batch View

In the Batch View, you can manually create and edit a new quantitation 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.

The Analysis mode includes a toolbar:



Use the toolbar or the equivalent commands in the Batch View shortcut menu to create the sample list and submit samples for acquisition. See “[Toolbar](#)” on [page 414](#) or “[Batch View Shortcut Menu](#)” on [page 418](#).

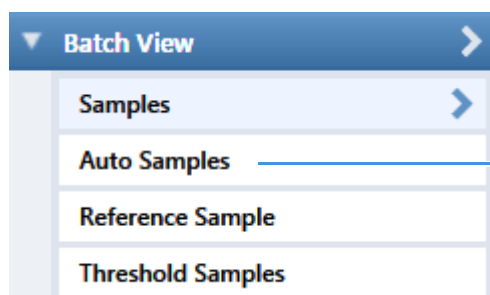
See the following topics:

- [Samples Page](#)
- [Auto Samples Page](#)
- [Reference Sample Page](#)
- [Threshold Samples Page](#)

❖ To open the Batch View

1. Click **Analysis** in the navigation pane of the current mode.
2. Click **Batch View**.

The Batch View navigation pane opens.



Available only when you activate Intelligent Sequencing in the Configuration console

Samples Page

To open the Samples page, click **Samples** in the Batch View navigation pane.

This section contains information about the following topics:

- [Samples Page Features](#)
- [Creating a New Batch](#)
- [Editing a Batch](#)
- [Submitting a Batch](#)

Samples Page Features

The Samples page is divided into two panes:

- Samples pane

Use the samples pane to create a batch. See [Samples Pane](#).

- Compound Active Status pane

Use the Compound Active Status pane to make specific compounds active or inactive. See “[Compound Active Status Pane](#)” on [page 420](#).

Samples pane

The screenshot displays the 'Batch View - Batch_A [Quan]' window. At the top, there is a toolbar with a dropdown menu for 'Local Method' (set to 'Method_Quan'), an 'Update' button, and fields for 'Instrument' (Thermo Scientific Instrument) and 'User'. Below the toolbar is a table with the following columns: Status, Filename, Sample type, Groups, Qual Processing, Level, Sample ID, Sample name, Vial position, Injection volume, Conversion Factor, Channel, Barcode Expected, Barcode Actual, and Sample Volume. The table contains three rows of data for samples 1, 2, and 3, all with a status of 'Unknown' and a sample volume of 1. Below the table is a 'Compound Active Status' pane with a table containing two rows: one for FENTHION-CE20-R20-TL75-QED at RT 1.91, and another for Sulfisomidine at RT 2.72. Both compounds have their 'Active' checkboxes checked.

Status	Filename	Sample type	Groups	Qual Processing	Level	Sample ID	Sample name	Vial position	Injection volume	Conversion Factor	Channel	Barcode Expected	Barcode Actual	Sample Volume
▶ 1	Unknown1	Unknown		<input type="checkbox"/>					10.0	1.000	Auto			1
2	Unknown2	Unknown		<input type="checkbox"/>					10.0	1.000	Auto			1
3	Unknown3	Unknown		<input type="checkbox"/>					10.0	1.000	Auto			1

	RT	Compound	Active
▶ 1	1.91	FENTHION-CE20-R20-TL75-QED	<input checked="" type="checkbox"/>
2	2.72	Sulfisomidine	<input checked="" type="checkbox"/>

Compound Active Status pane

Tip To resize the panes, drag the separator that divides the panes.

Samples Pane

The samples pane includes the following features:

- [Column Display](#)
- [Status Indicators](#)
- [Groups](#)
- [Qual Processing](#)
- [Sample Weight Calculation](#)
- [Instrument Methods](#)
- [Toolbar](#)
- [Batch View Sample List](#)
- [Batch View Shortcut Menu](#)

Column Display

The sample list contains many columns of information. You can scroll to see all the columns, and you can customize which ones to display and their display order.

❖ To scroll the sample list

Use the horizontal scroll bar at the bottom of the sample list to view all the information.

When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name, while the other columns scroll right and left.

❖ To customize the column display

1. Right-click the sample list and choose **Modify Columns** from the shortcut menu.

The Modify Columns dialog box opens. See “[Modify Columns dialog box](#).”

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

These columns appear to the right of the sample list's fixed columns: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.

3. To arrange the order of the columns, do the following:

- a. In the Displayed Columns pane, select a column name.
- b. Use **Up** or **Down** 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, and the last column in the list represents the rightmost column in the Batch View sample list.

Note The following columns are fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

- a. In the Displayed Columns pane, select the column width.

5	Sample ID	100
▶ 6	Sample name	100
7	Vial position	100

- b. Type a new value for the width.

5. Repeat [step 4](#) for all columns whose widths you want to change, and 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.

Figure 124. Modify Columns dialog box

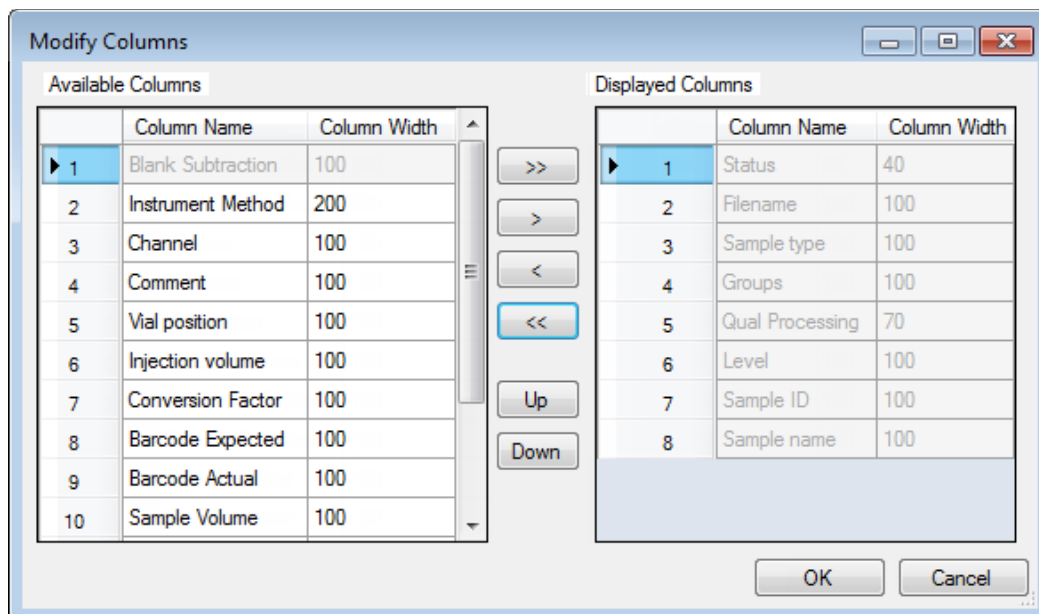












Table 94. Button descriptions for the Modify Columns dialog box




Button	Description
	Moves all columns to the Displayed Columns pane.
	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.	
	Moves the selected column to the Available Columns pane.
	Moves all columns except fixed columns.
	Moves the selected column name in the Displayed Columns pane one row up in the column order.
	Moves the selected column name in the Displayed Columns pane one row down in the column order.

Status Indicators

Status indicators show the current status of each sample during the acquisition and processing.

-  Sample is not acquired.
-  Sample is acquired but not processed.
-  Sample is acquired and processed.
-  Sample is currently acquiring.

Local Method: Method_Alprazolam Update

	Status	Filename	Sample type	Groups	Qual Processing	Sample ID	Sample name	Vi pe
1		Solvent_A	Solvent		<input type="checkbox"/>			1
2		Cal_5	Cal Std		<input type="checkbox"/>			2
3		Unknown1	Unknown		<input type="checkbox"/>			3

Status indicators




Groups

Use the Groups feature to assign samples to a group.

❖ To create a group



- For each sample, type the name of a group in the Groups column.
Repeat this for each sample that you want to include in a group.
- Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
	Benzo26473	groupB, groupA
	Benzo25557	groupB
	Benzo26154	groupB, groupA

Qual Processing

Use the Qual Processing feature to indicate samples to be processed with the qualitative peak processing criteria specified in the method.

Status	Filename	Sample type	Groups	Qual Processing
	VitWaterEquanMaxA001	Unknown		<input checked="" type="checkbox"/>
	VitWaterEquanMaxA002	Unknown		<input checked="" type="checkbox"/>

The Qualitative View displays processed data for the selected samples. See “[Qualitative View](#)” on [page 475](#).

Sample Weight Calculation

Use the sample weight features to calculate the conversion factor for a sample. The application uses different methods to calculate the conversion factor for liquid or solid calculation types.

Liquid: $SampleVolume \div DilutionFactor$

Solid: $(SampleVolume \times DilutionFactor) \div SampleWeight$

Manual: The application does not calculate the Conversion Factor. Instead, you can enter the Conversion Factor value.

Follow these procedures:

- [To display the features for calculating sample weight](#)
- [To calculate the conversion factor for a liquid sample](#)
- [To calculate the conversion factor for a solid sample](#)
- [To manually specify the conversion factor for a sample](#)

❖ To display the features for calculating sample weight

If the Conversion Factor, Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns are not visible, right-click and choose **Enable Sample Weight Calculation** from the shortcut menu.

Conversion Factor	Sample Volume	Dilution Factor	Sample Weight	Calculation Type	Final Units
1.000	1	1	1	Liquid ▼	
1.000	1	1	1	Solid ▼	
1.000	1	1	1	Manual ▼	

❖ To calculate the conversion factor for a liquid sample

Note The application uses the following formula to calculate the Conversion Factor:
 $SampleVolume \div DilutionFactor$

1. From the **Calculation Type** list, select **Liquid**.

For a liquid sample, the Sample Weight value is not editable.

2. In the Sample Volume column, type the volume in ng/mL for your sample.
3. In the Dilution Factor column, type the value for the dilution.

For example, if you have 1000 ng/mL of a substance that is too concentrated for the mass spectrometer, you can dilute it by 1000. Then your injection volume is 1, your conversion factor is 1000, and your sample amount is 1000.

4. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

❖ To calculate the conversion factor for a solid sample

Note The application uses the following formula to calculate the Conversion Factor:
 $(SampleVolume \times DilutionFactor) \div SampleWeight$

1. From the **Calculation Type** list, select **Solid**.
2. In the Sample Weight column, type the weight in ng for your sample.
3. In the Sample Volume column, type the volume in ng/ml for your sample.
4. In the Dilution Factor column, type the value for the dilution.

For example, if you have 1000 ng/ml of a substance that is too concentrated for the mass spectrometer, you can dilute it by 1000. Then your injection volume is 1, your conversion factor is 1000, and your sample amount is 1000.

5. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

❖ To manually specify the conversion factor for a sample

Note The application uses the specified conversion factor when it calculates the amount for the sample.

1. From the **Calculation Type** list, select **Manual**.

For a manually calculated sample, the only available columns are the Conversion Factor and the Final Units.


2. In the Conversion Factor column, type the conversion factor to use for your sample.
3. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

Instrument Methods

Use the Instrument Methods column to specify instrument methods for the samples.

Note By default, the Instrument Method column is not displayed in the Batch View sample list.

❖ To specify instrument methods for samples

1. Display the Instrument Method column in the sample list:
 - a. Right-click the sample list and choose **Modify Columns** from the shortcut menu.
The Modify Columns dialog box opens.
 - b. In the Available Columns pane, select **Instrument Method**.
 - c. Click  to move the Instrument Method column to the Displayed Columns pane.
 - d. Click **OK**.

The application displays the Instrument Method column, defaulting to the instrument method specified in the master method.

2. Click the Instrument Method column and select an instrument method from the list.

This list contains all the available instrument methods. Instrument methods from external sources are prefixed with “Ext:”.

You can specify a different instrument method for each sample.

Batch View - Batch_8266 [Quan]

Local Method: Instrument:

	Status	Groups	Filename	Sample type	Qual Processing	Instrument Method
4			Unknown4	Unknown	<input type="checkbox"/>	Ext: Instrument1
5			Unknown5	Unknown	<input type="checkbox"/>	Ext: Instrument2
6			Unknown6	Unknown	<input type="checkbox"/>	Ext: Instrument3

When you submit the batch for acquisition, the application saves a copy of the selected instrument methods to the following folders:

External instrument methods:

...\\TraceFinderData\\3.3\\Projects\\...\\batch\\Methods\\method\\ExternalMethods

Local instrument methods:

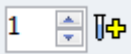
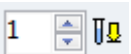









...\\TraceFinderData\\3.3\\Projects\\...\\batch\\Methods\\method

Toolbar

The Analysis mode includes this toolbar for creating and submitting a batch.



Table 95. Toolbar icons

Icon	Description
	Adds the specified number of new, empty samples to the end of the sample list. See the instructions “To add samples to the list” on page 422 .
	Inserts a new, empty sample or samples above the selected sample. See the instructions “To insert samples into the list” on page 423 .
	Removes the selected samples from the sample list. See the instructions “To remove samples from the list” on page 424 .
	Adds imported samples from a CSV, an XML, or an SLD file to the sample list. See the instructions “To import samples into the list” on page 423 .
	Submits only the selected samples for acquisition, processing, or report generation. See the instructions “To submit samples in the batch” on page 433 .
	Submits the batch for acquisition, processing, or report generation. See the instructions “To submit samples in the batch” on page 433 .
	Submits only the selected peaks for processing. See the instructions “To submit selected peaks for processing” on page 433 .
	Opens the Acquisition mode where you can use a batch template to define a standard sequence composed of various sample types to be assembled into a batch of samples. See “Working in Data Review” on page 447 .
	Opens the Acquisition mode where you can create a batch template that contains the basic settings and sample types for your batches. See “Using the Acquisition Mode” on page 347 .
	Opens the Quick Acquisition window where you can quickly submit a single sample. See Appendix A, “Using Quick Acquisition.”
	Opens the Audit Viewer where you can view audit logs. See Chapter 13, “Using the Audit Viewer.” Available only when you enable Auditing in the Administrator Console. Refer to the instructions in the <i>TraceFinder Administrator Console User Guide</i> .

Batch View Sample List

The sample list displays all the quantitative data for the samples of a batch.

Status indicators for each sample indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The sample list includes the following columns of information:

Figure 125. Batch View sample list

Local Method: Method_Alprazolam_Quan Update Instrument: Thermo Scientific Instrument

	Status	Filename	Sample type	Groups	Qual Processing	Level	Sample ID	Sample name	Vial position	Injection volume
1		UnknownA1	Unknown		<input type="checkbox"/>		1		CStk1-01:7	10.0
2		UnknownA2	Unknown		<input type="checkbox"/>		1		CStk1-01:7	10.0
3		UnknownA3	Unknown		<input type="checkbox"/>		1		CStk1-01:7	10.0

Calculation Type	Conversion Factor	Dilution Factor	Sample Weight	Sample Volume	Final Units
Liquid	1.000	1	1	1	
Liquid	1.000	1	1	1	
Liquid	1.000	1	1	1	

Instrument Method	Channel	Barcode Expected	Barcode Actual	Comment
Instrument1	Auto			
Instrument1	Auto			
Instrument1	Auto			

Table 96. Batch View sample list columns (Sheet 1 of 2)








Column	Description
Status	<p> Sample is not acquired.</p> <p> Sample is acquired but not processed.</p> <p> Sample is acquired and processed.</p> <p> Sample is currently acquiring.</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed () , and the Unknown Screening View shows the Status for the samples as acquired but not processed () .</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed () .</p>
Groups	Threshold group to which a sample belongs. Samples can be viewed by group in the Comparative View of Data Review.
Filename	Name of the raw data file that contains the sample data.
Sample Type	<p>Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC Std, or Unknown</p> <p>Default: Unknown</p>
Qual Processing	Indicates samples to be processed with the qualitative peak processing criteria specified in the method. The Qualitative View displays processed data for the selected samples.
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.
Vial Position	The tray vial number used for an autosampler acquisition.
Injection Volume	<p>The injection volume (in microliters) of the injected sample.</p> <p>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 displayed range.</p> <p>The Injection Volume value set in the master method overwrites the value in the instrument method.</p> <p>Valid range: 0.1 through 5000 µL</p>

Table 96. Batch View sample list columns (Sheet 2 of 2)

Column	Description
Calculation Type	<p>Liquid: The application calculates the Conversion Factor as</p> $\text{SampleVolume} \div \text{DilutionFactor}$ <p>Solid: The application calculates the Conversion Factor as</p> $(\text{SampleVolume} \times \text{DilutionFactor}) \div \text{SampleWeight}$ <p>Manual: Sample Volume, Dilution Factor, Sample Weight, and Final Units columns are not available, and the Conversion Factor value is editable.</p>
Conversion Factor	<p>Editable only when Calculation Type is Manual.</p> <p>Default: 1</p>
Sample Volume	Default: 1
Dilution Factor	Default: 1
Sample Weight	<p>Available only when Calculation Type is Solid.</p> <p>Default: 1</p>
Final Units	<p>Specifies the calculated amount in the Data Review view or in reports.</p> <p>Default: 1</p>
Instrument Method	Specifies the instrument to use for the acquisition. This column is hidden by default. To display this column, see “To customize the column display” on page 408.
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. The Channel column is available only when you have activated multiplexing in the Configuration console. See “Multiplexing” on page 61.
Barcode Expected	A user-entered barcode for the vial.
Barcode Actual	An actual barcode for the vial. This value is not editable.
Comment	A user-defined comment for the sample.

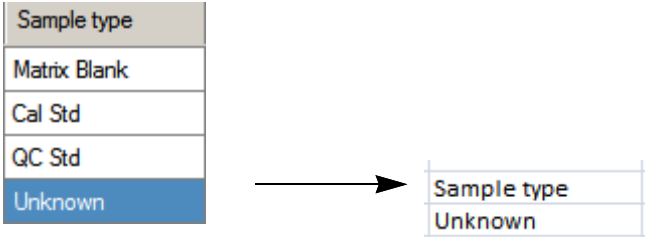
Batch View Shortcut Menu

The Batch View includes a shortcut menu for creating a batch.

Table 97. 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 423 .
Browse in Raw File (Move)	Opens a dialog box where you can select a raw data file to use for the selected sample row. The application removes the raw data file from the source location.
Browse in Raw File (Copy)	Opens a dialog box where you can select a raw data file to use for the selected sample row. The application copies the raw data file from the source location.
Map Raw Files to Samples	Opens a dialog box where you can select multiple raw data files to use for the selected 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 408 .
Enable/Disable Sample Weight Calculation	Displays or hides the Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information into a text editor or spreadsheet application. You cannot paste this data back into the Batch View sample list.

Table 97. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
Copy with Headers	<p>Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information into another text editor or spreadsheet application. You cannot paste this data back into the sample list.</p> <p>For example</p>  <p>Copy with Headers from TraceFinder</p> <p>Paste into an Excel spreadsheet.</p>
Paste	Pastes a single column of copied data from another text editor or spreadsheet application 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.
Edit Instrument Method	<p>Opens the Instrument Setup window where you can edit the parameters of the instrument method.</p> <ul style="list-style-type: none"> • When you edit an external method, the application updates the method in the ... \Xcalibur\methods folder. • When you edit an internal method, the application updates the method in the ... \TraceFinderData\3.3\Projects\... \batch\Methods\method folder. <p>For detailed information about editing instrument methods, see “Working with Instrument Methods” on page 108.</p>

Compound Active Status Pane

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 sample list, select a sample.

All compounds in the selected sample are listed in the Compound Active Status pane.

Compound Active Status

	RT	Compound	Active
▶ 1	1.91	FENTHION-CE20-R20-TL75-QED	<input checked="" type="checkbox"/>
2	2.72	Sulfisomidine	<input checked="" type="checkbox"/>

The default active/inactive status is determined by the identification settings in the local method. For information about setting the identification parameters, see [“Identification”](#) on [page 152](#).

- To display compounds alphabetically, right-click and choose **Sort by Compound Name** from the shortcut menu.
 - To display compounds from shorter to longer retention time, right-click and choose **Sort by Retention Time** from the shortcut menu.
2. Select or clear the **Active** check box for the compound.

For instructions about changing the active/inactive status in the Data Review view, see [“Inactive and Excluded Compounds”](#) on [page 496](#).

Compound Active/Inactive Status

You can specify which compounds are active or inactive in the Local Method View or the Batch View.

Figure 126. Active and inactive compounds in the Local Method View

Local Method View - Batch_2_Method_Vitamin1						
Master method: Method Vitamin1						
Acquisition List	Identification	Detection	Calibration	Calibration levels	Chk Std levels	Real Time View
	RT	Compound	Compound type	Active	CAS No	
1	5.88	1-Butanol, 4-(butylnitrosoamino)-	Target Compound	<input type="checkbox"/>	3817116	
2	16.68	3,3'-Diaminodiphenylmethane	Target Compound	<input checked="" type="checkbox"/>	19471126	

For details about setting the status on the Identification page, see [“Identification”](#) on [page 152](#).

Figure 127. Active and inactive compounds in the Batch View

Batch View - Batch_2 [Quan]							
Local Method:		Method_Vitamin1_Quan			Update		
	Status	Filename	Sample type	Groups	Qual Processing	Level	Sample ID
▶ 1		VitWaterEquanMaxA001	Unknown		<input type="checkbox"/>		CStkl-01:3
2		VitWaterEquanMaxA002	Unknown		<input type="checkbox"/>		CStkl-01:4

Compound Active Status			
	RT	Compound	Active
▶ 1	5.88	1-Butanol, 4-(butylnitrosoami...	<input type="checkbox"/>
2	16.68	3,3'-Diaminodiphenylmethane	<input checked="" type="checkbox"/>
3	2.91	4-Methyl-2,6,7-trioxa-1-phosp...	<input checked="" type="checkbox"/>

For details about setting the status in the Batch View, see “[Compound Active Status Pane](#)” on [page 420](#).

Creating a New Batch

In the Batch View, you can create a new batch.

Follow these procedures:

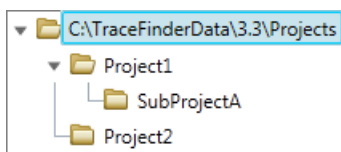
- [To create a new batch](#)
- [To add samples to the list](#)
- [To insert samples into the list](#)
- [To import samples into the list](#)
- [To remove samples from the list](#)
- [To copy a sample](#)
- [To reinject a sample](#)
- [To edit sample values](#)
- [To browse in raw data files](#)
- [To customize the column display](#)

❖ To create a new batch

1. Choose **File > New > Batch** from the main menu.

The Create New Batch dialog box opens, displaying all drives that contain projects. See “[Create New Batch Dialog Box](#)” on [page 428](#).

2. Select a drive from the list.



Tip The application displays all configured and enabled repositories.

3. Select the folder where you want to store your batch.

Tip To activate the Create button, you must enter a unique batch name. If the Create button is not activated, you have entered a batch name that is already used.

To create a new folder for the storage location, see “[Editing Folders for Batches](#)” on page 429.

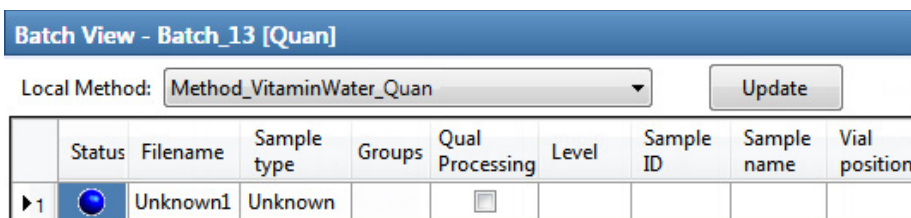
4. Select **Quan** from the Type list.

The batch list displays all batches in the selected folder. The Method list displays all methods for the quantitation type.

5. Select a master method from the Master Method list.

6. Click **Create**.

A new batch opens with one Unknown sample.




The batch name in the title bar indicates that you are creating a quantitation batch.

When you create a batch using a quantitation method that includes unknown screening features, the title bar indicates that the method includes unknown screening.

Batch View - Batch_X [Quan with Unknown]


❖ 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** icon, .





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 will insert new, Unknown samples, and then 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** icon .

The application inserts the Unknown samples above the selected sample.

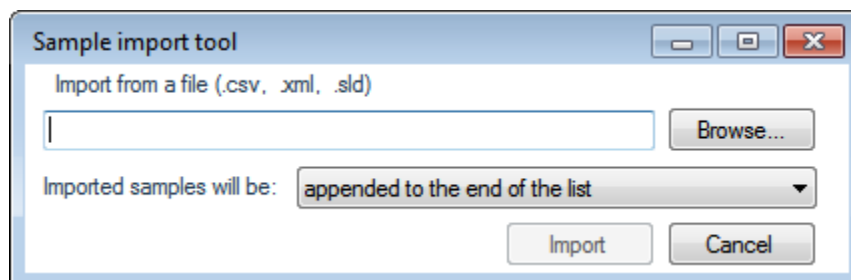
	Status	Filename	Sample type	Groups
1		cal_std_5	Cal Std	
2		Unknown2	Unknown	
3		Unknown1	Unknown	
4		cal_std_10	Cal Std	

Inserted samples →

❖ **To import samples into the list**

1. Choose **Batch > Import Samples** from the main menu, or click the **Import Samples** icon, .

The Sample Import Tool dialog box opens.



From this dialog box, you can import samples from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file that contains the samples 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 sample list.

When you import samples from an Xcalibur sequence file (.sld), the application makes the following column name substitutions:

Xcalibur column	TraceFinder column
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conversion Factor

When you import samples from an Xcalibur sequence file (.sld), the application makes the following sample type substitutions:

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	QC Std
Std Bracket	Cal Std

- (Optional) When using multiplexing, select a channel for each imported sample. Imported samples default to Auto.

Note The Channel column is available only when you have activated multiplexing in the Configuration console. See “[Multiplexing](#)” on [page 61](#).

❖ To remove samples from the list

- Select the samples that you want to remove.

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

- Right-click and choose **Remove Selected Samples** from the shortcut menu.

❖ To copy a sample

- Select the sample that you want to copy.
- Right-click and choose **Insert Copy Sample** from the shortcut menu.

The application inserts the copy above the selected sample.

❖ To reinject a sample

- In the sample list, select the sample that you want to reinject.
- Right-click and choose **Reinject This Sample** from the shortcut menu.

The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

❖ **To edit sample values**

1. For each sample, do one of the following:

Type a new file name over the current filename.

–or–

Double-click the Filename column and locate a raw data file to use for the sample.

–or–

Right-click and choose **Browse in Raw File** from the shortcut menu, and then locate a raw data file to use for the sample.

By default, the application sets the Sample Type to Unknown.

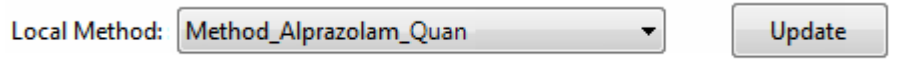
2. For each sample, click the Sample Type column and select a sample type from the list.

Available sample types			
Matrix Blank	Solvent	QC Std	Unknown
Cal Std			

3. For each Cal Std or QC Std sample, select a level from the Level list.

The sample levels are defined in the master method. If there are no levels to select in the Level list, do the following:

- a. Return to the Method Development mode.
- b. Open the method.
- c. Click the **Compounds** tab.
- d. Click the **Calibration Levels** tab.
- e. Add the levels.
- f. Save the method.
- g. Return to the Batch View in the Analysis mode, and then click **Update**.



The application updates the local method with the new sample levels.

For detailed instructions about specifying calibration levels, see [“Calibration Levels”](#) on page 207.

4. Type a vial position in the Vial Position column for each sample.
5. Type a volume in the Injection Volume column for each sample.

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

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

Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name, while the other columns scroll right and left.

For instructions to automatically copy or fill values in these columns, see [Appendix C, “Using Copy Down and Fill Down.”](#)

❖ To browse in raw data files

1. Do one of the following:

Double-click the Filename column.


–or–

Right-click and choose **Browse in Raw File** from the shortcut menu.

The What Raw File Would You Like to Use dialog box opens.

2. Select a raw data file to use for the sample or use the CTRL key to select multiple files, and then click **Open**.

The application overwrites the selected, unacquired sample in the batch with the first “browsed in” file and adds any additional browsed in files below the selected sample.

For all browsed-in raw data files, the application sets the Status to Acquired, , and sets the Sample Type to Unknown.

Note You cannot overwrite an acquired sample. When you select a sample that is acquired, the application adds all browsed in files below the selected sample.

❖ 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. See [“Modify Columns dialog box” on page 427](#).

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

All the columns you select appear after the Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:
 - a. In the Displayed Columns pane, select a column name.
 - b. Use **Up** or **Down** 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, and the last column in the list represents the rightmost column in the Batch View sample list.

Note The following columns are fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:
 - a. In the Displayed Columns pane, select the column width.

7	Vial position	69
▶ 8	Injection volume	100
9	Calculation Type	100

- 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.

Modify Columns Dialog Box

Use the Modify Columns dialog box to select the columns that you want to display.

Figure 128. Modify Columns dialog box

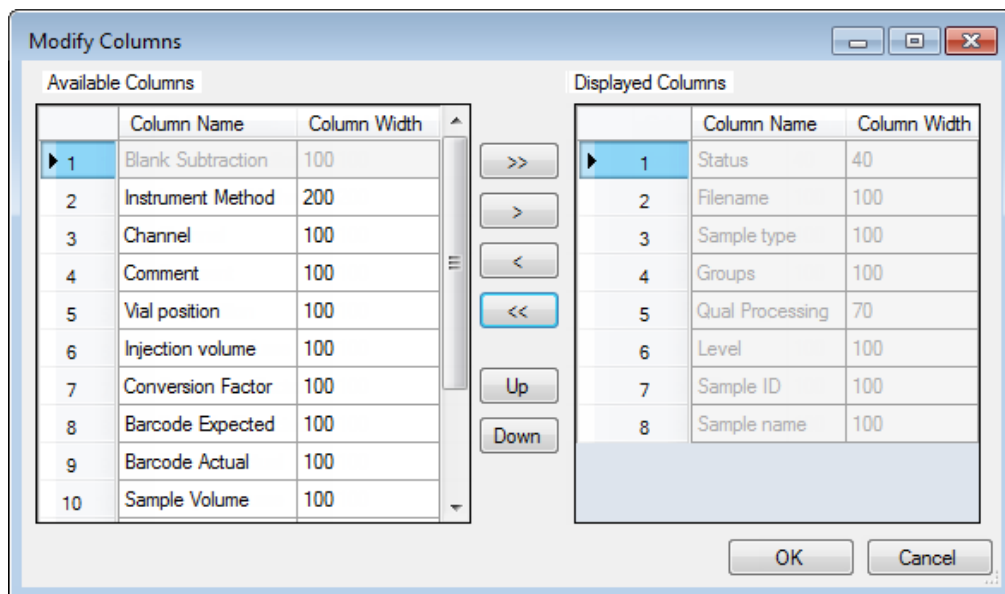








Table 98. Button descriptions for the Modify Columns dialog box

Button	Description
	Moves all columns to the Displayed Columns pane.
	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.	
	Moves the selected column to the Available Columns pane.
	Moves all columns except those that are fixed.
	Moves the selected column name in the Displayed Columns pane one row up in the column order.
	Moves the selected column name in the Displayed Columns pane one row down in the column order.

Create New Batch Dialog Box

Use the Create New Batch dialog box to select a folder and method for your batch and to name the new batch.

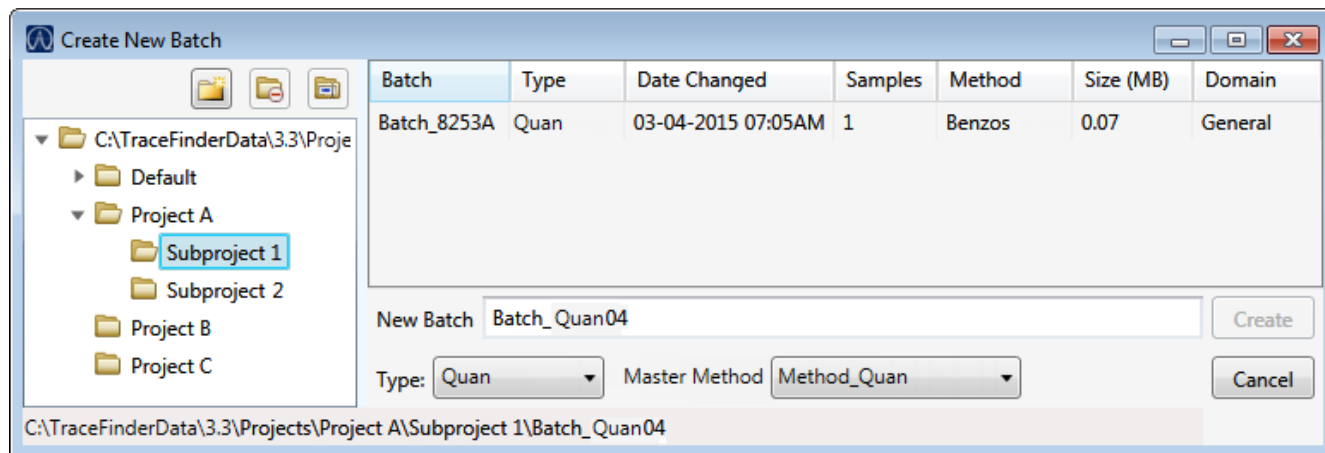


Table 99. Create New Batch dialog box parameters (Sheet 1 of 2)




Parameter	Description
 Create New Folder	<p>Adds one of the following:</p> <ul style="list-style-type: none"> • When a drive is selected, adds a new project-level folder to the drive. • When a project folder is selected, adds a subproject-level folder to the selected project. • When a subproject folder is selected, adds a lower-level folder to the subproject. <p>Or, right-click and choose Create Folder from the shortcut menu.</p>

Table 99. Create New Batch dialog box parameters (Sheet 2 of 2)

Parameter	Description
 Delete Folder	With no confirmation prompt, immediately removes the selected folder. You cannot delete a folder that contains lower-level folders; you must delete the lower-level folders first. Or, right-click and choose Delete from the shortcut menu.
 Rename Folder	Renames the selected folder. Or, right-click and choose Rename from the shortcut menu.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
New batch parameters	
New Batch	Name of the new batch to create. Note If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Type	Type of batch to create: Quan, Screening, or Unknown Only.
Method	Method used to create the new batch.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is created.
Buttons	
Create	Creates the specified batch and opens the Batch View for the new batch.
Cancel	Closes the Create New Batch dialog box without creating a batch.


Editing Folders for Batches

From the Create New Batch dialog box, you can create new folders for your batches. You can also delete or rename folders.

Use these procedures:

- [To create new project folders](#)
- [To delete project folders](#)
- [To rename project folders](#)

❖ To create new project folders

1. In the Create New Batch dialog box, select the folder for which you will create a new lower-level folder.
 - You can select the main TraceFinderData\3.3\Projects folder and create a new folder under it.
 - You can select one of the existing folders and create a lower-level folder under it.
2. Click the **Create Folder** icon, .


The application adds a new lower-level folder to the selected folder.

3. Select the new folder name and type a name for the folder.

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

Note After you add a lower-level folder, you cannot rename the parent folder.


❖ To delete project folders

1. In the Create New Batch dialog box, select the folder to delete.
2. Click the **Delete Folder** icon, .

With no confirmation prompt, the application immediately removes the selected folder.

Note You cannot delete folders that contains lower-level folders; you must delete the lower-level folders first.

❖ To rename project folders

1. In the Create New Batch dialog box, select the folder to rename.
2. Click the **Rename Folder** icon, .

Note You cannot rename folders that contain lower-level folders.

3. Type a new name for the folder and press ENTER.

The application saves the new folder name.

Editing a Batch

In the Batch View, you can open a saved batch and edit the sample 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 “ready to acquire” batch.

Follow these 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 open a saved batch

1. Choose **File > Open > Batch** from the main menu.

The Open Batch dialog box opens. See [Open Batch dialog box](#).

2. Select a project and a subproject.
3. Select **Quan** or **Any** from the Type list.

The batch list displays all batches created with quantitation methods (or all methods of all types when you select Any).

4. Select a batch from the list.
5. Click **Open**.

The selected batch opens in the Batch View.

Open Batch Dialog Box

Use the Open Batch dialog box to select a batch to open.

Figure 129. Open Batch dialog box

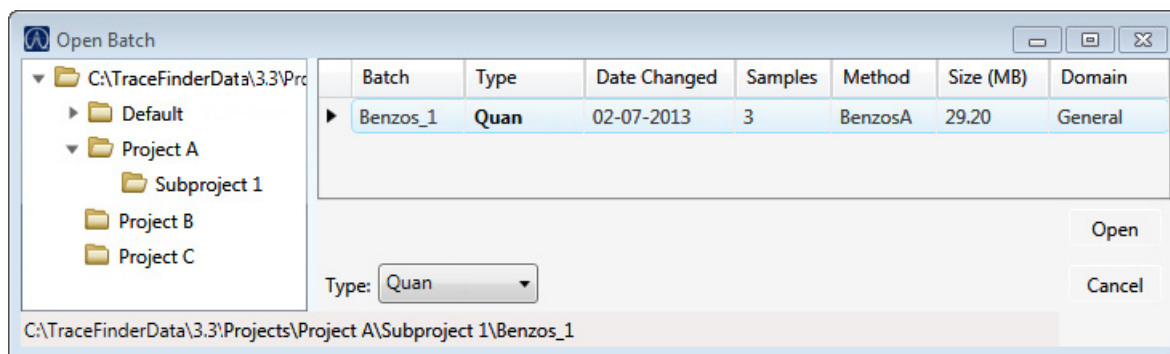


Table 100. Open Batch dialog box parameters (Sheet 1 of 2)

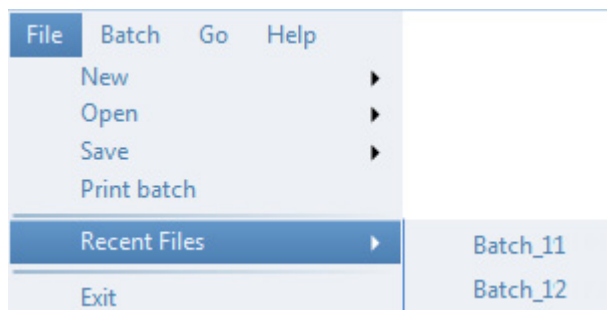
Parameter	Description
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date the batch was last updated.

Table 100. Open Batch dialog box parameters (Sheet 2 of 2)

Parameter	Description
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is stored.
Buttons	
Type	Type of batch to display in the Batch list: Quan, Screening, Unknown Only, or Any.
Open	Opens the Batch View for the selected batch.
Cancel	Closes the Open Batch dialog box without opening a batch.

❖ **To open a recent batch**

Choose **File > Recent Files > *batch*** from the main menu.



The selected batch opens in the Batch View.

❖ **To edit samples in a batch**

Use the commands described in “Working in the Batch View” on page 406.





You can add new samples, edit samples, or delete samples.

❖ **To reinject a sample from a previously acquired batch**

1. In the sample list, select the sample that you want to reinject.
2. Right-click and choose **Reinject This Sample** from the shortcut menu.

The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The 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	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

When you submit all samples in this batch, the application acquires all samples (including previously acquired samples).

- To save this batch with the new samples for reinjection, choose **File > Save > Batch** from the main menu.

The batch is saved as a prepared batch that is ready to submit. You can open this batch from the Reinject Samples page in the Acquisition mode and submit the batch. The application acquires only the samples that have not been previously acquired.

Submitting a Batch


In the 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 436](#).

For a description of commands in the shortcut menu, see “[Batch View shortcut menu commands](#)” on [page 418](#).

Follow these procedures:



- [To submit selected peaks for processing](#)
- [To submit samples in the batch](#)
- [To view the output files](#)

❖ To submit selected peaks for processing

- In the Peak List, select the **Selected** check box for the peaks that you want to process.
- Click the **Submit ... for Processing** icon, .

The application processes the selected peaks and updates the data in the Data Review panes.

❖ To submit samples in the batch

- Do one of the following:
 - To submit all samples in the batch, click the **Submit Batch** icon, .
 - To submit specific samples, select the samples and click the **Submit Selected Samples** icon, .

The Submit Options dialog box opens. See “[Submit Options dialog box](#)” on page 436.

Note You can also submit only selected peaks for processing. See “[To submit selected peaks for processing](#)” on page 433.

- To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.
 - When all submitted samples have been previously acquired, this option is (by default) not selected.
 - When one or more samples in the batch have not been acquired, this option is (by default) selected.

Tip You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

- To process the submitted samples, select the **Process Data** check box.

The application displays processing options for the method.

If the quantitation method includes unknown screening features, the application also displays unknown screening options. For specifying processing data for batches that also use unknown screening features, see “[To submit samples in the batch](#)” on page 633 of Chapter 11, “[Using the Analysis Mode for Unknown Screening Batches](#).”

- Select the check box for the quantitation options that you want to use.

Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

Quantitate: Performs quantitation.

- (Optional) Select the **Create Reports** check box.
- (Optional with multiplexing activated) Select the **Priority Sequence** check box.

The application acquires the priority batch on the next available channel or the assigned channel.

- (Optional without multiplexing activated) 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.

Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.

- a. Select the **Use** check box for the device that you want to use for this acquisition.
- b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

This is usually the autosampler.

- c. 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.

- d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.

9. To start the selected processes, click **OK**.

The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Analysis mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT When your batch also uses unknown screening features, after the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages for the unknown screening features (“[Editing the Processing Pages](#)” on [page 311](#)) and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Submit Options Dialog Box

Use the Submit Options dialog box to submit a batch for acquisition, processing, or reporting.

Figure 130. Submit Options dialog box

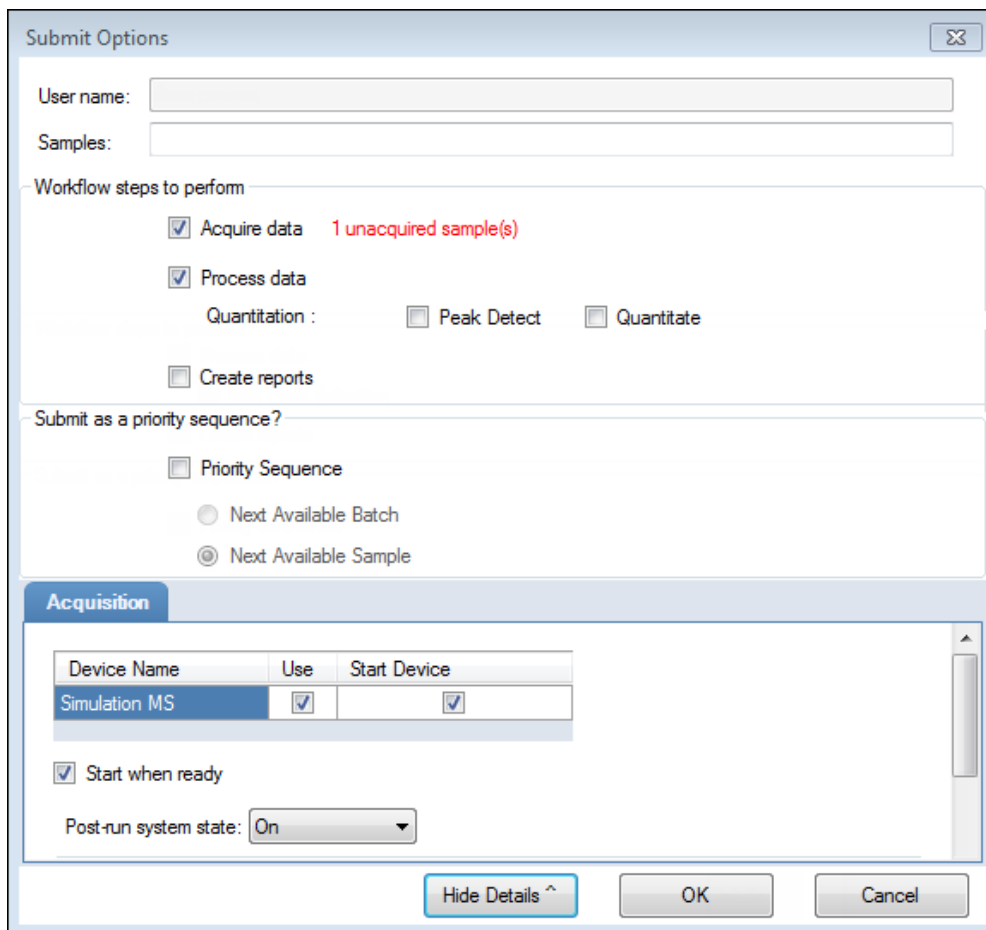


Table 101. Submit Options dialog box parameters (Sheet 1 of 3)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Workflow Steps to Perform	
Acquire Data	Submits the current batch to acquisition. <ul style="list-style-type: none"> When all submitted samples have been previously acquired, this option is (by default) not selected. When one or more samples in the batch have not been acquired, this option is (by default) selected.

Table 101. Submit Options dialog box parameters (Sheet 2 of 3)

Parameter	Description
Process Data	<p>Processes the data for the current batch using any of the following options:</p> <p>Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.</p> <p>Quantitate: Performs quantitation.</p> <p>Note Quantitation methods can include unknown screening features. For specifying processing data for batches that also use unknown screening features, see “To submit samples in the batch” on page 633.</p>
Create Reports	Creates reports for the current batch.
Submit as a Priority Sequence?	
Priority Sequence	<p>With multiplexing activated, places the batch immediately after the currently acquiring batch.</p> <p>Without multiplexing activated, specifies one of the following priority options to place the batch in the queue:</p> <p>Next Available Batch: Places the batch immediately after the currently acquiring batch.</p> <p>Next Available Sample: Places the batch immediately after the currently acquiring sample.</p> <p>Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.</p>
Acquisition pane	
Device Name	<p>Lists all configured instruments.</p> <p>If the instrument that 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.</p> <p>Available only when you select the Acquire Data check box.</p>
Use	<p>Specifies the instruments used for this acquisition.</p> <p>Available only when you select the Acquire Data check box.</p>
Start Device	<p>Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler.</p> <p>Available only when you select the Acquire Data check box.</p>

Table 101. Submit Options dialog box parameters (Sheet 3 of 3)

Parameter	Description
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.
Post-run System State	Specifies the system state after it acquires the last batch: On (default), Standby, or Off.
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.

❖ **To view the output files**

Locate the files to view from the following directories:

The application writes saved batches to the project folder:

... \TraceFinderData\3.3\Projects\...

For each acquired sample, the application writes an RSX file to the batch Data folder:

... \TraceFinderData\3.3\Projects\...\Data

The application saves method information to the batch Methods folder:

... \TraceFinderData\3.3\Projects\...\Methods

The application writes the reports to the batch Reports folder:

... \TraceFinderData\3.3\Projects\...*batch*\Reports

Saving a Batch to a New Location

You can move the current batch to a different project folder, or you can make a copy of the current batch and save the copy to a different project folder.

Follow these procedures:

- [To save a batch to another project folder](#)
- [To move a batch to another folder](#)
- [To create a new project folder](#)
- [To delete project folders](#)
- [To rename project folders](#)

❖ To save a batch to another project folder

1. Choose **File > Save > Save Batch As** from the Batch View main menu in the Analysis mode.

The Save Batch As dialog box opens. See [“Save Batch As Dialog Box”](#) on page 441.

2. Select a storage location.

The default storage location is C:\TraceFinderData\3.3\Projects.

3. Select or create a project folder.

4. Type a name for the new batch.

If you are saving the batch to a different folder, you must give it a unique name. You cannot overwrite an existing batch in a folder.

5. Click **Save**.

When you save the batch to a different folder, the reports reflect the original project folders and the application does not save the calibration history.

❖ To move a batch to another folder

1. Choose **File > Save > Move Batch** from the Batch View main menu in the Analysis mode.

The Save Batch As dialog box opens. See [“Save Batch As Dialog Box”](#) on page 441.

2. Select a storage location.

The default storage location is C:\TraceFinderData\3.3\Projects.

3. Select or create a project folder.


4. Type a name for the new batch.

You must give the batch a unique name in the new subproject folder. You cannot overwrite an existing batch.

5. Click **Save**.

When you move the batch, the reports reflect the original project and subproject folders and the application does not save the calibration history.

❖ To create a new project folder

1. In the Save Batch As dialog box, select the folder for which you will create a new lower-level folder.
 - You can select the main TraceFinderData\3.3\Projects folder and create a new folder under it.
 - You can select one of the existing folders and create a lower-level folder under it.
2. Click the **Create Folder** icon, .


The application adds a new lower-level folder to the selected folder.

3. Select the new folder name and type a name for the folder.

Folder names can contain spaces and special characters, except for the following special characters: \ / : + ? " < >

Note After you add a lower-level folder, you cannot rename the parent folder.


❖ To delete project folders

1. In the Save Batch As dialog box, select the folder to delete.
2. Click the **Delete Folder** icon, .

With no confirmation prompt, the application immediately removes the selected folder.

Note This feature is not available for folders that contain lower-level project or batch folders; you must first delete the lower-level project or batch folders.

❖ To rename project folders

1. In the Save Batch As dialog box, select the folder to rename.
2. Click the **Rename Folder** icon, .

Note This feature is not available for folders that contain lower-level project or batch folders; you must first delete the lower-level project or batch folders.

3. Type a new name for the folder and press ENTER.

The application saves the new folder name.

Save Batch As Dialog Box

Use the features in the Save Batch As dialog box to save a batch to a new name or to move a batch to a different project folder.

Figure 131. Save Batch As dialog box

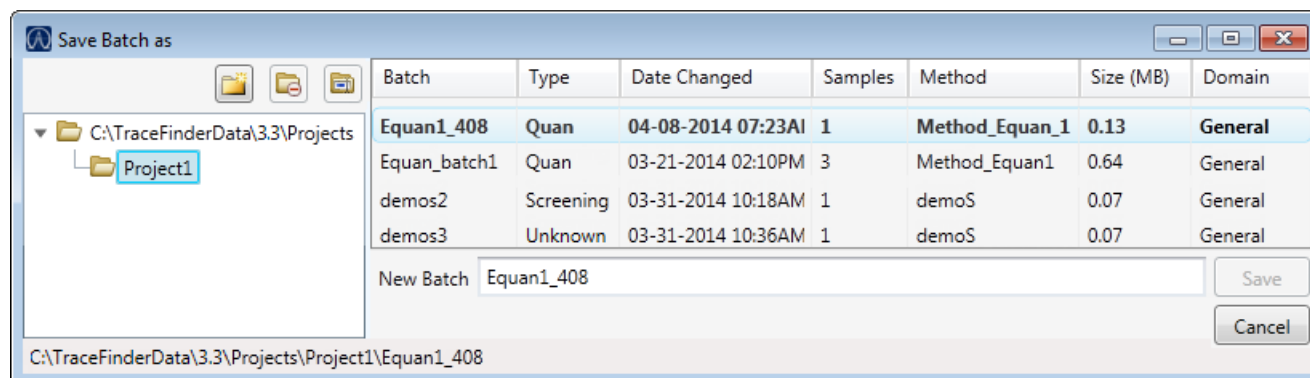


Table 102. Save Batch As dialog box parameters (Sheet 1 of 2)




Parameter	Description
 Create New Folder	Adds one of the following: <ul style="list-style-type: none"> When a drive is selected, adds a new project-level folder to the drive. When a project folder is selected, adds a subproject-level folder to the selected project. When a subproject folder is selected, adds a lower-level folder to the subproject. Or, right-click and choose Create Folder from the shortcut menu.
 Delete Folder	With no confirmation prompt, immediately removes the selected folder. You cannot delete a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders. Or, right-click and choose Delete from the shortcut menu.
 Rename Folder	Renames the selected folder. You cannot rename a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders. Or, right-click and choose Rename from the shortcut menu.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.

Table 102. Save Batch As dialog box parameters (Sheet 2 of 2)

Parameter	Description
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
New batch parameters	
New Batch	Name of the new batch to create. Note If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is created.
Buttons	
Save	Saves the batch to the specified name and folder and opens the Batch View for the new batch.
Cancel	Closes the Save Batch As dialog box without saving the batch.
Shortcut menu commands	
Create Folder	Adds one of the following: <ul style="list-style-type: none"> • When a drive is selected, adds a new project-level folder to the drive. • When a project folder is selected, adds a subproject-level folder to the selected project. • When a subproject folder is selected, adds a lower-level folder to the subproject.
Delete Folder	Immediately removes the selected folder. There is no prompt to confirm that you want to delete the selected folder. You cannot delete a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders.
Rename Folder	Renames the selected folder. You cannot rename a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders.
Expand Child Nodes	Expands all project and subproject folders in the Project tree.
Collapse Child Nodes	Collapses all project and subproject folders in the Project tree.

Auto Samples Page


The Auto Samples page identifies the Solvent or Matrix Blank samples to use for any Auto Sample or Auto Sample and Reinject failure actions as specified on the Intelligent Sequencing page of the method. See “Editing the Intelligent Sequencing Page” on page 228.

Each sample type that you specify for a failure action on the Intelligent Sequencing page must be defined in the samples list on the Auto Samples page.

❖ To add an auto sample type

1. Click **Auto Samples** in the Batch View navigation pane.

The Auto Samples page opens. See [Auto Samples page](#).

2. Right-click and choose **Add Auto Sample** from the shortcut menu, or click the **Add New Auto Sample** icon, .

The application adds a Solvent sample to the sample list.

You can add, insert, or remove samples from this list as you would any sample list. See “Samples Page” on page 406.

3. To change the sample type to a Matrix Blank, click the Sample Type column and select **Matrix Blank** from the list.
4. In the Injection Volume column for the sample, type a volume.

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

5. In the Number of Injections column, type the number of injections available in the designated Solvent or Matrix Blank vial.

After auto sample injections have occurred, you can return to this page to view the number of Injections Used in each vial.

6. In the Vial Position column, type the vial position for the Solvent or Matrix Blank sample.

Auto Samples Page

Use the Auto Samples page to specify the sample types to use with Intelligent Sequencing.

Figure 132. Auto Samples page

	Sample Type	Injection Volume	Injections Used	Number of Injections	Vial Position
	Solvent	1.0	0	1	10
	Matrix Blank	1.0	0	10	11
	Matrix Blank	1.0	0	10	12

Table 103. Auto Samples page parameters

Column	Description
Sample Type	The sample type for the auto sample injection as specified on the Intelligent Sequencing page—either Solvent or Matrix Blank. Default: Solvent
Injection Volume	The injection volume used for the sample acquisition as specified on the Samples page. Valid range: 0.1 through 5000 μ L
Injections Used	The number of times a vial has been used. The count is cumulative across all batches.
Number of Injections	The number of injections available in the designated Solvent or Matrix Blank vial.
Vial Position	Vial position for this sample type as specified on the Samples page.

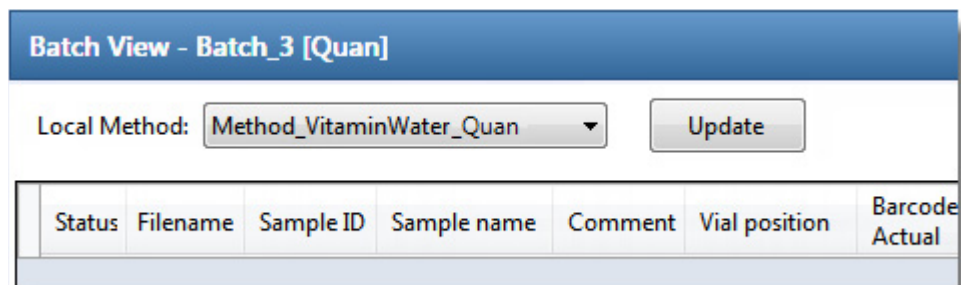
Reference Sample Page


The Reference Sample page displays the reference samples that you selected for this batch.

❖ To specify a chromatogram reference sample

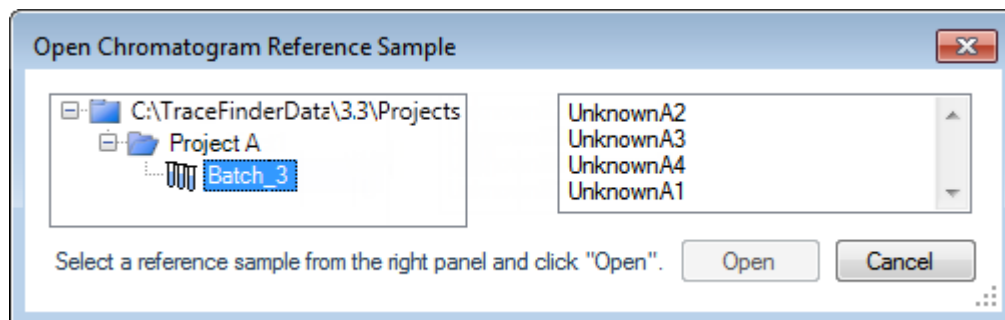
1. In the Batch View, click **Reference Samples**.

An empty reference sample table opens.



2. Click the **Add Reference Sample** icon, , or right-click and choose **Add Reference Sample** from the shortcut menu.

The Open Chromatogram Reference Sample dialog box opens.



Note If you are using a new method, no reference samples appear here. You must first process a batch using the current master 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 application displays only batches that were created using the current master method.

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

The application displays all the processed samples in the selected batch. Before using a sample as a reference sample, you must have processed the sample with the current master method.

7. Click **Open**.

Threshold Samples Page

For each group in a batch, you can specify a sample in the group as the threshold sample to use in the Comparative View.

❖ To specify a threshold sample

1. In the Batch View, click **Threshold Samples**.
2. Click the Sample list for each group and select a sample in the group to be the threshold sample.

	Group	Sample
▶	groupb	Benzo26473 ▼
		Benzo26473
		Benzo25557
		Benzo26154

The Comparative View uses the threshold method and amount you specified in the method, the group you created on the Samples page, and the threshold sample you selected on this page to define the threshold guide that it displays in the sample peak plots.

For information about specifying the method to use for creating a threshold guide, see [“Threshold” on page 223](#).

For information about creating groups, see [“Groups” on page 410](#).

For information about using the threshold guide in the Comparative View, see [“Comparative View” on page 468](#).

Working in Data Review

In the Data Review view, you can view the data generated by the master method. Use Data Review to verify the data for a compound before you generate reports.

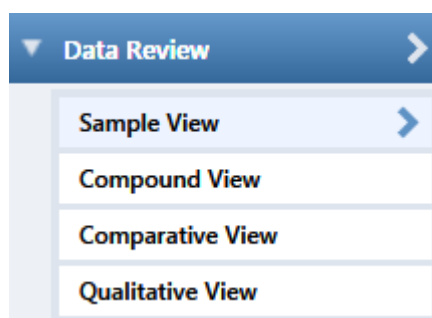
❖ To open the Data Review view

1. Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.

2. Click **Data Review**.

The Data Review navigation pane opens.



Choose from a Sample View, Compound View, Comparative View, or Qualitative View to analyze the data generated by the master method.

❖ To move, dock, or float Data Review panes

Follow the instructions in [Appendix D, "Moving Data Review Panes."](#)

❖ To restore the default layout

Choose **View > Restore Default Layout**.

The Sample View, Compound View, Comparative View, and Qualitative View have their own defaults for which panes are displayed and in which location.

See the following topics:

- [Sample View](#)
- [Compound View](#)
- [Comparative View](#)
- [Qualitative View](#)
- [Features Common to All Data Review Pages](#)

Sample View

The Sample View displays the following information in three different panes: a list of all samples in the current batch, the compound results for all compounds in the method, and peak plots for all compounds found in the currently selected sample.

These are the default panes and their locations:

Sample Peaks pane Samples pane Compound Results pane

Samples					Compound Results		
Flags	Status	Filename	Sample Type	Flags	Flag Details	Compound	e
1	●	B_25557	Unknown			FENTHION-CE20	d
2	●	B_26154	Unknown			Sulfisomidine	d

Sample Peaks

Peak Plot Size

FENTHION-CE20-R20-TL75-QED

RT: 2.05
AA: 67156904.79
AH: 8297169.53
SN: 128.06

Relative Intensity

RT(min)

Sulfisomidine

RT: 2.74
AA: 83969917.96
AH: 13279603.06
SN: 488.86

Relative Intensity

RT(min)

When you select a sample in the [Samples Pane](#), the associated [Compound Results Pane](#) flags any compound with errors in the selected sample. The associated [Sample Peaks Pane](#) displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the selected sample. The Sample Peaks pane highlights the compound selected in the Compound Results pane.


The Sample View display includes the following features:

- [Samples Pane](#)
- [Compound Results Pane](#)
- [Sample Peaks Pane](#)
- [Caution Flags](#)
- [Viewing Sample View Panes](#)

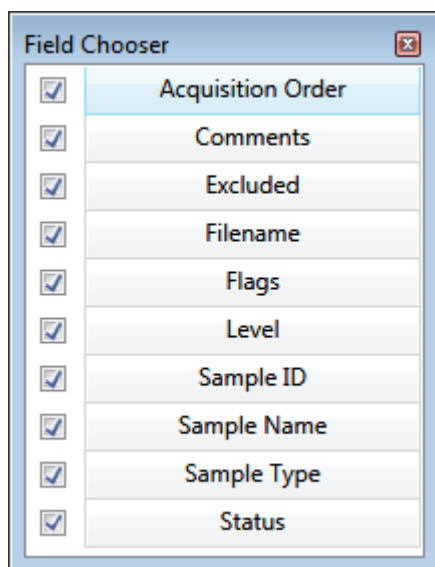
Samples Pane

Use the Samples pane in the Sample View to select a specific sample. The associated [Compound Results Pane](#) displays all compounds in the method and flags any compound with errors in the selected sample.

❖ To hide or display columns in the Samples pane

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Samples pane.



Note The Field Chooser also lists any custom columns that you defined in the Configuration Console. See [“Creating Custom Columns”](#) on page 63.

2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

The application immediately displays or hides the column in the Samples pane.


3. When you are finished modifying the column display, click  to close the Field Chooser.

Figure 133. Samples pane

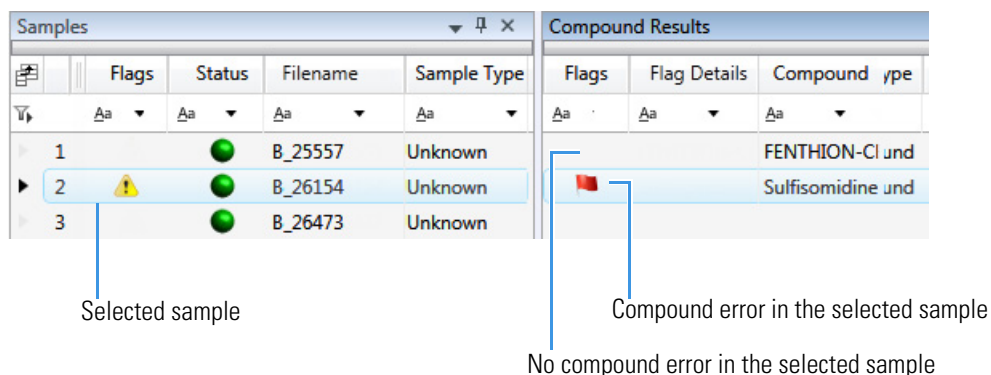










Table 104. Samples pane columns

Column	Description
Flags	Caution flag displayed when a compound in the sample has an error. See “Caution Flags” on page 454.
Status	<ul style="list-style-type: none">  Sample is not acquired.  Sample is acquired but not processed.  Sample is acquired and processed.  Sample is currently acquiring. <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed () , and the Unknown Screening View shows the Status for the samples as acquired but not processed () .</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed () .</p>
Sample Name	A user-defined name that identifies a sample.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC Std, or Unknown.
Comments	User-defined comments for the sample.
Excluded	Turns a compound on or off in the calibration curve in the Compound Details pane.
Filename	A user-defined name that identifies a sample.
Level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined, alphanumeric string that identifies a sample.

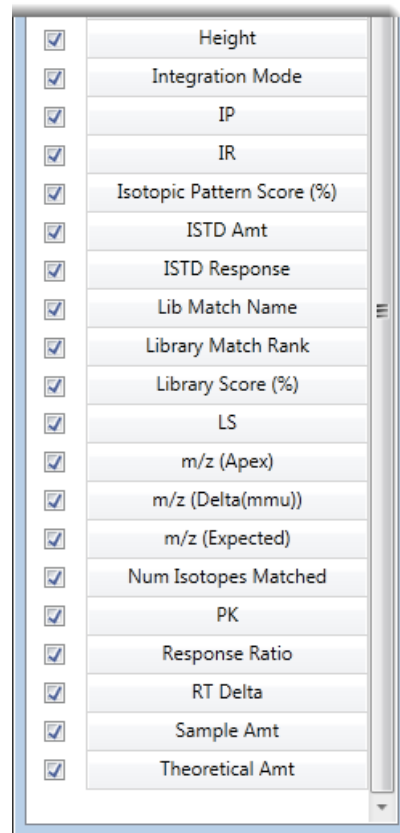
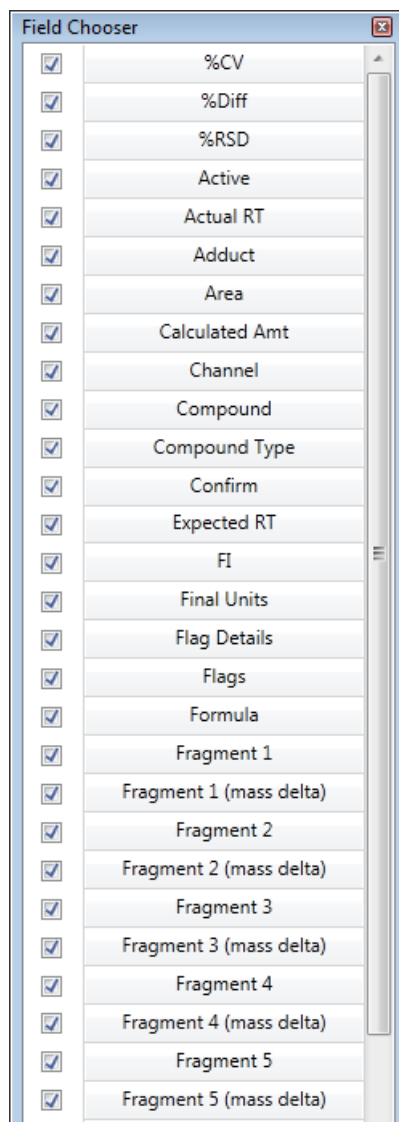
Compound Results Pane

Use the Compound Results pane in the Sample View to select a specific compound in the selected sample. The associated [Sample Peaks Pane](#) highlights the selected compound.

❖ To hide or display columns in the Compound Results pane

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Compound Results pane.



2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

The application displays or hides the column in the Compound Results pane.


3. When you are finished modifying the column display, click  to close the Field Chooser.

Figure 134. Compound Results pane

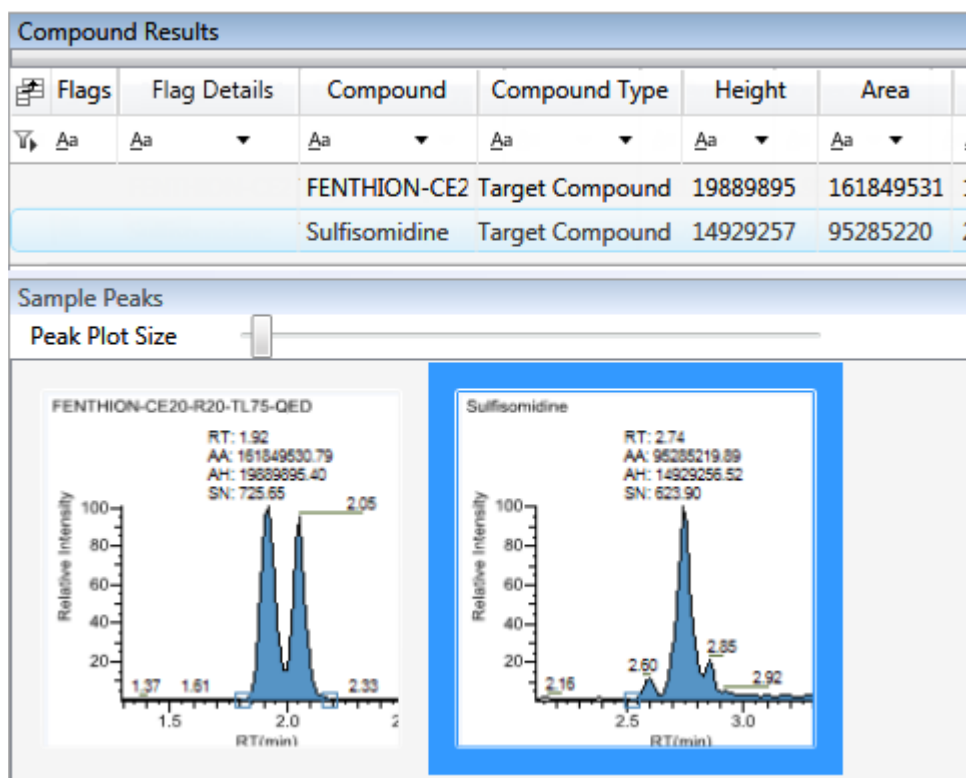


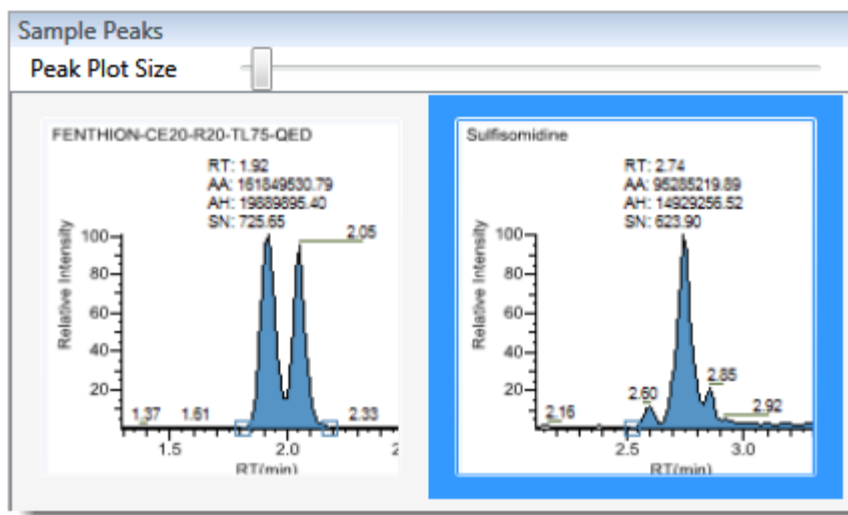
Table 105. Compound Results pane columns

Column	Description
Flags	Caution flag displayed when the compound has an error. See “Caution Flags” on page 454.
Compound	Compound names as identified in the library.
Compound Type	Specified compound type: Target Compound or Internal Standard.

The remainder of the columns in the results list are common to the Compound Results pane in the Sample View and the Sample Results pane in both the Compound View and the Comparative View. See “Common Column Parameters” on page 490.

Sample Peaks Pane

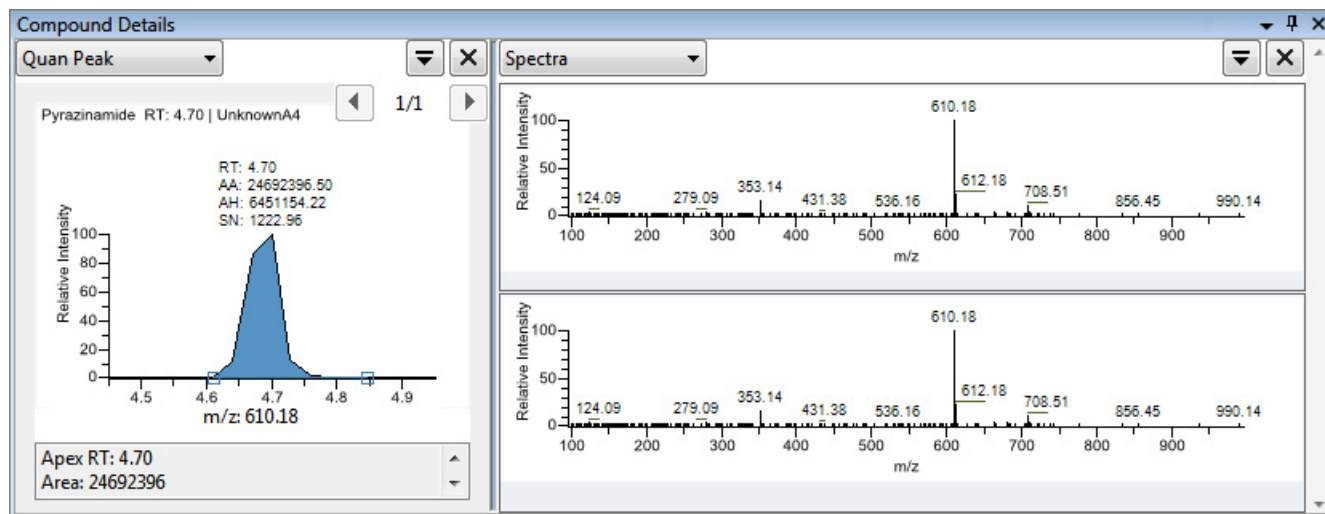
The Sample Peaks pane in the Sample View displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the Compound Results pane. The application highlights the chromatogram for the compound that is currently selected in the Compound Results pane.



❖ To display details for a compound

Double-click the chromatogram in the Sample Peaks pane.

The Compound Details pane opens.



The Compound Details pane displays information about the quantitative peak, calibration curve, confirming ion, internal standard, reference peak, ion overlay, and spectra for the compound.

For a detailed description of the available information in the Compound Details pane, see [“Compound Details”](#) on [page 498](#).

Caution Flags


In the Sample View, the application displays caution flags in both the Samples pane and the Compound Results pane.

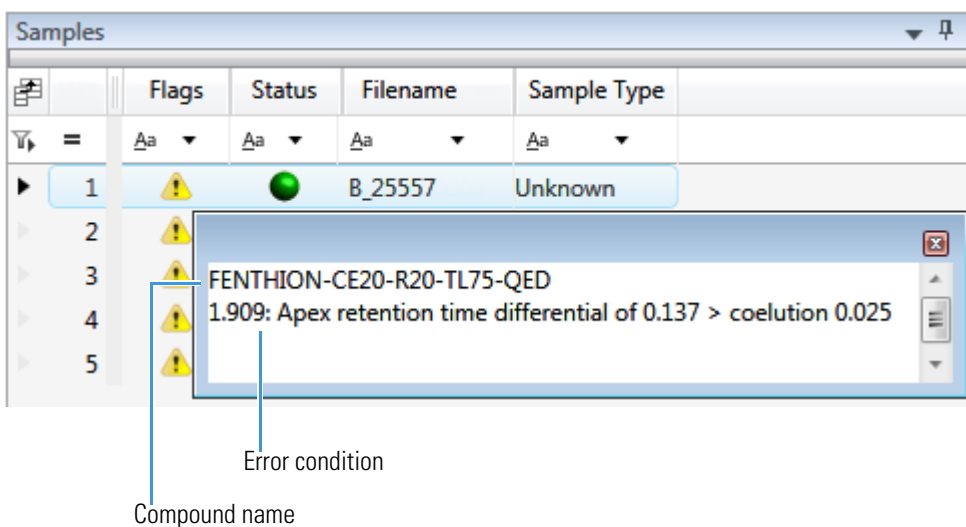
See the following topics:

- [Flags in the Samples Pane](#)
- [Flags in the Compound Results Pane](#)
- [Error Indicators in the Sample Peaks Pane](#)

Flags in the Samples Pane

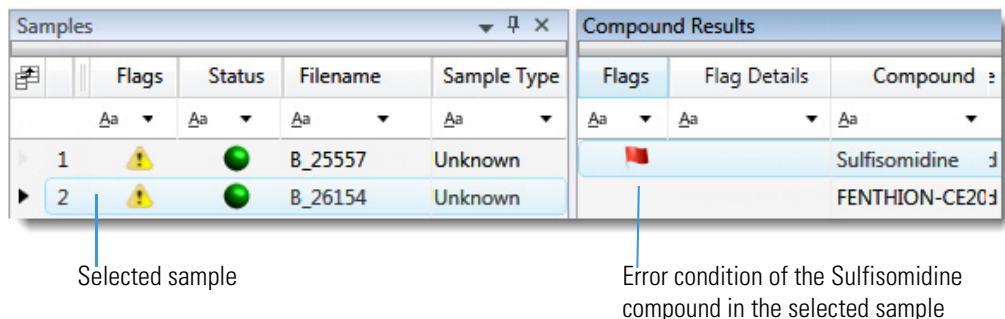
The Flags column in the Samples pane displays a caution flag if any compound in the sample is not in compliance with the method criteria.


Click the caution flag icon, , to display the details. Information in the pop-up box shows the compound that is in error and describes the exact error condition.




Flags in the Compound Results Pane







The Flags column in the Compound Results pane displays a flag if the compound in the selected sample is not in compliance with the method criteria.



Hold your cursor over the flag icon, , to display details for the compound in the selected sample.

	Sulfisomidine	Target Compound	14929257
	2.732: Ion Ratio of 141.4 is not between 78.96 and 118.96		
	2.732: Ion Ratio of 109.68 is not between 47.11 and 87.11		

Flags in the Compound Results pane indicate the following:

-  A red flag for compounds that have violated (or are activated by) any of the values set in the method. See “[Editing the QAQC Page](#)” on [page 217](#).
-  A red flag for compounds that are outside the specified ion ratio range. See [Ion ratio failure flag](#).
-  An orange flag for compounds that are below the LOQ, below the LOD, or between the LOD and LOQ values specified in the method. For descriptions of these limits, see “[Limits](#)” on [page 218](#).
-  A green flag for “found” compounds that are over the LOR amount specified in the method. For a description of the LOR limit, see “[Limits](#)” on [page 218](#).
-  A yellow flag for compounds that are equal to or below the LOR amount specified in the method.
-  A yellow flag for compounds that are not found in Calibrator or QC sample types. The Compound Results pane does not flag compounds that are not found in Specimen sample types.

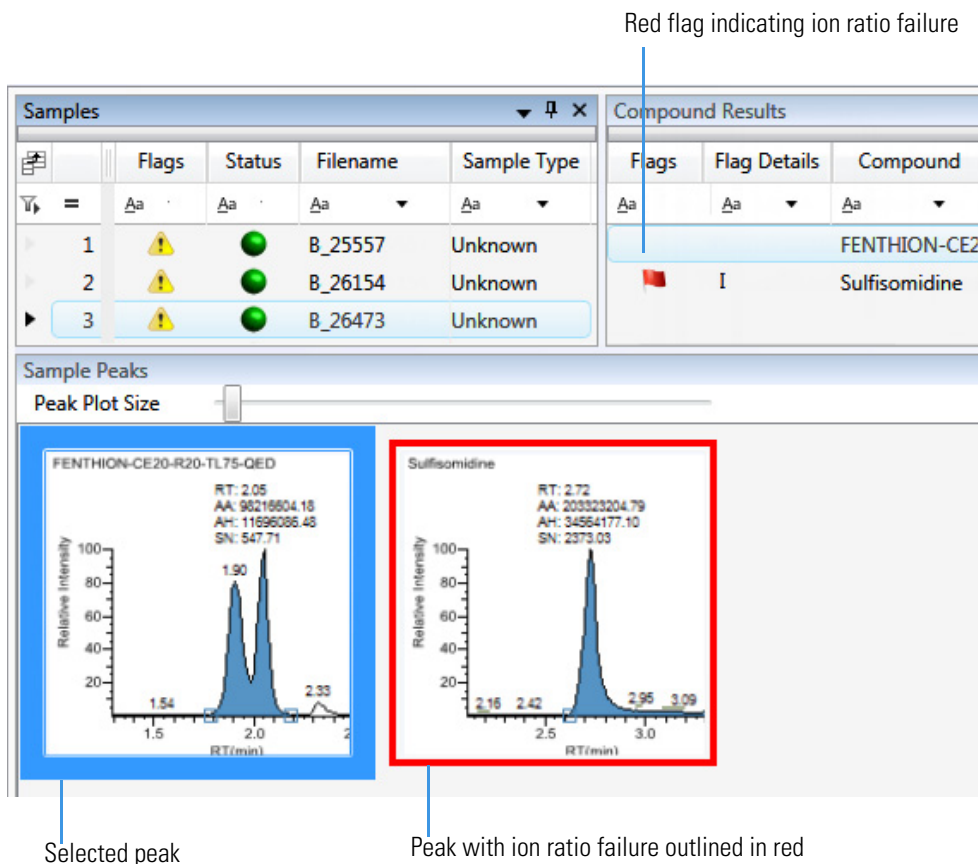
No flag for compounds that have no errors or where no report options are selected.

Note These criteria for flag states do not apply to Matrix Blank sample types when the compound is an internal standard.

Error Indicators in the Sample Peaks Pane

In the Sample Peaks pane, peak plots are outlined with the color of their associated error flag. In the following example, the FENTHION peak plot is highlighted in blue to indicate that FENTHION is the selected compound, and the Sulfisomidine peak plot is outlined in red to indicate that the Sulfisomidine compound in the selected sample is outside the specified ion ratio range.

Figure 135. Ion ratio failure flag



Viewing Sample View Panes

The Sample View displays data using multiple panes: Samples, Compound Results, Sample Peaks, and Compound Details. You can display, hide, or move any of these panes.

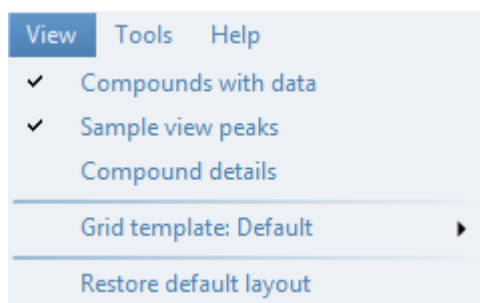
❖ To display or hide a Sample View pane

From the View menu, choose from the following:

- **Compounds with Data:** Displays or hides the Compound Results pane.
- **Sample View Peaks:** Displays or hides the Sample Peaks pane.
- **Compound Details:** Displays or hides the Compound Details pane.

Note The Samples pane is required for the Sample View display. You cannot hide the Samples pane.

A check mark indicates a displayed pane.



Compound View

The Compound View uses three different panes to display a list of all compounds available in the method, all samples in the current batch, and the peak plots for all compounds found in each sample.

These are the default panes and their locations:

Sample Peaks pane Compounds pane Sample Results pane

The screenshot displays the Compound View interface with three main panes:

- Compounds Pane:** A table listing compounds. The first row is highlighted:

Flag	Compound	Compound
Aa	FENTHION-CE2	Target Compound
Aa	Sulfisomidine	Target Compound
- Sample Results Pane:** A table listing samples. The first row is highlighted:

Flags	Flag Details	Status	Filename
1		●	B_25557
2		●	B_26154
3		●	B_26473
- Sample Peaks Pane:** Displays chromatograms for selected samples. The first plot is for sample B_25557, showing a peak at RT: 2.05. Other plots show peaks for B_26154 (RT: 1.92) and B_26473 (RT: 2.05).

When you select a compound in the **Compounds Pane**, the **Sample Results Pane** flags any sample that contains errors associated with the selected compound. The **Sample Peaks Pane** highlights the selected compound, displays the name of the sample in which the compound was found, and, for the compound, displays the chromatogram, retention time, area, height, and signal-to-noise ratio.


The Compound View includes the following features:

- [Compounds Pane](#)
- [Sample Results Pane](#)
- [Sample Peaks Pane](#)
- [Caution Flags](#)

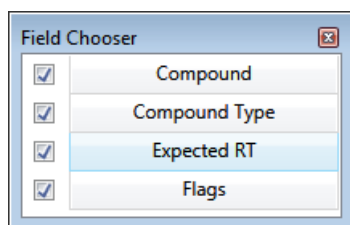
Compounds Pane

Use the Compounds pane in the Compound View to select a specific compound. The [Sample Results Pane](#) displays all samples in the batch and flags any sample that contains errors associated with the selected compound.

❖ To hide or display columns in the Compounds pane

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Compounds pane.



2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

The application immediately displays or hides the column in the Compounds pane.


3. When you are finished modifying the column display, click  to close the Field Chooser.

Figure 136. Compounds pane

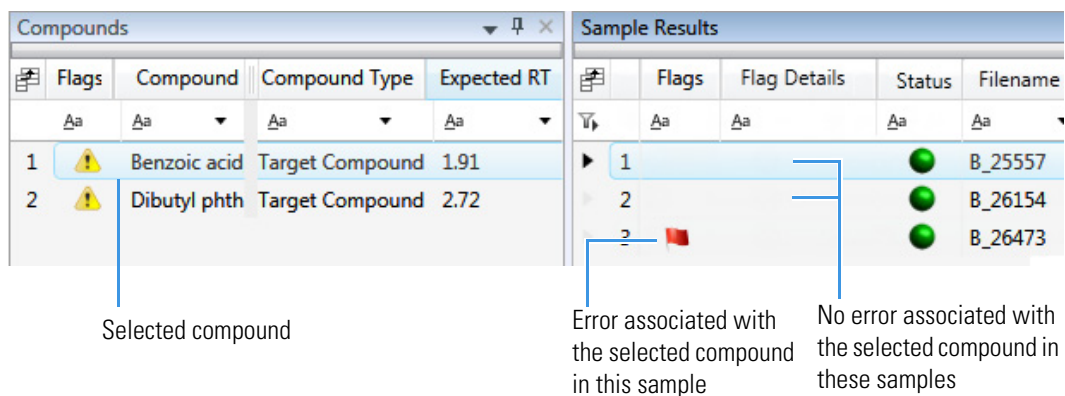



Table 106. Compounds pane columns

Column	Description
Flags	Caution flag displayed when a compound has an error in any of the samples.
Compound	Compound names as identified in the library. If there is no library selected in the method template, the compound name is identified as <i>peak@RT</i> .
Compound Type	Specified compound type: Target Compound or Internal Standard.
Expected RT	Expected retention time for the compound.

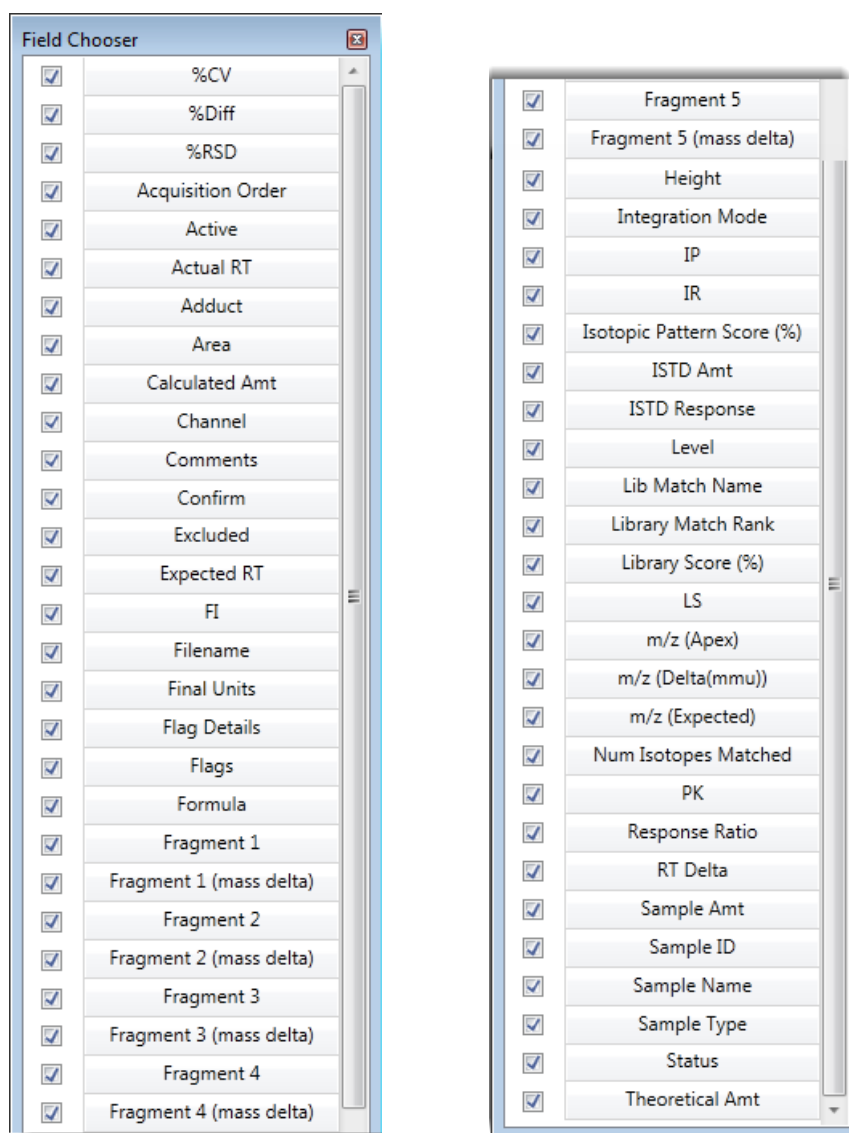
Sample Results Pane

Use the Sample Results pane in the Compound View to select a specific compound in a specific sample. The Sample Peaks pane highlights the selected compound and displays the name of the sample in which the compound was found and the following information about the compound: chromatogram, retention time, area, height, and signal-to-noise ratio. See [Sample Results pane](#).

❖ To hide or display columns in the Sample Results pane

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Sample Results pane.



Note The Field Chooser also lists any custom columns that you defined in the Configuration Console. See [“Creating Custom Columns”](#) on page 63.

2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

The application immediately displays or hides the column in the Sample Results pane.


3. When you are finished modifying the column display, click  to close the Field Chooser.

Figure 137. Sample Results pane

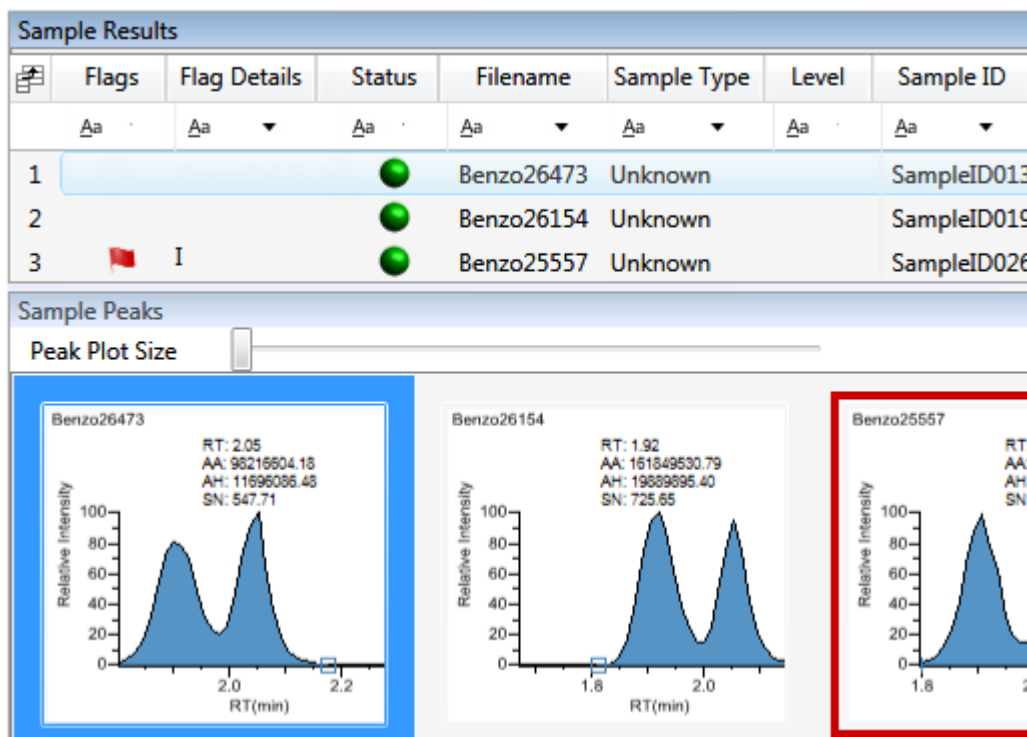









Table 107. Sample Results pane columns (Sheet 1 of 2)

Column	Description
Acquisition Order	Sequentially numbers the samples.
Flags	Caution flag displayed when a compound within the sample has an error.
Flag Details	Indicates the type of error: <ul style="list-style-type: none"> • I: Confirming ion coelution failure or Ion ratio failure • A: Amount error • B: Matrix blank error • H: Peak not found

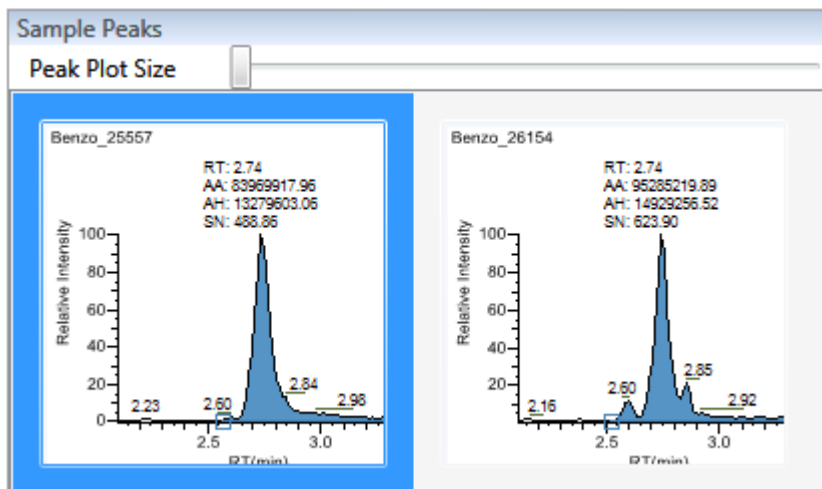
Table 107. Sample Results pane columns (Sheet 2 of 2)

Column	Description
Status	<p> Sample is not acquired.</p> <p> Sample is acquired but not processed.</p> <p> Sample is acquired and processed.</p> <p> Sample is currently acquiring.</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed () , and the Unknown Screening View shows the Status for the samples as acquired but not processed () .</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed () .</p>
Filename	A user-defined name that identifies a sample.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC Std, or Unknown.

The remainder of the columns in the Sample Results pane are common to both the Sample View and the Compound View displays. See [“Common Column Parameters”](#) on [page 490](#).

Sample Peaks Pane

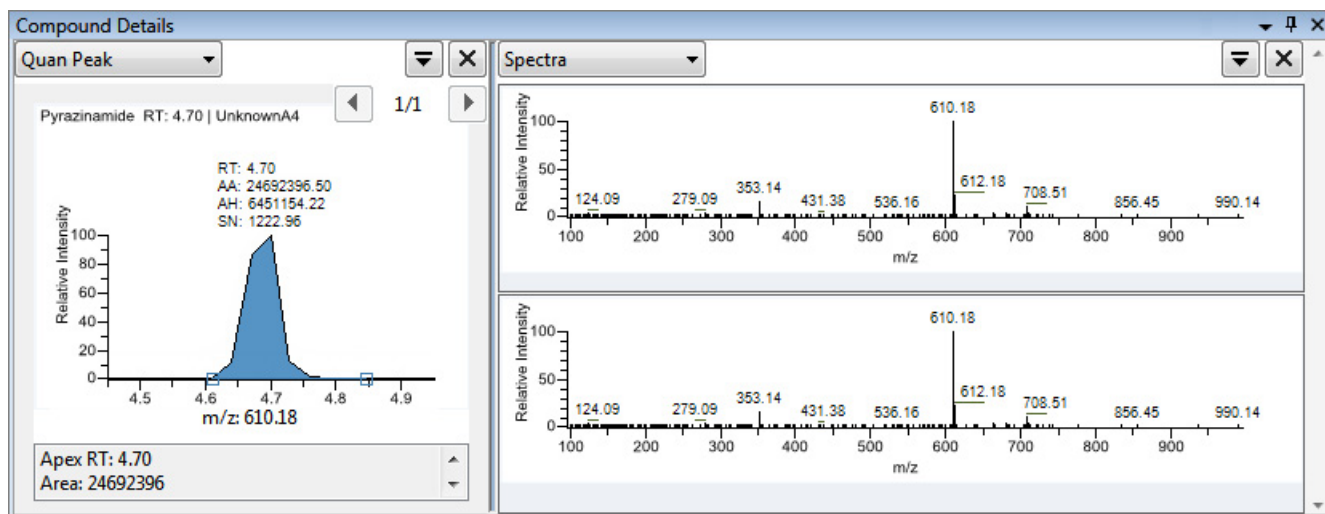
The Sample Peaks pane in the Compound View displays the compound chromatogram, retention time, area, height, and signal-to-noise ratio associated with the selected compound in each of the samples in the batch. The application highlights the compound chromatogram for the sample that is currently selected in the Sample Results pane.



❖ To display details for a compound

1. Double-click the chromatogram in the Sample Peaks pane.

The application adds the Compound Details pane to the window.



The Compound Details pane displays information about the quantitative peak, calibration curve, confirming ion, internal standard, reference peak, ion overlay, and spectra for the compound.

For details about the available information in the Compound Details pane, see [“Compound Details”](#) on page 498.

Caution Flags

In the Compound View, the application displays caution flags in both the Compounds pane and in the Sample Results pane.

See the following topics:

- [Flags in the Compounds Pane](#)
- [Flags in the Sample Results Pane](#)
- [Error Indicators in the Sample Peaks Pane](#)


Flags in the Compounds Pane

The Flags column in the Compounds pane displays a caution flag if the compound in any of the samples is not in compliance with the method criteria.

Compounds			Sample Results				
Flags	Compound	Expected RT	A	Flags	Flag Details	Status	Filename
⚠	FENTHION-CE20-R20-	2.08	1	🟢		🟢	B_25557
⚠	Sulfisomidine	1.92	2	🔴	I	🟢	B_26154
			3	🟡	H	🟢	B_26473

Selected Sulfisomidine compound

Flags for the Sulfisomidine compound in each sample

Click the caution flag icon, , to display the details. Information in the pop-up box shows the sample where the compound is in error and describes the exact error condition.

Compounds	
Flags	Compound
⚠	FENTHION-CE20-R20-TL75-QED


Benzo_25557
1.909: Apex retention time differential of 0.137 > coelution 0.025



Sample name

Error condition





Flags in the Sample Results Pane

The Flags column in the Sample Results pane displays a flag if the selected compound in the sample is not in compliance with the method criteria.

Hold your cursor over the flag icon, , to display the details for the selected compound in the sample.

Sample Results					
	Flags	Flag Details	Status	Filename	Sample Type
▶		I		B_25557	Unknown
▶		1.909: Apex retention time differential of 0.137 > coelution 0.025			

Flags in the Sample Results pane indicate the following:

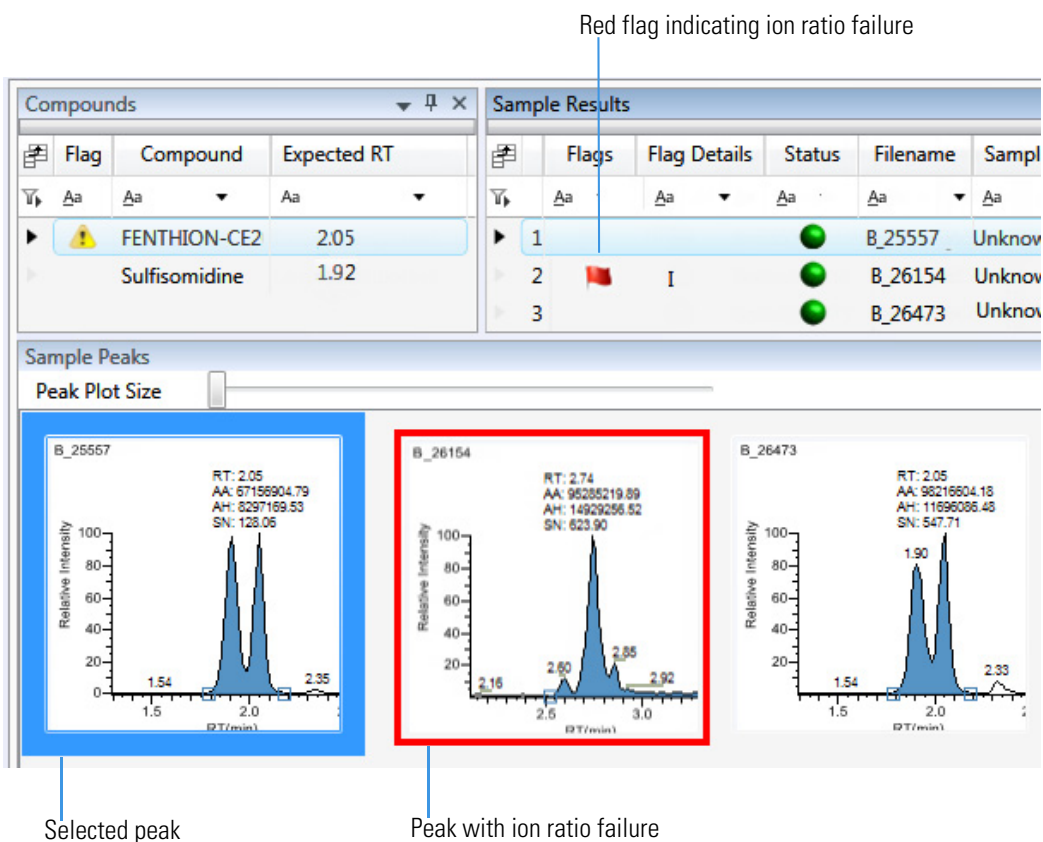
Flag	Description
	A green flag for compounds that are over the LOR amount specified in the method.
	A red flag for compounds that have violated (or are activated by) any of the values set in the method. See “Editing the QAQC Page” on page 217.
	A red flag for compounds that are outside the specified ion ratio range. See Ion ratio failure flag .
	An orange flag for compounds that are not found in Cal Std or QC Std sample types. “Not found” compounds are below the LOQ, below the LOD, or between the LOD and LOQ values specified in the method. The Sample Results pane does not flag compounds that are not found in Unknown sample types.
	No flag for compounds that have no errors or where no report options are selected.

Note These criteria for flag states do not apply to Matrix Blank sample types when the compound is an internal standard.

Error Indicators in the Sample Peaks Pane

In the Sample Peaks pane, peak plots are outlined with the color of their associated error flag. In the following example, the peak plot is highlighted in blue to indicate that Benzo_25557 is the selected sample and outlined in red to indicate that the FENTHION compound in the selected sample is outside the specified ion ratio range.

Figure 138. Ion ratio failure flag



Viewing Compound View Panes

The Compound View displays data using multiple panes: Compounds, Sample Results, Sample Peaks, and Compound Details. You can display, hide, or move any of these panes.

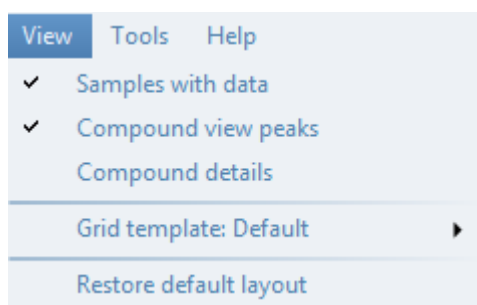
❖ To display or hide a Compound View pane

From the View menu, choose from the following:

- **Samples with Data:** Displays or hides the Sample Results pane.
- **Compound View Peaks:** Displays or hides the Sample Peaks pane.
- **Compound Details:** Displays or hides the Compound Details pane.

Note The Compounds pane is required for the Compound View display. You cannot hide the Compounds pane.

A check mark indicates a displayed pane.

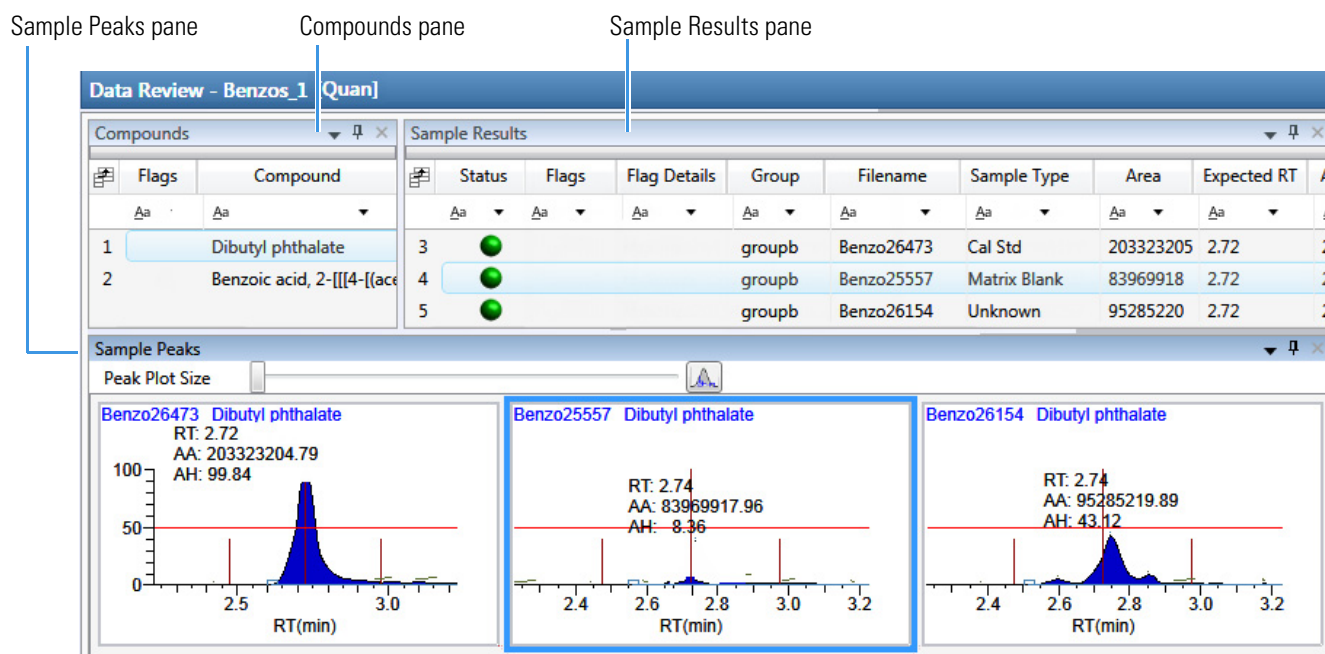


For procedures about creating docked, floating, or tabbed panes, see [“Moving Data Review Panes”](#) on [page 739](#).

Comparative View

The Comparative View uses three panes to display a list of all compounds available in the method, all samples in the current batch, and the sample peak plots for all compounds found in the samples with the horizontal threshold guide.

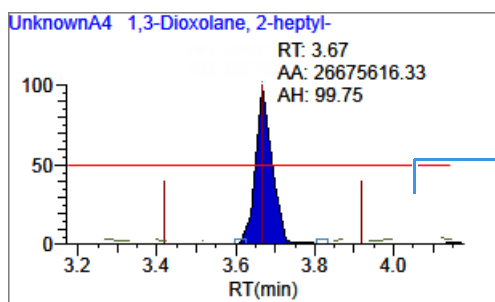
These are the default panes and their locations:



The panes in the Comparative View are identical to the Compound View with the addition of the Group column in the Sample Results. This column identifies any groups that a sample belongs to, as specified in the Batch View.

The following factors define the threshold guide that the Comparative View displays in the sample peak plots:

- The threshold method and amount that you specified in the method
- The group that you created on the Sample page
- The threshold sample that you selected on the Threshold Samples page



Horizontal guide indicates the threshold value as specified in the method.

See the following topics:

- [Configuring Sample Peaks Display Settings](#)
- [Manually Integrating Peaks](#)

For information about specifying the method to use for creating a threshold guide, see [“Threshold”](#) on [page 223](#).

For information about creating groups, see [“Groups”](#) on [page 410](#).

For information about specifying a threshold sample, see [“Threshold Samples Page”](#) on [page 446](#).

Configuring Sample Peaks Display Settings

The Sample Peaks pane in the Comparative View displays one row per compound and one column per sample. The Sample Peaks pane displays all samples in a group when you select any of the samples belonging to that group.

For information about creating groups, see [“Groups”](#) on [page 410](#).

❖ To change the Sample Peaks pane display

1. From the View menu, choose **Chromatogram Pane Settings**.

The Chromatogram Plot Settings dialog box opens. See [“Chromatogram Plot Settings Dialog Box”](#) on [page 472](#).

2. To change the number of rows or columns to fit in the Sample Peaks pane, type new values in the Number of Rows or Number of Columns boxes.

These values do not change the number of rows (compounds) and columns (samples) that are available in the Sample Peaks pane. These values determine how many rows and columns you want to view at one time in the display. The default is three rows and three columns.

In the following examples, the Number of Rows and Number of Columns are set to 1 ([Number of Rows equals 1 and Number of Columns equals 1](#)) and the Number of Rows and Number of Columns are set to 4 ([Number of Rows equals 4 and Number of Columns equals 4](#)).

Figure 139. Number of Rows equals 1 and Number of Columns equals 1

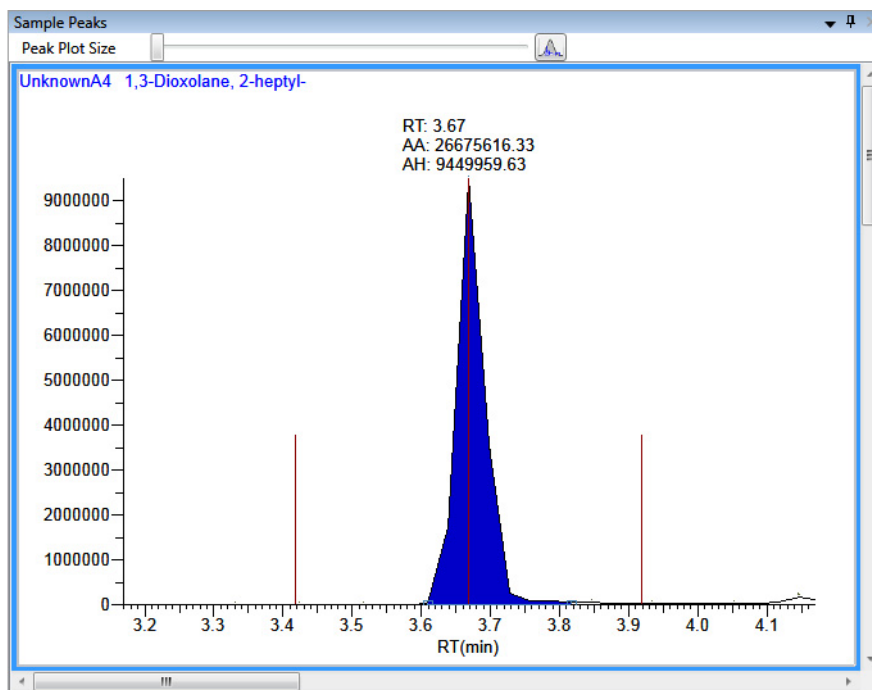
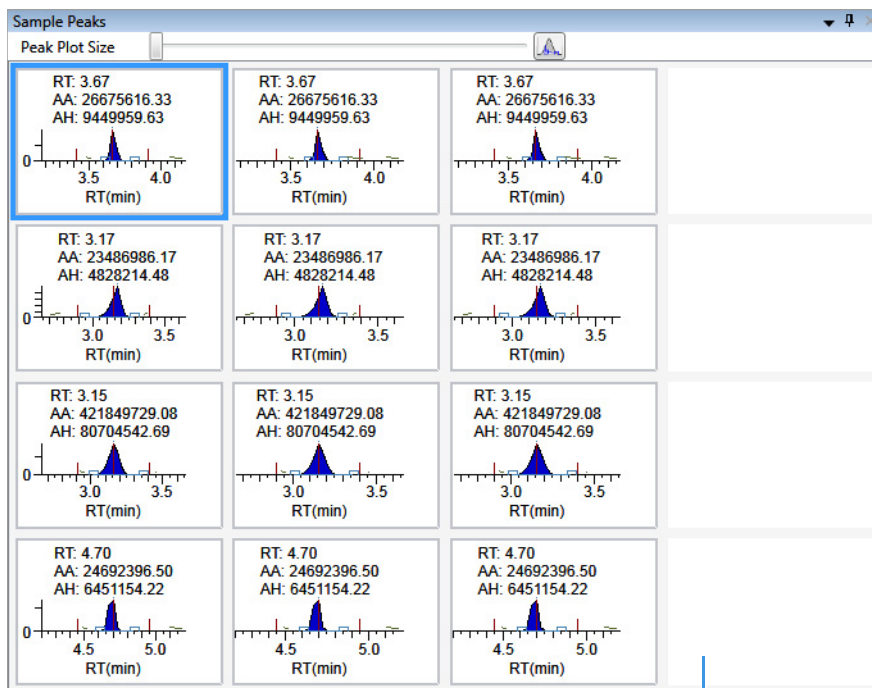


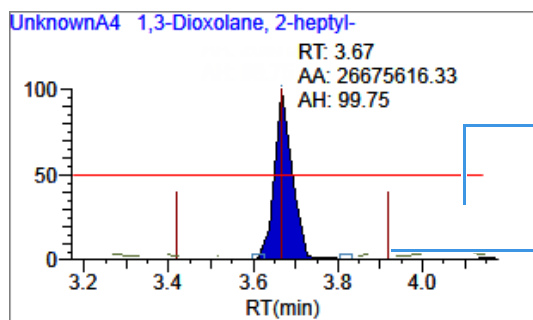
Figure 140. Number of Rows equals 4 and Number of Columns equals 4



Because there are only three samples, this column is empty.

3. To change the display type for the y -axis scale, select one of the following:

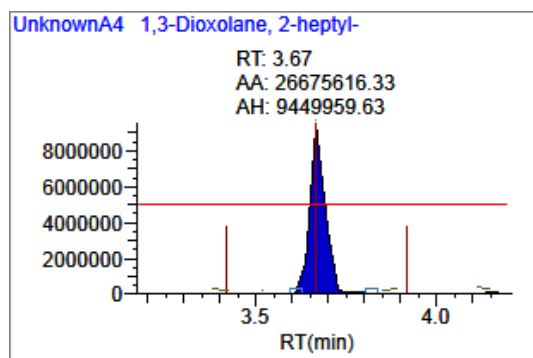
- **Relative:** Displays the y -axis scale from 0 through 100.



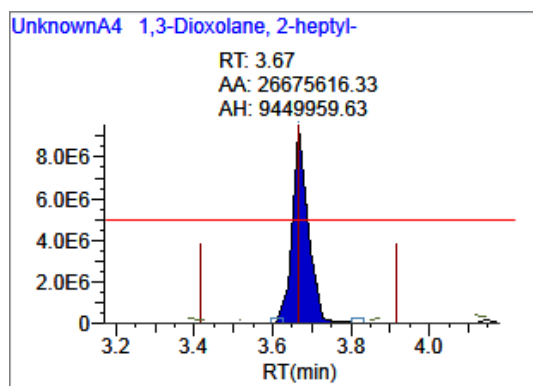
Horizontal bar indicates the threshold value as specified in the method.

Vertical bars indicate the expected retention time and window, as specified in the method.

- **Absolute:** Displays the y -axis scale from 0 to the actual value of the most intense peak in the group.



- **Label in Scientific Notation:** Displays the y -axis scale in scientific notation.



Note The Sample Peaks pane displays a y axis only in the first chromatogram in each row. The limits of the scale are determined by the most intense peak in the group.

4. Specify which labels you want to display in the sample peak plots.

For an example of all available peak plot labels, see [Peak Plot Labels](#).

Chromatogram Plot Settings Dialog Box

Use the Chromatogram Plot Settings dialog box to change the Sample Peaks pane display.

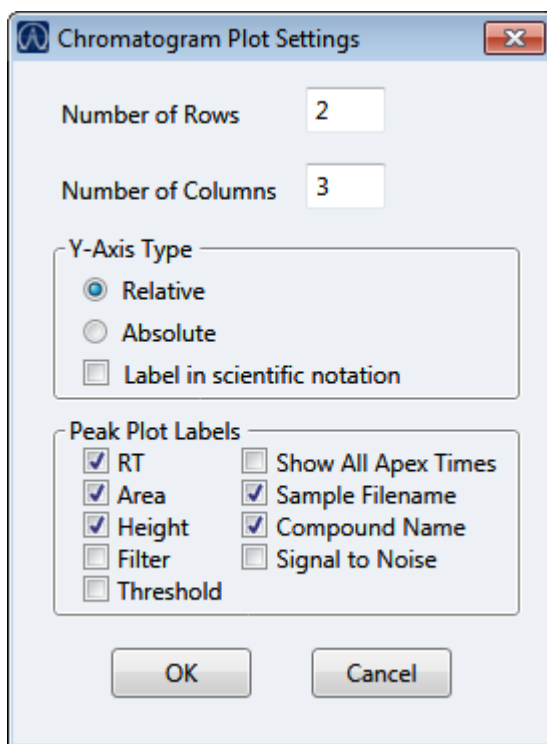


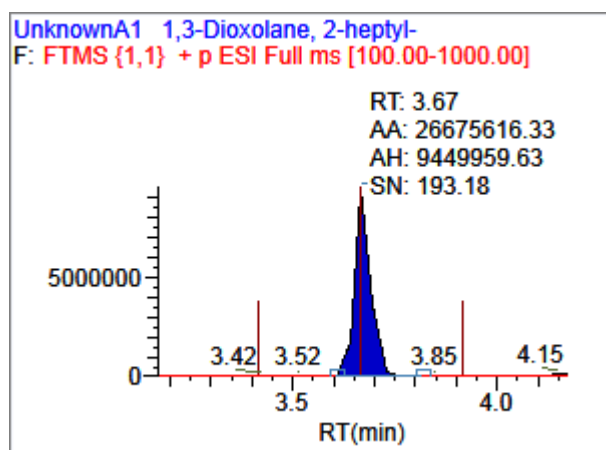
Table 108. Chromatogram Plot Settings dialog box parameters (Sheet 1 of 2)

Parameter	Description
Number of Rows	Specifies the number of rows visible in the Sample Peaks pane. When Number of Rows equals 1, the application scales the height of all chromatograms to fill the Y dimension of the Sample Peaks pane. Default: 3
Number of Columns	Specifies the number of columns visible in the Sample Peaks pane. When Number of Columns equals 1, the application scales the width of all chromatograms to fill the X dimension of the Sample Peaks pane. Default: 3
Y-Axis Type	Displays the <i>y</i> -axis scale as Relative (to the most intense peak), Absolute, or in scientific notation.

Table 108. Chromatogram Plot Settings dialog box parameters (Sheet 2 of 2)

Parameter	Description
Peak Plot Labels	Displays or hides the following peak labels: <ul style="list-style-type: none">• RT• Area• Height• Filter• Threshold• Show All Apex Times• Sample Filename• Compound Name• Signal to Noise

Example with all peak labels displayed:

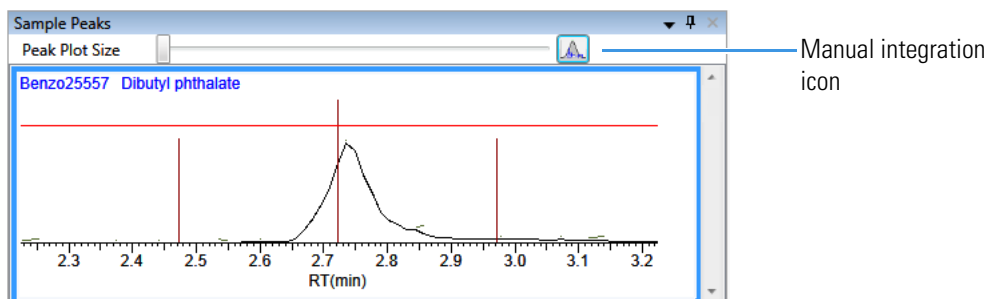


Manually Integrating Peaks

Use the manual integration feature to manually add a peak. You can manually add a peak in a chromatogram plot only when the application fails to identify a peak.

❖ To manually integrate a peak

1. In the Sample Peaks plot, click the **Manual Integration** icon.



The cursor changes to look like this:

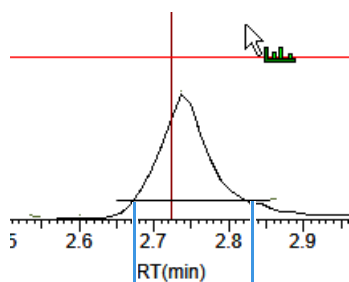


2. Integrate a peak as follows:

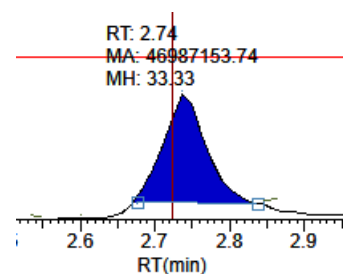
- a. Drag the cursor to define the beginning and ending base points for the new peak.

Note You must drag the cursor inside the x axis and y axis.

- b. Click outside the plot to refresh the display.



Click the first base point, and then drag to the second base point.



Click outside the plot to refresh the view.

The application identifies the peak and indicates the manual integration in the labels.

3. To zoom in on an area, do the following:

- a. Drag the cursor below the x axis or to the left of the y axis.

The plot zooms to fit the defined X or Y dimension into the entire pane. The application zooms all compounds in the row to the same scale.

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

Qualitative View

The Qualitative View uses several different panes to display qualitative information for the selected sample. See [Displaying Qualitative View Panes](#).

If the application finds no detected peaks for the selected sample, you can manually add peaks.

To see processed data for a sample in the Qualitative View, you must select the Qual Processing parameter for that sample in the Batch View before you process the batch. See “[Batch View Sample List](#)” on [page 415](#).

These are the default panes and their locations:

Samples pane

Flags	Status	Filename	Sample Type
	●	BuspironeB1 Unknown	
	●	BuspironeB2 Unknown	

Peaks pane

Filter: + c ESI Full ms [200.00-800.00]

Peak RT	SI	RSI	MP	Est Amt	Library Hit
1.63	161	570	4	0.000	Sulfasomizole

Sample chromatogram

Filter: + c ESI Full ms [200.00-800.00]

Relative Intensity vs RT(min)

Peak details

RT: 1.63
AA: 15933608054.13
AH: 664538778.45
SN: 146.16

Relative Intensity vs RT(min)

Spectrum

Relative Intensity vs m/z

Library hits

Rank	SI	RSI	MP	Library ε
=	=	=	=	Aa
1	332	978	0	2-Hexan
2	320	966	0	Sulfisom
3	314	959	0	Propane

Sample chromatogram pane

Peak Chromatogram pane

Spectrum pane

Library Hits pane

The Qualitative View displays data in the following panes:

- [Samples Pane](#)
- [Peaks Pane](#)
- [Sample Chromatogram Pane](#)
- [Peak Chromatogram Pane](#)
- [Spectrum Pane \(Library and Data\)](#)
- [Library Hits Pane](#)

Displaying Qualitative View Panes

The Qualitative View displays data using multiple panes: Samples, Peaks, Sample Chromatogram, Peak Chromatogram, Spectrum, and Library Hits. You can display, hide, or move any of these panes.

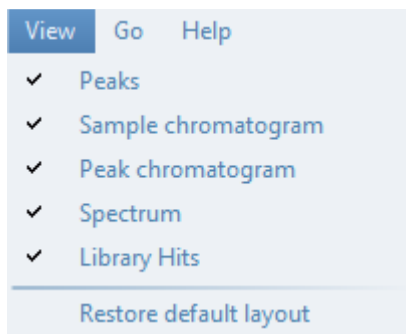
❖ To display or hide a Qualitative View pane

From the View menu, choose to display or hide the following:

- **Peaks**
- **Sample Chromatogram**
- **Peak Chromatogram**
- **Spectrum**
- **Library Hits**

Note The Samples pane is required for the Qualitative View display. You cannot hide the Samples pane.

A check mark indicates a displayed pane.




For procedures about creating docked, floating, or tabbed panes, see “[Moving Data Review Panes](#)” on [page 739](#).

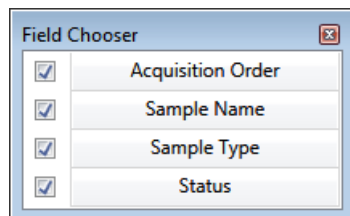
Samples Pane

Use the Samples pane in the Qualitative View to select a specific sample. The associated [Peaks Pane](#) displays all peaks found in the selected sample.

❖ To hide or display columns in the Samples pane

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Samples pane.



2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

The application immediately displays or hides the column in the Samples pane.


3. Click  to close the Field Chooser.

Figure 141. Samples pane

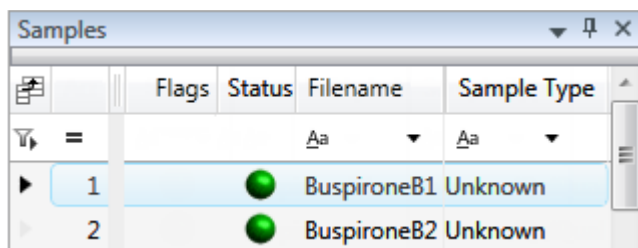









Table 109. Samples pane columns (Sheet 1 of 2)

Column	Description
Acquisition Order	Sequentially numbers the samples.
Flags	Caution flag displayed when a compound in the sample has an error. See “Caution Flags” on page 454.

Table 109. Samples pane columns (Sheet 2 of 2)

Column	Description
Status	<p> Sample is not acquired.</p> <p> Sample is acquired but not processed.</p> <p> Sample is acquired and processed.</p> <p> Sample is currently acquiring.</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed () and the Unknown Screening View shows the Status for the samples as acquired but not processed () .</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed () .</p>
Filename	A user-defined name that identifies a sample.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC Std, or Unknown.

Peaks Pane

The Peaks pane in the Qualitative View works with the Samples pane to display graphical values for a unique sample and peak combination. For detailed descriptions of parameters in the Peaks pane, see “Peaks Pane” on page 481.

Follow these procedures:

- [To display peaks for a specific compound](#)
- [To remove a peak](#)
- [To hide or display columns in the Peaks pane](#)

❖ To display peaks for a specific compound

1. From the Samples pane, select a sample.

The Peaks pane displays the retention times for peaks identified in the selected sample, the values for the best match methods for each peak, and the library match.

The method specifies which technique to use for identifying peaks: peaks within a specific retention time range, as a minimum percentage of the height or area of the largest peak, or as a minimum percentage of the nearest internal standard peak. You can change the method for identifying peaks in the Method Template Editor. See “Creating a Method Template” on page 243.

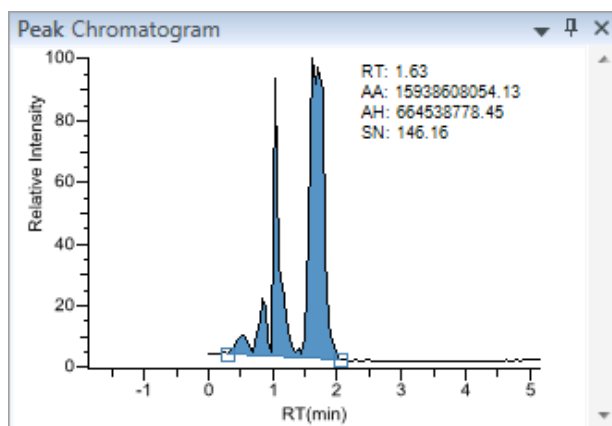
2. In the Peaks pane, select a peak in the sample.

Peaks						
Filter: + c ESI Full ms [200.00-800.00]						
Peak RT	SI	RSI	MP	Est Amt	Library Hit	
9.82	124	732	0	0.000	Phenomorphane	
1.63	161	570	4	0.000	Sulfasomizole	

The application displays the selected peak in the [Peak Chromatogram](#) pane, displays the Qual Data and Qual Library sections in the [Spectrum](#) pane, and locates the selected peak in the [Sample Chromatogram](#) pane.

- The Qual Data section shows spectrum data for the peak in the raw data file.
- The Qual Library section shows actual spectrum for the identified library compound.

Figure 142. Peak Chromatogram pane



Note 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.

Figure 143. Spectrum pane

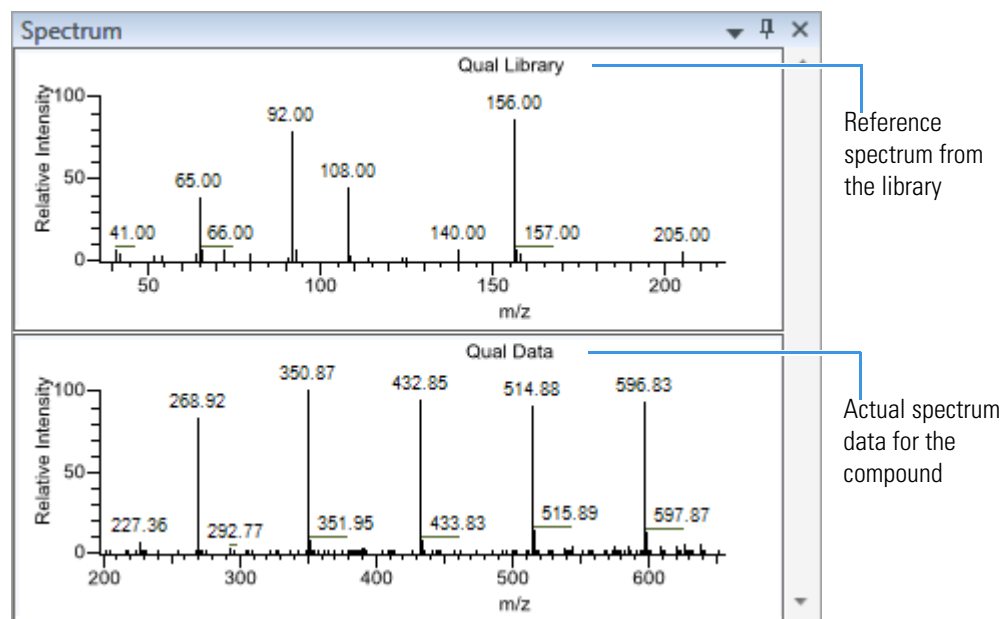
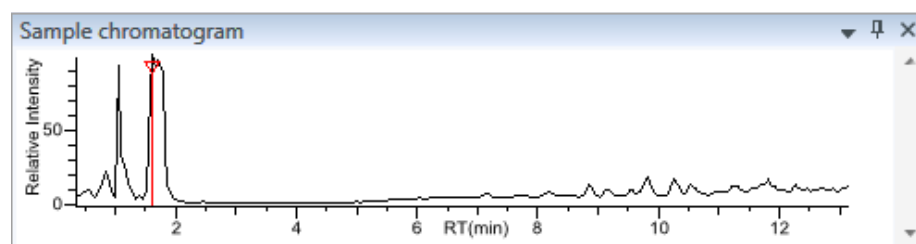


Figure 144. Selected peak in the Sample Chromatogram pane




❖ To remove a peak

1. Select a peak in the Sample Chromatogram pane.
2. Right-click the Peak Chromatogram pane and choose **Remove Qual Peak** from the shortcut menu.

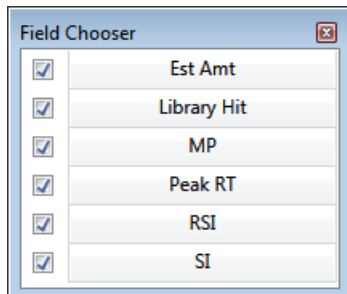
The application removes the selected peak from all Qualitative View panes.

Note There is no undo for this action, but you can manually add a peak to redefine a removed peak. See “[Sample Chromatogram Pane](#)” on [page 482](#).

❖ **To hide or display columns in the Peaks pane**


1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Peaks pane.



2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

The application immediately displays or hides the column in the Peaks pane.

3. When you are finished modifying the column display, click  to close the Field Chooser.

Peaks Pane

Use the features in the Peaks pane to display graphical values for each sample and peak combination.

Figure 145. Peaks pane

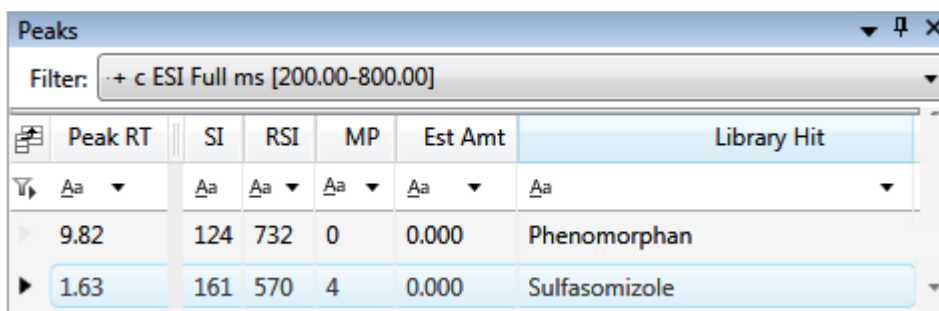
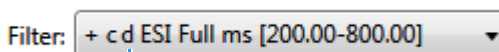


Table 110. Peaks pane parameters (Sheet 1 of 2)

Parameter	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

Table 110. Peaks pane parameters (Sheet 2 of 2)

Parameter	Description
Peak RT	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) A method used to search the NIST library. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
MP	Match probability.
Est Amt	Estimated amount of the compound.
Library Hit	Library compound that matches the identified peak.

Sample Chromatogram Pane

The Sample Chromatogram pane in the Qualitative View displays all peaks in the selected sample. The peak selected in the Peaks pane displays a red marker. See “[Sample Chromatogram Pane](#)” on page 484.

❖ To zoom in on a peak

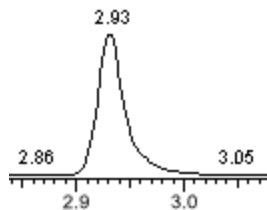
1. In the Sample Chromatogram pane, drag the cursor to delineate a rectangle around the peak.

The delineated area expands to fill the view.

2. To restore the default view, right-click the Sample Chromatogram pane and choose **Reset Scaling** from the shortcut menu.

❖ To manually add a peak

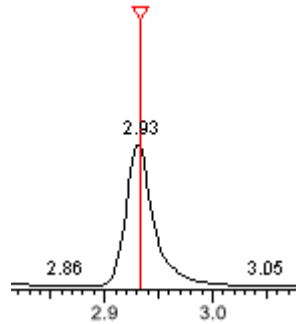
1. Zoom in to better identify which peak to add to the results set.



2. Right-click the Sample Chromatogram pane, and choose **Add Qual Peak** from the shortcut menu.

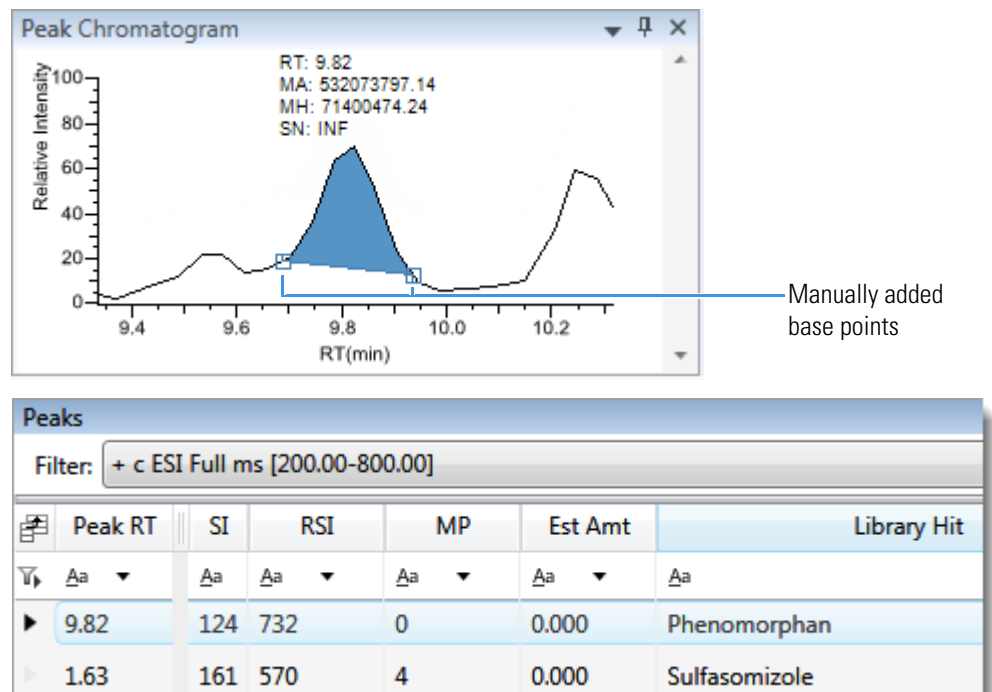
- Click to indicate the left and right base points for the peak.

The application marks the peak in the Sample Chromatogram pane.



The application places the peak delimiter tags at the base point locations and automatically updates the peak values in the Peaks pane and Peak Chromatogram pane. See [Peak Chromatogram pane with a manually added peak](#).

Figure 146. Peak Chromatogram pane with a manually added peak



Sample Chromatogram Pane

Use the features in the Sample Chromatogram pane to display peaks in the selected sample.

Figure 147. Sample Chromatogram pane

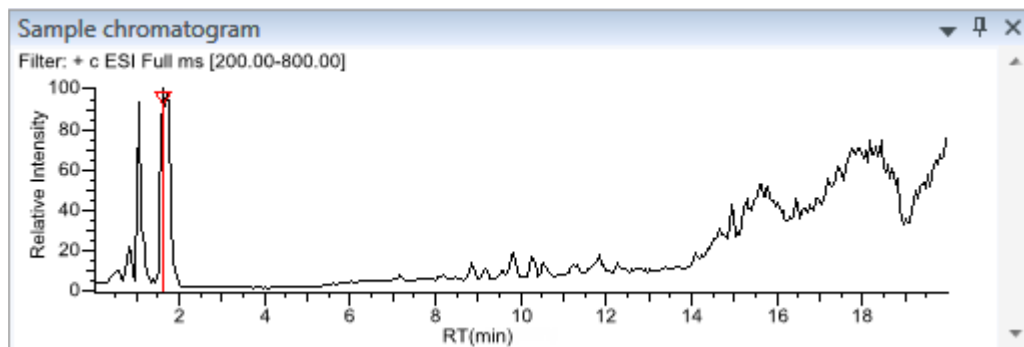


Table 111. Sample chromatogram pane shortcut menu commands

Command	Description
Add Qual Peak	Select the beginning and ending base points for a new qualitative peak. Available only when no peak is detected.
Reset Scaling	Resets the original scaling after a zoom operation.

Peak Chromatogram Pane

The Peak Chromatogram pane in the Qualitative View displays the selected peak. For a description of commands in the shortcut menu, see “Peak Chromatogram Pane” on page 486.

Follow these 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](#)

❖ 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.

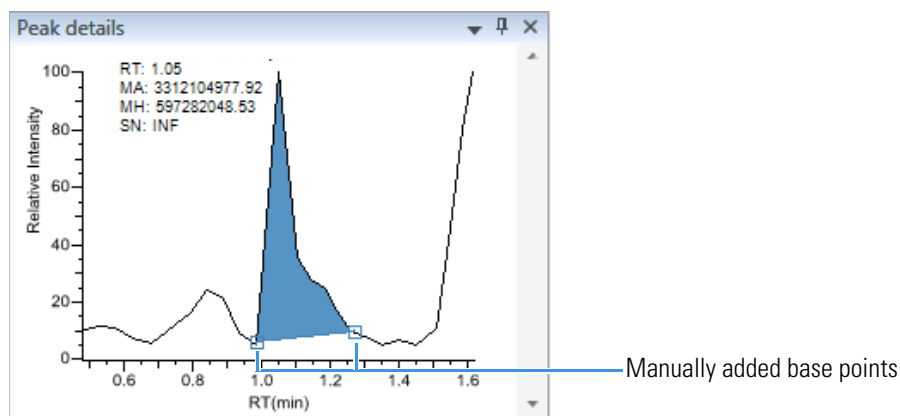
❖ To manually add a peak

1. Right-click anywhere in the Peak Chromatogram pane, and choose **Add Qual Peak** from the shortcut menu.

If a peak is already detected, the Add Qual Peak command is not activated.

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 peak

Right-click the Peak Chromatogram pane, and choose **Remove Qual Peak** from the shortcut menu.

The application removes the peak displayed in the Peak Chromatogram pane. All data for this peak are removed from the Qualitative View panes.

❖ To switch between method and manual integration modes

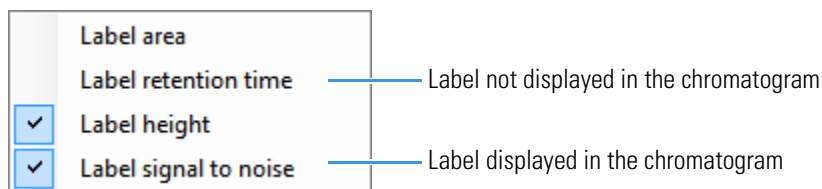
Right-click the Peak Chromatogram pane and choose either **Method Integration** or **Manual Integration** from the shortcut menu.

Initially, the method integration and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the Peak Chromatogram plots update and the result set updates 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 Peak Chromatogram pane and hold the cursor over **Peak Labels**.
2. Choose to display labels for the peak retention time (RT), peak height (AH), peak area (AA), or signal-to-noise (SN).



3. To remove a label, choose the label type again to clear it.

Peak Chromatogram Pane

Use the features in the Peak Chromatogram pane to display the selected peak.

Figure 148. Peak Chromatogram pane

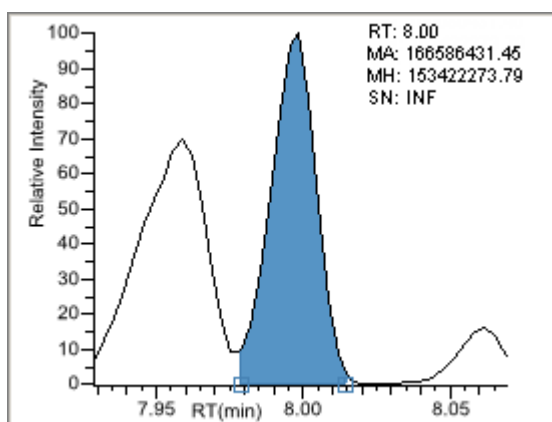


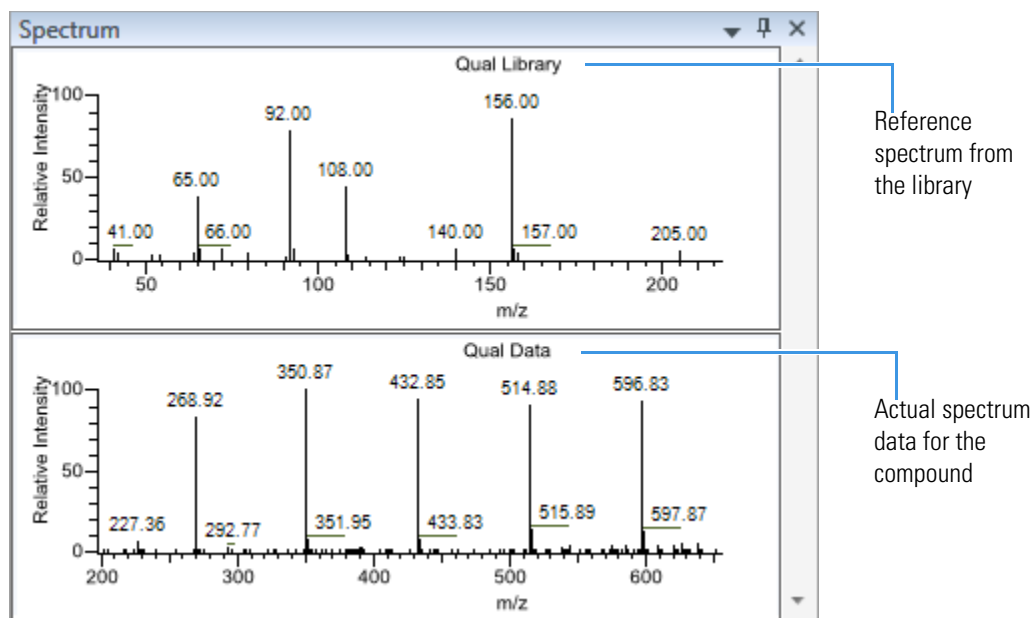
Table 112. Peak Chromatogram pane shortcut menu commands

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 to Noise).
Remove Qual Peak	Available only for manually added peaks. Removes the peak displayed in the Peak Chromatogram pane.

Spectrum Pane (Library and Data)

The Spectrum pane in the Qualitative View displays the reference spectrum from the library and the spectrum data for the selected sample. The top pane displays the spectrum for the identified compound found in the reference library; the bottom pane displays the actual spectrum data for the selected peak.

Figure 149. Spectrum pane



❖ To zoom in on a peak

1. In either spectrum 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 spectrum plot and choose **Reset Scaling** from the shortcut menu.

Library Hits Pane

The Library Hits pane in the Qualitative View displays the best library matches for the selected peak. Use this pane to select a different library entry for the peak. For detailed descriptions of the Library Hits pane parameters, see [Library Hits pane](#).

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	7.95	13829174	10605061	0.000	0.000	P

P flag

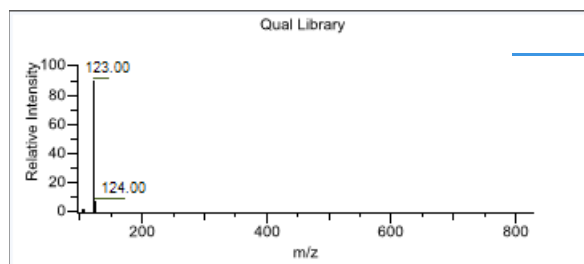
❖ To change the library entry for a selected peak

In the Library Hits pane, select the check box for the library entry that you want to use to identify the selected peak.

- In the Spectrum pane, the reference spectra change to show the spectra for the selected library entry.
- In the Peaks pane, the SI, RSI, MP, and Compound values update to reflect the selected library entry.

Rank	SI	RSI	MP	Library entry	
<input type="radio"/>	=	=	=	Aa	
<input checked="" type="radio"/>	1	332	978	0	2-Hexanone
<input type="radio"/>	2	320	966	0	Succinic anhydride
<input type="radio"/>	3	314	959	0	Propane, 1-(ethenyl-oxo)-

Selected library entry in the Library Hits pane



Reference spectra for Hexanone

Peak RT	SI	RSI	MP	Est Amt	Library Hit
0.00	332	978	0	0.000	2-Hexanone
4.46	145	860	0	0.000	Methane, bis(2-chloroethoxy)-

Peak list for Hexanone

Figure 150. Library Hits pane

<input type="checkbox"/>	Rank	SI	RSI	MP	Library entry
<input type="radio"/>	=	=	=	=	Aa
<input checked="" type="radio"/>	1	332	978	0	2-Hexanone
<input type="radio"/>	2	320	966	0	Succinic anhydride
<input type="radio"/>	3	314	959	0	Propane, 1-(ethenyloxy)-:

Table 113. Library Hits pane parameters

Parameter	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) A method used to search the NIST library.
RSI	(Reverse search index) A method used to search the NIST library. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
MP	Match probability.
Library Entry	Library compound that matches the identified peak.

Features Common to All Data Review Pages

The following parameters and features are common to all quantitation batch data review pages:

- [Common Column Parameters](#)
- [Inactive and Excluded Compounds](#)
- [Compound Details](#)
- [Exporting Compounds](#)

Common Column Parameters

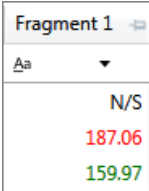
Table 114. Common parameters for Compound Results and Sample Results tables (Sheet 1 of 7)

Column	Description
%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.
%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. Note This RSD value is not the same as the RSD value used with the Average RF curve type in the method. See “Calibration” on page 204. The application uses this %RSD value in Data Review and in the Compound Calibration Report when you acquire multiple samples for the same QC Std or Cal Std samples.
Active	Displays or hides a compound for a particular sample. <ul style="list-style-type: none"> • When a compound is marked inactive, the application does not remove its data and calculated values from the result set. Instead, the application masks the appearance of that compound for that particular sample and grays the compound in the compounds list. • 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 Compound Details pane. It is no longer part of the result set. <p>In a Sample View, the Active parameter is in the Compound Results pane.</p> <p>In a Compound View, the Active parameter is in the Sample Results pane.</p>
Acquisition Order	Sequentially numbers the samples.

Table 114. Common parameters for Compound Results and Sample Results tables (Sheet 2 of 7)

Column	Description																								
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.																								
Adduct	The most intense adduct for the retention time for a compound.																								
Area	The area obtained by integrating peak intensities from the start to the end of the peak. When the Response Ratio is specified as Area, this column displays an asterisk (*Area).																								
Calculated Amt	The amount present in the sample, as determined using the calibration curve and the response ratio.																								
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. The Channel column is available only when you have activated multiplexing in the Configuration console. See “Multiplexing” on page 61.																								
Confirm	The number of criteria confirmed out of the total number specified in the method.																								
Expected RT	Expected retention time for the compound.																								
FI	<p>Fragment Ions flag. The application displays one of these indicators:</p> <ul style="list-style-type: none"> • A green circle (pass) when the measured m/z value of any of the fragments is within the mass tolerance specified in the method. On the Isotopes page in the Spectrum pane, the All Isotopes and Multi-Isotopes flags are also green. • A red square (fail) when the measured m/z value of none of the fragments is within the mass tolerance specified in the method. On the Isotopes page in the Spectrum pane, the All Isotopes and Multi-Isotopes flags are also red. • A blank when there are no fragments detected. <p>To display a list of fragments and their pass/fail status, hold your cursor over the indicator.</p> <table border="1"> <thead> <tr> <th>Frag #</th> <th>Found</th> <th>Expected m/z</th> <th>Measured m/z</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>●</td> <td>159.97000</td> <td>159.97183</td> </tr> <tr> <td>2</td> <td>●</td> <td>182.02000</td> <td>182.02444</td> </tr> <tr> <td>3</td> <td>■</td> <td>132.96000</td> <td>132.96091</td> </tr> <tr> <td>4</td> <td>■</td> <td>160.98000</td> <td>0.00000</td> </tr> <tr> <td>5</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	Frag #	Found	Expected m/z	Measured m/z	1	●	159.97000	159.97183	2	●	182.02000	182.02444	3	■	132.96000	132.96091	4	■	160.98000	0.00000	5			
Frag #	Found	Expected m/z	Measured m/z																						
1	●	159.97000	159.97183																						
2	●	182.02000	182.02444																						
3	■	132.96000	132.96091																						
4	■	160.98000	0.00000																						
5																									
Filename	Name of the raw data file that contains the sample data.																								
Final Units	Specifies the calculated amount. Default: 1																								

Table 114. Common parameters for Compound Results and Sample Results tables (Sheet 3 of 7)

Column	Description
Flag Details	Indicates all errors found in the compound. Type of error: <ul style="list-style-type: none"> • I: Confirming ion coelution failure • A: Amount error • B: Matrix blank error • PK: Peak not found • LS: Library matching error • IP: Isotope error • FI: Fragment ions error • IR: Ion ratio error
Flags	Caution flag displayed when a compound within the sample has an error.
Formula	The formula for the peak as specified in the compound database.
Fragment <i>n</i>	Displays the measured <i>m/z</i> for the fragment ion. The application displays a separate column for each found fragment. <ul style="list-style-type: none"> • For each fragment found in the compound database that passes the filter in the method, the Compounds table displays the <i>m/z</i> value in green text. • For each fragment found in the compound database that does not pass the filter in the method, the Compounds table displays the <i>m/z</i> value in red text. • For each fragment that is not found in the compound database, the Compounds table displays N/S (none specified).  <ul style="list-style-type: none"> — N/S: Fragment not found in the compound database — 187.06: Fragment found but does not meet method parameters — 159.97: Fragment found and meets method parameters
Fragment <i>n</i> (Delta (ppm/mmu))	The difference between the expected fragment ion <i>m/z</i> from the compound database and the measured fragment ion <i>m/z</i> . The application displays a separate delta column for each identified fragment.
Group	Threshold group to which a sample belongs. You can view samples by group in the Comparative View of Data Review.
Height	The distance from the peak maximum to the peak base, measured perpendicular to the ordinate. When the Response Ratio is specified as Height, this column displays an asterisk (*Height).
Integration Mode	Integration mode specified in the method. See “ Quan Peak ” on page 499 .

Note Compounds can have a maximum of five fragments, and the Compounds table has a maximum of five Fragment columns. When a compound contains fewer than five fragments, all remaining Fragment columns display N/S.

Table 114. Common parameters for Compound Results and Sample Results tables (Sheet 4 of 7)

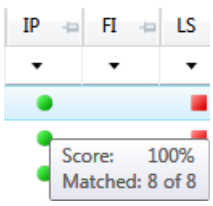
Column	Description
IP	<p>Isotopic Pattern flag. The application displays one of these indicators:</p> <ul style="list-style-type: none"> • A green circle (pass) when the score percentage is higher than the specified fit threshold percentage. • A red square (fail) when the score percentage is lower than the specified fit threshold percentage. • A blank when the parameter is not scored. <p>To display the score of matched isotopes, hold your cursor over the indicator.</p> 
IR	<p>Ion Ratio flag. The application displays one of these indicators:</p> <ul style="list-style-type: none"> • A green circle when the ion ratio is within the acceptable ion ratio range. • A red square when the ion ratio is not within the acceptable ion ratio range.
Isotopic Pattern Score (%)	The percentage of the number of total isotopes to the number of matched isotopes.
ISTD Amt	Amount of internal standard.
ISTD Response	Response of the internal standard.
Lib Match Name	<p>The name of the best matching compound in the library search. When the application finds a match in the library, this column displays the matching library entry with the highest score.</p> <ul style="list-style-type: none"> • When the application does not perform a library search, this column displays “N/A” in black text. • When the application does not perform an MS/MS scan, this column displays “N/A” in red text.








Table 114. Common parameters for Compound Results and Sample Results tables (Sheet 5 of 7)

Column	Description
Library Match Rank	<p>Displays the ranking of the library match. When the application finds a match in the library, this column displays the library entry's relative rank, in the format "x of y", where</p> <ul style="list-style-type: none"> x = the rank of the highest scoring library match. y = the total number of library matches from the list of matches for a particular adduct that contains the highest scoring match. <p>Results are as follows when the application performs both a library search and an MS/MS scan and both the library entry and the formula match the target compound:</p> <ul style="list-style-type: none"> A library score that is higher than or equal to the score threshold meets the criteria, and the values in this column appear in green. A library score that is lower than the score threshold fails to meet the criteria, and the values in this column appear in red. <p>When the application does not perform a library search, this column displays "N/A" in black text.</p> <p>When the application does not perform an MS/MS scan, this column displays "N/A" in red text.</p>
Library Score (%)	<p>The score from the library fit. When the application finds a match in the library, this column displays the highest score associated with the Lib Match Name parameter.</p> <p>Results are as follows when the application performs both a library search and an MS/MS scan and both the library entry and the formula match the target compound:</p> <ul style="list-style-type: none"> A library score that is higher than or equal to the score threshold meets the criteria, and the values in this column appear in green. A library score that is lower than the score threshold fails to meet the criteria, and the values in this column appear in red. <p>When the application does not perform a library search, this column displays "N/A" in black text.</p> <p>When the application does not perform an MS/MS scan, this column displays "N/A" in red text.</p> <p>Valid range: 1 through 100%</p>
LS	<p>Library Search flag. The application displays one of these flags:</p> <ul style="list-style-type: none"> A green circle when the library search is successful. A red square when the library search is not successful.
<i>m/z</i> (Apex)	<p>Mass-to-charge ratio found in the spectra for the peak. Assumes that the charge is 1.</p> <p>When the application successfully integrates the peak, this column displays the charged <i>m/z</i> value for the compound, which is the highest intensity in the apex scan.</p> <p>When the application cannot successfully integrate the peak, this column displays "N/F" (not found).</p>

Table 114. Common parameters for Compound Results and Sample Results tables (Sheet 6 of 7)

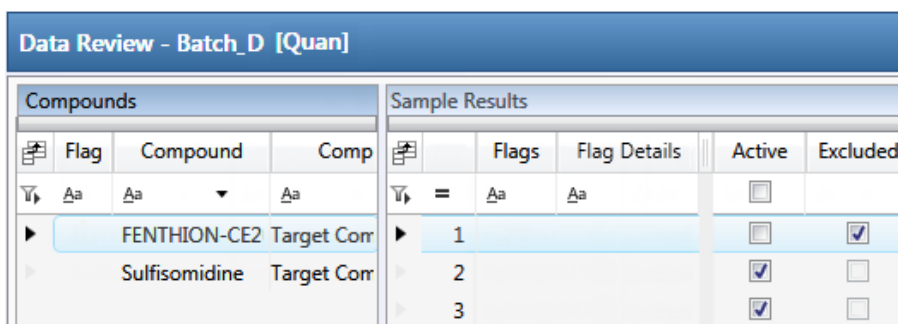
Column	Description
<i>m/z</i> (Delta (mmu))	<p>Difference between the <i>m/z</i> (Expected) and <i>m/z</i> (Apex). Assumes that the charge is 1.</p> <p>When the <i>m/z</i> (Apex) column displays <i>m/z</i> value for the compound, this column displays the delta <i>m/z</i> corresponding to the highest intensity in the apex scan.</p> <ul style="list-style-type: none"> When the mass tolerance is specified in ppm in the master method, then $m/z \text{ (Delta)} = 1\,000\,000 \times ([m/z \text{ (Apex)} - m/z \text{ (Expected)}] \times m/z \text{ (Expected)})$. When the mass tolerance is specified in mmu in the master method, then $m/z \text{ (Delta)} = 1000 \times m/z \text{ (Apex)} - m/z \text{ (Expected)}$.
<i>m/z</i> (Expected)	<p>Mass-to-charge ratio from the compound database. Assumes that the charge is 1.</p> <ul style="list-style-type: none"> When an adduct is found, the application displays the neutral mass value for the compound (calculated from the neutral formula) \pm the mass of the most intense adduct ion found for the compound. When no adduct is found, the application displays the neutral mass value for the compound \pm the mass of the first adduct entered in the compound database. <p>For details about defining adducts for the compound database, see “Specifying Adducts” on page 53.</p> <p>For details about adding adducts to compounds, see “Editing Compounds in the Database” on page 84.</p> <p>Note When the adduct is a gain, the adduct mass is a positive number. When the adduct is a loss, the adduct mass is a negative number. The resulting mass value after adding or subtracting the adduct mass is always a positive number.</p>
Num Isotopes Matched	<p>The number of isotopes matched in the expected calculated isotope spectra relative to the total number of isotopes used in the score calculation, in the format “x of y”, where</p> <ul style="list-style-type: none"> x = the number of isotopes matching the elemental composition used for the Isotopic Pattern Score calculation. y = the total number of isotopes considered in the Isotopic Pattern Score calculation. This is the number of isotope peaks expected to be above the spectral noise.
PK	<p>Peak found</p> <p>The application displays one of these flags:</p> <ul style="list-style-type: none"> A green circle when the peak is found. A red square when the peak is not found.
Response Ratio	<p>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.</p>
RT Delta	<p>Difference between the expected retention time and the measured retention time.</p>

Table 114. Common parameters for Compound Results and Sample Results tables (Sheet 7 of 7)

Column	Description
Sample Amt	The injected volume multiplied by the conversion factor. For example, if you have 1000 ng/mL of a substance that is too concentrated for the mass spectrometer, you can dilute it by 1000. Then your injection volume is 1, your conversion factor is 1000, and your sample amount is 1000.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC Std, or Unknown.
Status	<p> Sample is not acquired.</p> <p> Sample is acquired but not processed.</p> <p> Sample is acquired and processed.</p> <p> Sample is currently acquiring.</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed () , and the Unknown Screening View shows the Status for the samples as acquired but not processed () .</p> <p>Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed () .</p>
Theoretical Amt	Theoretical amount of the compound expected in the sample.
Excluded	Turns a compound on or off in the calibration curve in the Compound Details pane.

Inactive and Excluded Compounds

Use the Active and Excluded columns to control which compounds are used for calculating the calibration curve and for reporting.



Data Review - Batch_D [Quan]						
Compounds				Sample Results		
Flag	Compound	Comp	Flags	Flag Details	Active	Excluded
Aa	FENTHION-CE2 Target Corr	Aa	1		<input type="checkbox"/>	<input checked="" type="checkbox"/>
	Sulfisomidine Target Corr		2		<input checked="" type="checkbox"/>	<input type="checkbox"/>
			3		<input checked="" type="checkbox"/>	<input type="checkbox"/>

Follow these 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 Sample Results pane.

All compounds in the selected sample appear 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.
 - When a compound is marked inactive, the application does not remove its data and calculated values from the result set. Instead, the application masks the appearance of that compound for that particular sample and grays the compound name in the compounds list.
 - 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. The calibration point is no longer part of the result set.
3. In the Sample Results pane, select or clear the **Active** check box.

Use the horizontal scroll bar at the bottom of the table to scroll to the Active column.

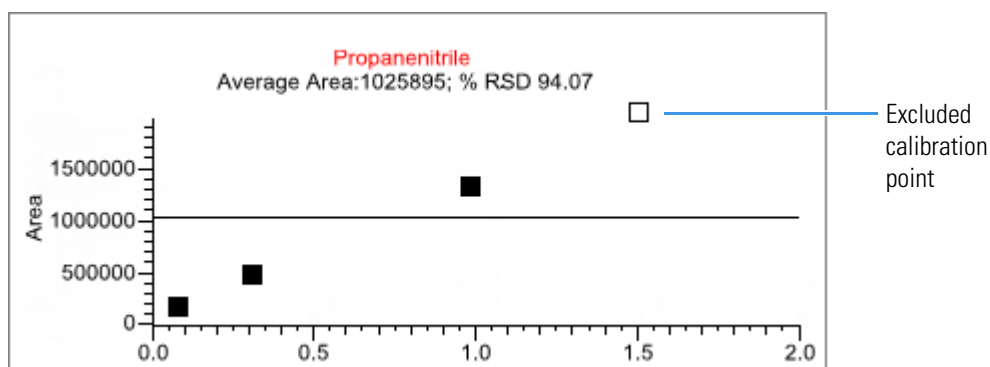
❖ To exclude a calibration point

In the sample list, select the **Excluded** check box for the sample.

Note Only calibration samples have the Excluded check box available.

Use the horizontal scroll bar at the bottom of the table to scroll to the Excluded column.

The application displays a value that is no longer used for calibration as an empty box in the graphical view of the calibration curve.



Compound Details

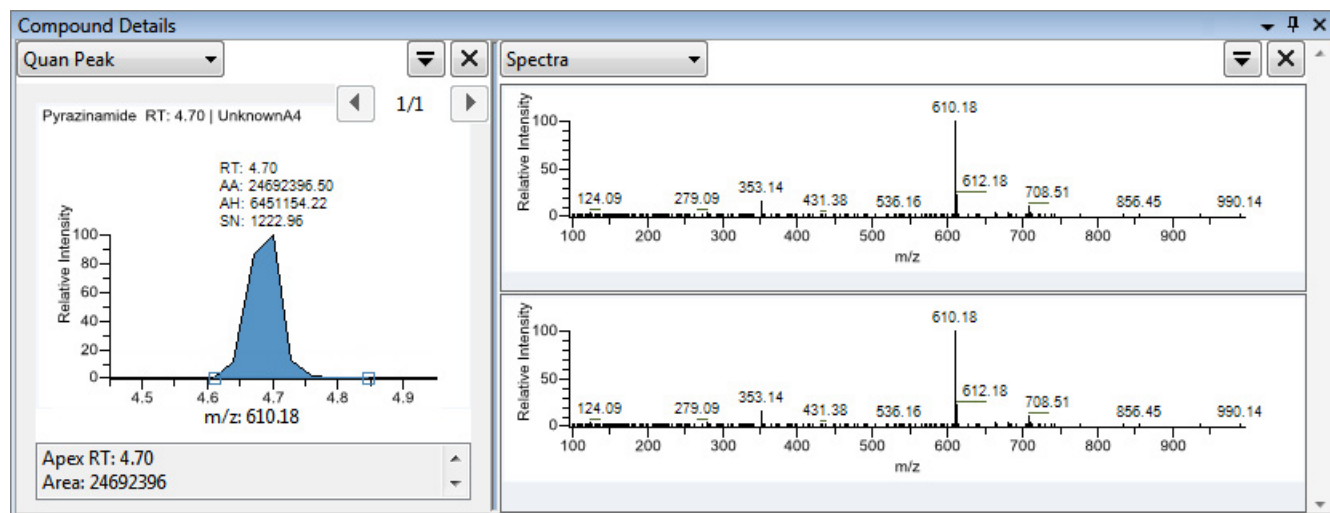
Use the Compounds Details pane to display any of the following types of data:

- [Quan Peak](#)
- [Confirming Ions](#)
- [Calibration Curve](#)
- [Ion Overlay](#)
- [ISTD](#)
- [Reference Peak](#)
- [Spectra](#)
- [Library Match](#)
- [Isotope](#)
- [Fragments](#)

❖ To open the Compound Details pane

1. Double-click the chromatogram in the Sample Peaks pane.

The Compound Details pane opens.



By default, the first display pane shows the quantitative peak for the selected compound.

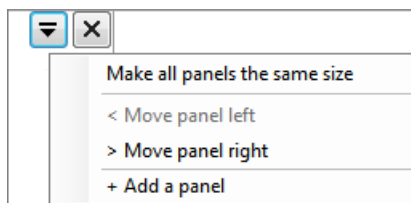
2. In the second pane, select the additional type of data that you want to display.

Follow these procedures to change the display of the peak data in either of the panes:

- [To change the peak panes](#)
- [To zoom in on a peak](#)

❖ **To change the peak panes**

In any of the peak panes, click  to view a list of commands.



Command	Description
Make All Panels the Same Size	Evenly divides the area to make all panes the same width. This command does not change the pane height.
Move Panel Left	Moves the current panel one space to the left. This command is not available when the current pane is the leftmost pane.
Move Panel Right	Moves the current panel one space to the right. This command is not available when the current pane is the rightmost pane.
Add a Panel	Adds an empty peak pane to the display. You can display a maximum of four peak panes.

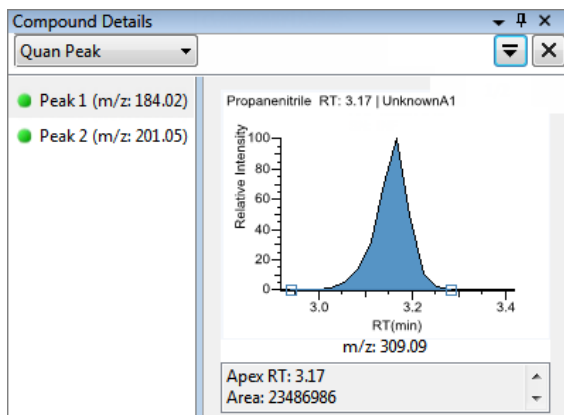
❖ **To zoom in on a peak**

1. In any of the views, drag your cursor to delineate a rectangle around the peak or spectra. 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.

Quan Peak

A compound can have multiple quantitative peaks. You can switch between quantitative peaks, but you cannot view multiple quantitative peaks at the same time. The Quan Peak pane uses a unique shortcut menu. See “[Quan Peak pane shortcut menu commands](#)” on page 503.

Figure 151. Quantitative peak pane with multiple quantitative peaks



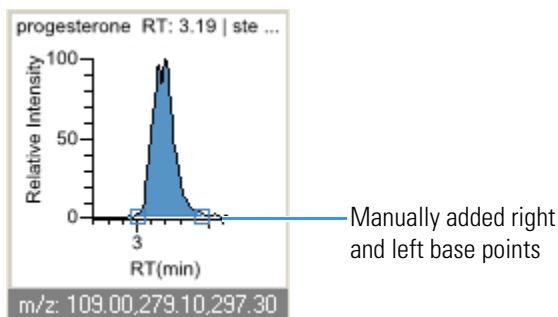
Follow these procedures to modify the quantitative or confirming ion peak data:

- To manually add a peak
- To remove a manually created peak
- To switch between method and manual integration modes
- To change the displayed information for detected peaks
- To modify the peak detection settings

❖ To manually add a peak

1. Right-click anywhere in the quantitative peak pane, and choose **Add Quan Peak** from the shortcut menu.
2. Click the left base of the peak that you want to identify.
3. Drag to the right base and release the mouse.

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 pane, and choose **Cancel Add Peak** from the shortcut menu.

The application cancels the Add Peak operation. If you have already completed adding the peak, select the peak and then choose **Remove Quan Peak** from the shortcut menu.

❖ To manually integrate a quantitative peak

1. Hold your cursor over one of the two peak delimiter tags in the 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 peak delimiter tag to another location and automatically update the peak values (area, height, and so forth) into the result set.

The generated reports for these data identify the manual modifications.

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 application originally calculates the method values based on the processing method parameters. The manual values are a result of what you have edited.

❖ To switch between method and manual integration modes

Right-click the chromatogram view and choose either **Method Integration Settings** or **Manual Integration Settings** from the shortcut menu.

Initially, the method integration and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the chromatogram plots update and the result set updates 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 peak pane 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 are cleared for labels that are not displayed.

3. To remove a label, choose the label type again and clear it.

Label settings are globally applied to quantitative peaks, confirming ion 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

- Right-click the chromatogram view and choose one of the following from the shortcut menu:
 - Peak Detection Settings > Edit Local Method Peak Detection Settings:** Makes changes to the selected compound for all samples in this batch.
 - Peak Detection Settings > Edit User Defined Peak Detection Settings:** Makes changes to the selected compound for only the selected sample. The application saves these changes with the batch and stops applying the local method detection settings to the compound for this sample only.

The Peak Detection Settings dialog box opens where you can adjust detection settings that were specified in the method. The title bar of the dialog box lists the selected compound and indicates whether you are making changes to only the selected sample or to the local method.

Figure 152. Peak Detection Settings dialog box



2. Edit any of the detection settings.

For detailed descriptions of all detection settings, see “Detection” on page 154.

3. To save your changes to this compound, click **Apply**.

- When you are editing a single sample, the application makes changes to the selected compound for this sample. If the sample is a calibration sample type, this update changes the calibration curve which, in turn, affects all calculated amounts.
- When you are editing the local method, the application makes changes to the selected compound for all samples in this batch.

Note The Peak Detection Settings commands are also available in the Confirming Ions pane.

Table 115. Quan Peak pane shortcut menu commands (Sheet 1 of 2)

Command	Description
Method Integration Settings	<p>Use Local Method Peak Detection Settings: Applies the local method integration settings to the selected compound.</p> <p>To edit these peak detection settings, use the Peak Detection Settings > Edit Local Method Peak Detection Settings command.</p> <p>Use User Peak Detection Settings: Applies the user-customized method integration settings to the selected compound.</p> <p>To edit these user-customized settings, use the Peak Detection Settings > Edit User Defined Peak Detection Settings command.</p>
Manual Integration Settings	Displays manual integration settings.
Add Quan Peak –or– Remove Quan 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. Not available for analog compounds.
Send RT to Method	Sets the current retention time as the expected retention time for the compound in the local method.
Peak Labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).

Table 115. Quan Peak pane shortcut menu commands (Sheet 2 of 2)

Command	Description																																								
Show Peak Info	Displays peak information for the selected compound, as in this example: <div data-bbox="769 417 1214 831" data-label="Table"> <table border="1"> <thead> <tr> <th colspan="4">Propanenitrile</th> </tr> </thead> <tbody> <tr> <td>Quan ion m/z:</td> <td></td> <td></td> <td>309.09</td> </tr> <tr> <td>Integration mode:</td> <td></td> <td></td> <td>Method</td> </tr> <tr> <td>Left RT:</td> <td>2.94</td> <td>Area:</td> <td>23486986</td> </tr> <tr> <td>Apex RT:</td> <td>3.17</td> <td>Height:</td> <td>4828214</td> </tr> <tr> <td>Right RT:</td> <td>3.28</td> <td>Noise:</td> <td>0.00</td> </tr> <tr> <td>Data file:</td> <td colspan="3">UnknownA3</td> </tr> <tr> <td>Filter:</td> <td colspan="3">FTMS {1,2} + p ESI Full ms2</td> </tr> <tr> <td>Detector:</td> <td colspan="3">MS</td> </tr> <tr> <td>Trace:</td> <td colspan="3">Mass range</td> </tr> </tbody> </table> </div>	Propanenitrile				Quan ion m/z:			309.09	Integration mode:			Method	Left RT:	2.94	Area:	23486986	Apex RT:	3.17	Height:	4828214	Right RT:	3.28	Noise:	0.00	Data file:	UnknownA3			Filter:	FTMS {1,2} + p ESI Full ms2			Detector:	MS			Trace:	Mass range		
Propanenitrile																																									
Quan ion m/z:			309.09																																						
Integration mode:			Method																																						
Left RT:	2.94	Area:	23486986																																						
Apex RT:	3.17	Height:	4828214																																						
Right RT:	3.28	Noise:	0.00																																						
Data file:	UnknownA3																																								
Filter:	FTMS {1,2} + p ESI Full ms2																																								
Detector:	MS																																								
Trace:	Mass range																																								
Reset Scaling	Resets the original scaling after a zoom operation.																																								
Peak Detection Settings	<p>Edit User Defined Peak Detection Settings: Opens the Peak Detection Settings dialog box where you can make changes to the selected compound for this sample.</p> <p>Edit Local Method Peak Detection Settings: Opens the Peak Detection Settings dialog box where you can make changes to the selected compound for all samples in this batch.</p> <p>After you apply either of these updates, the application does not retain manual integration settings.</p>																																								

Confirming Ions

The Confirming Ions pane displays a list of peaks, a graphical view of all qualifying/confirming ions for the selected compound, and calculated ion ratios and ion ratio acceptance windows. A red border indicates that an ion ratio is outside of its window. See “Quantitative peak with multiple confirming ions” on page 507. The Confirming Ions pane uses a unique shortcut menu. See “Confirming Ions pane shortcut menu commands” on page 508.

In the peaks list, the application displays the mass of each confirming ion peak. When a peak is within the tolerance set, the peak status is green. When a peak is not within the tolerance set, the peak status is red.

Note For compounds with an analog detection type, the application displays “No Confirming Ions are Enabled” in the Confirming Ions pane.

Follow these procedures:

- To zoom in on a peak
- To remove a peak
- To customize the labels in the display
- To display surrounding apex times
- To manually integrate a peak
- To switch between method and manual integration modes

❖ **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 remove a peak**

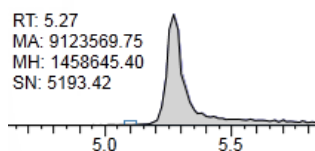
Right-click the Confirming Ions pane, and choose **Delete Peak** from the shortcut menu.

The application removes the peak displayed in the Confirming Ions pane. All data for this peak are removed from the Compound View panes.

❖ **To customize the labels in the display**

1. Right-click and choose **Peak Display Settings** from the shortcut menu.
The Peak Settings dialog box opens. For detailed descriptions of commands, see “[Peak Settings dialog box](#)” on page 509.
2. To display labels for the peak retention time (RT), mass area (MA), mass height (MH), or signal-to-noise (SN), select the appropriate check box.
3. Click **OK** in the Peak Settings dialog box.

Figure 153. Example of displayed labels

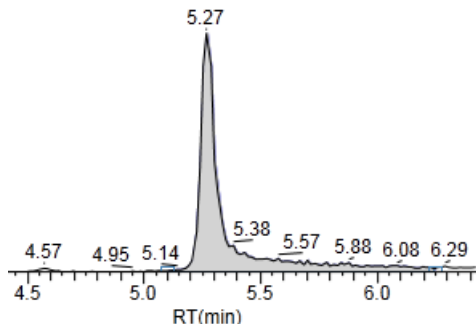


❖ **To display surrounding apex times**

1. Right-click and select **Peak Display Settings** from the shortcut menu.
The Peak Settings dialog box opens. For detailed descriptions of commands, see See “[Peak Settings dialog box](#)” on page 509.

2. Select the **Show All Apex Times** check box.
3. Click **OK** in the Peak Settings dialog box.

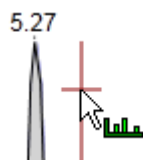
Figure 154. Example of displayed apex times



❖ **To manually integrate a peak**

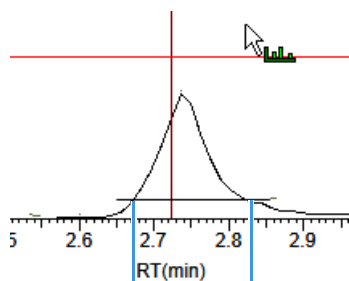
1. Right-click and choose **Swipe Manual Integration** from the shortcut menu, or click the **Swipe Manual Integration** icon, .

The cursor changes to indicate the manual integration mode.

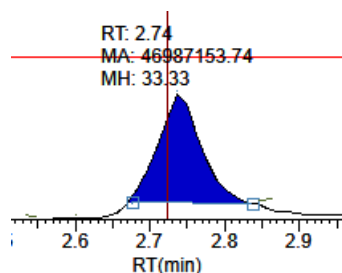


2. Drag the cursor to define the beginning and ending base points for the new peak.

Note You must drag the cursor inside the *x* axis and *y* axis.



Drag the cursor across the peak at the base points for the new peak.



The application identifies the peak and indicates the manual integration in the labels.

The application updates the area of the peak to the baseline that you have just added. When you regenerate the reports, they display the manually modified data.

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 application originally calculates the method values based on the processing method parameters. The manual values are a result of what you edited.

Note Because a Blank Report displays only the quantitation mass, when you manually integrate a confirming ion, the manual integration flag in the report is displayed on the quantitation mass.

❖ **To switch between method and manual integration modes**

Right-click the Confirming Ions pane and choose **Toggle Integration Settings (Manual or Method)** from the shortcut menu.

Initially, the method integration and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the Confirming Ions plots update and the result set updates 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.

Figure 155. Quantitative peak with multiple confirming ions

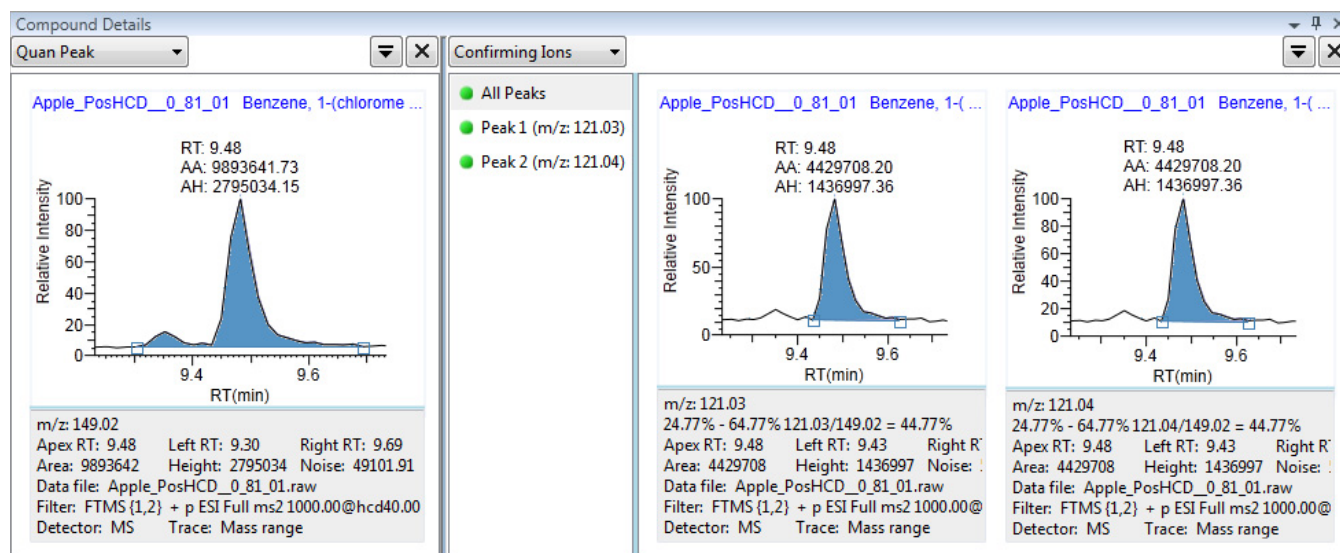
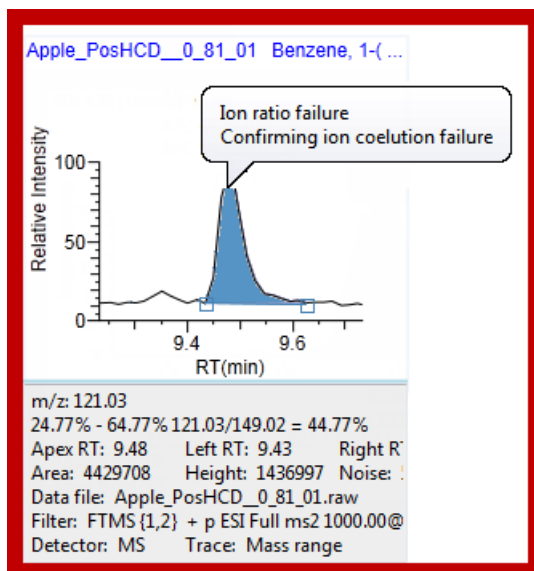


Figure 156. Confirming ion with coelution failure**Table 116.** Confirming Ions pane shortcut menu commands





Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Swipe Manual Integration	Switches to manual integration mode, where you can manually define the peak. Also available from the icon in the upper right corner,   .
Toggle Integration Settings (Manual or Method)	Switches the display between manual integration and method integration modes.
Delete Peak	Removes the peak and all data for this peak from all Compound View panes. Also available from the icon in the upper right corner,   .
Peak Display Settings	Opens the Peak Settings dialog box. See Peak Settings dialog box .
Peak Detection Settings	Edit User Defined Peak Detection Settings: Opens the Peak Detection Settings dialog box where you can make changes to the selected compound for this sample. Edit Local Method Peak Detection Settings: Opens the Peak Detection Settings dialog box where you can make changes to the selected compound for all samples in this batch. After you apply either of these updates, the application does not retain manual integration settings.

Figure 157. Peak Settings dialog box

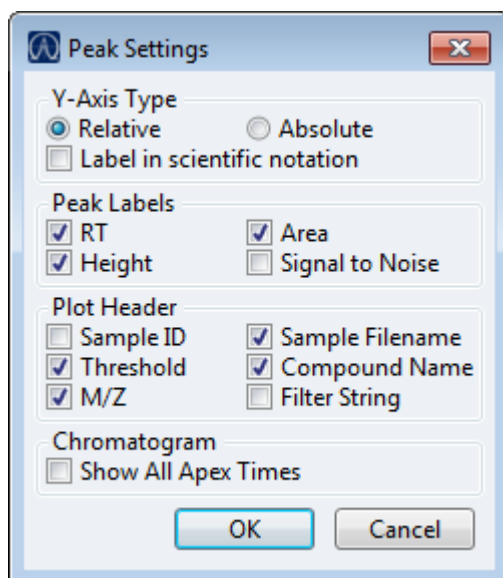


Table 117. Peak Settings dialog box parameters

Command	Description
Y-Axis Type	
Relative	Displays the <i>y</i> -axis scale from 0 through 100.
Absolute	Displays the <i>y</i> -axis scale from 0 to the actual value of the most intense peak in the group.
Label in Scientific Notation	Displays the <i>y</i> -axis scale in scientific notation.
Peak Labels	
RT	Displays the retention time (RT) label in the peak chromatogram pane.
Height	Displays the peak height (AH) label in the peak chromatogram pane.
Area	Displays the peak area (AA) label in the peak chromatogram pane.
Signal to Noise	Displays the signal-to-noise (SN) label in the peak chromatogram pane.
Plot Header	
Sample ID	Displays a user-defined, alphanumeric string that identifies a sample.
Threshold	Displays the peak threshold.
<i>m/z</i>	Displays the mass-to-charge ratio found in the spectrum for the peak. Assumes the charge is 1.

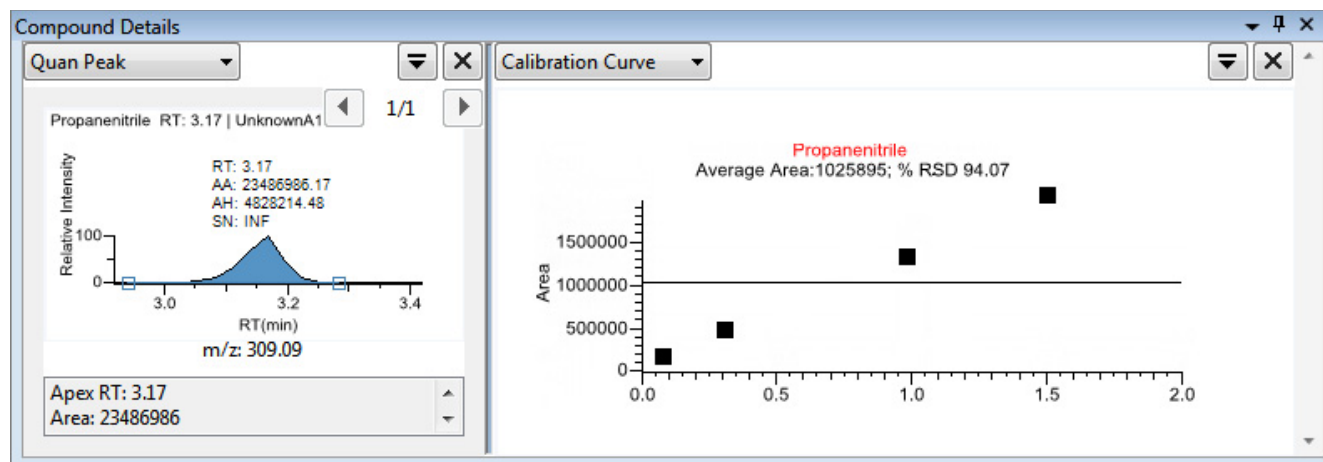
Table 117. Peak Settings dialog box parameters

Command	Description
Sample Filename	Displays the name of the current, selected sample where the peak was found.
Compound Name	Displays the matched compound name found in the library or compound database.
Filter String	Displays the filter used to identify the peak. Specified in the raw data file or the master method.
Chromatogram	
Show All Apex Times	Displays all surrounding apex times in the plot.

Calibration Curve

The Calibration Curve pane displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration. The Calibration Curve pane uses a unique shortcut menu. See [Calibration Curve pane shortcut menu commands](#).

Figure 158. Quantitative peak with a calibration curve plot



❖ **To manually exclude a calibration point**

In the sample 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.

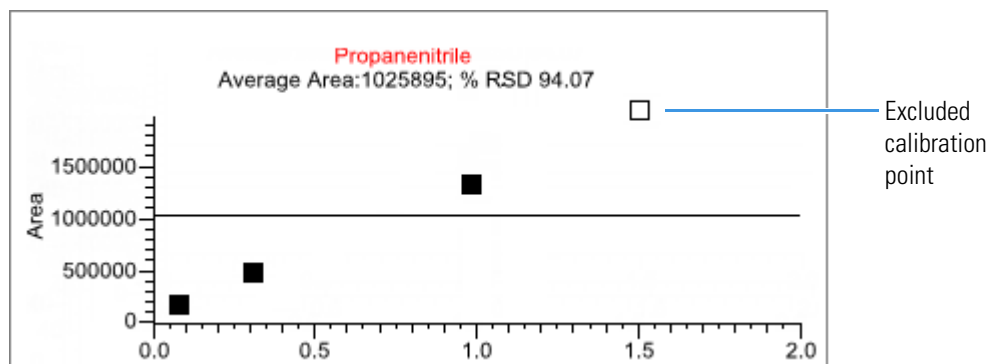


Table 118. Calibration Curve pane shortcut menu commands

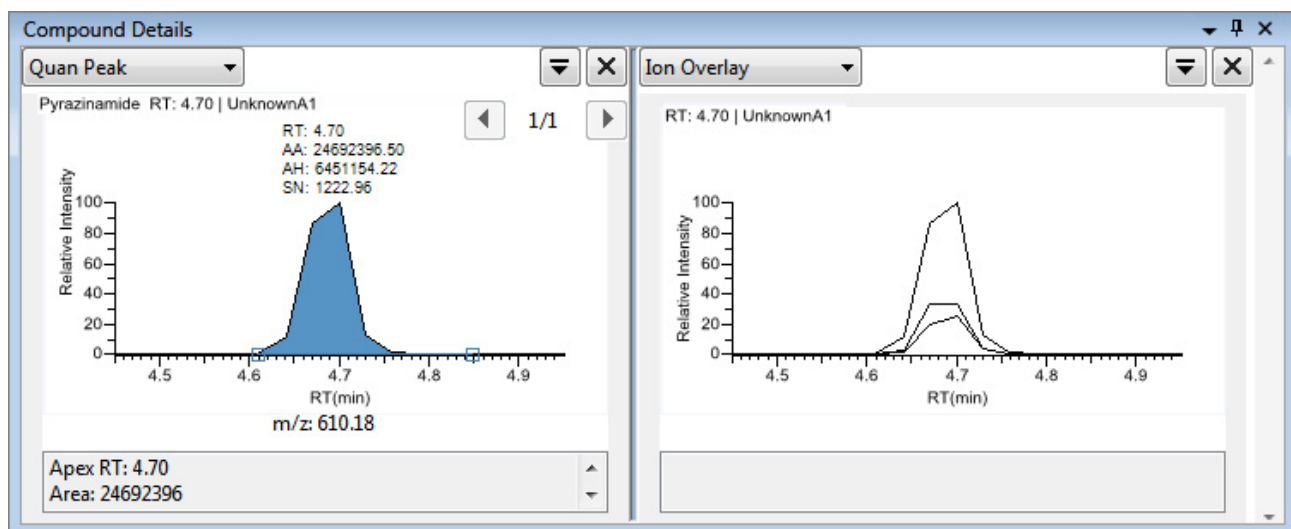
Command	Description
Standard Type	Sets the standard type to External or Internal.
Calibration Curve Type	Sets the calibration curve type to one of the following: <ul style="list-style-type: none"> Linear: Allows all settings with this exception: When Origin is set to Include, all Weighting values are 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	Saves the calibration curve settings.
Reset Scaling	Resets the original scale in the calibration curve pane.

Ion Overlay

The Ion Overlay pane represents an overlay of the entire ion set—quantification and qualifying/confirming—for the selected compound. Use this pane to graphically review the peak apex alignment and coeluting peak profiles.

Note For compounds with an analog detection type, the application displays “No Data” in the Ion Overlay pane.

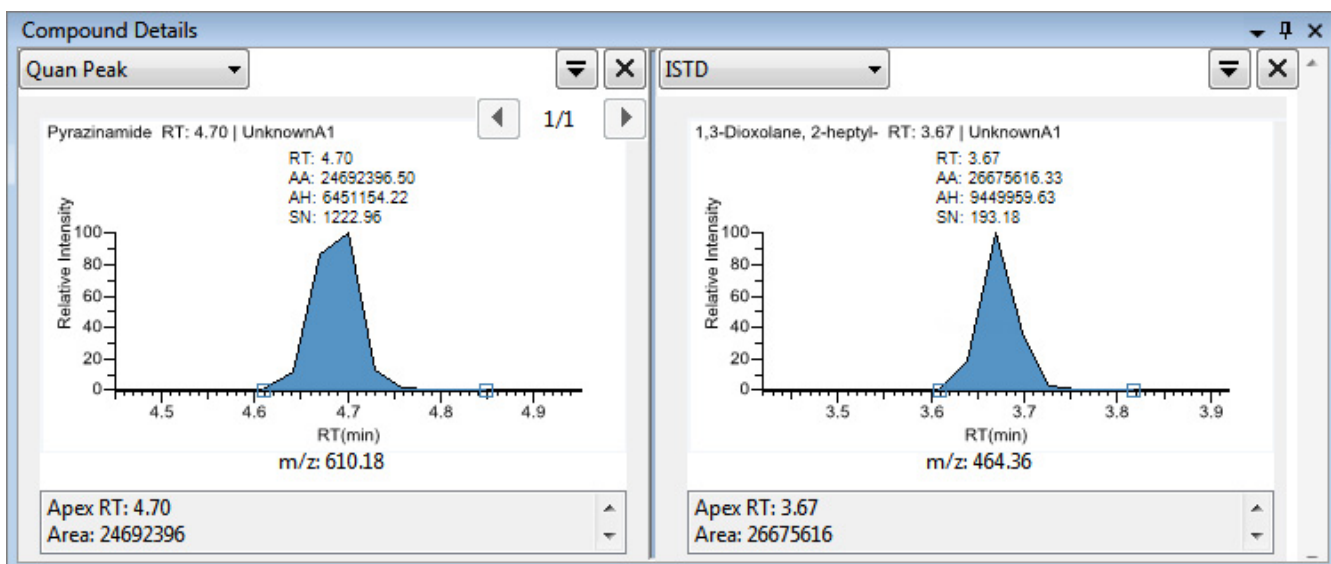
Figure 159. Quantitative peak with confirming ion overlay



ISTD

The ISTD pane displays the internal standard specified for the compound in the method. See [“To specify an internal standard type for a compound”](#) on page 204.

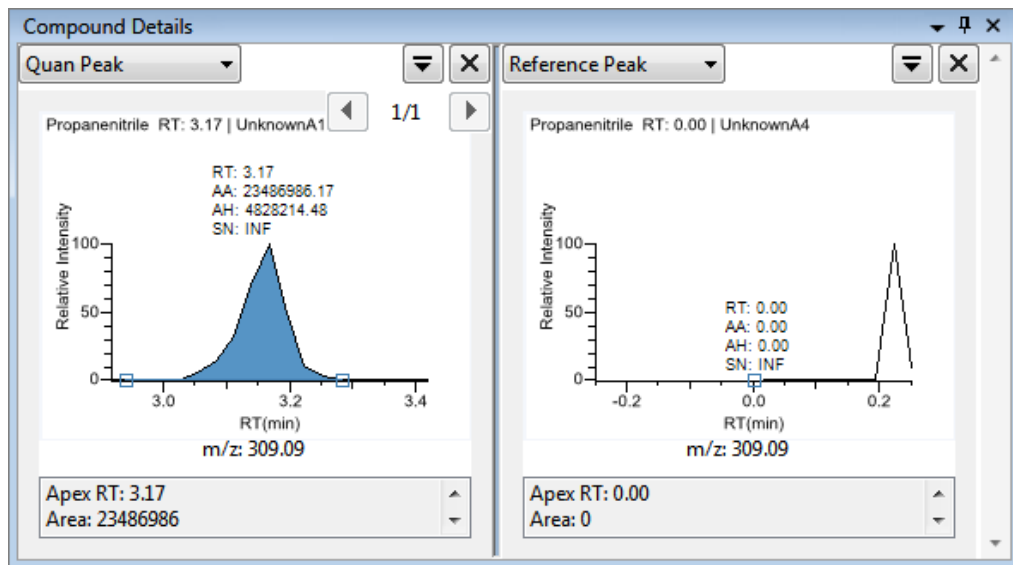
Figure 160. Quantitative peak with an internal standard



Reference Peak

The Reference Peak pane displays the reference peak as specified in the method.

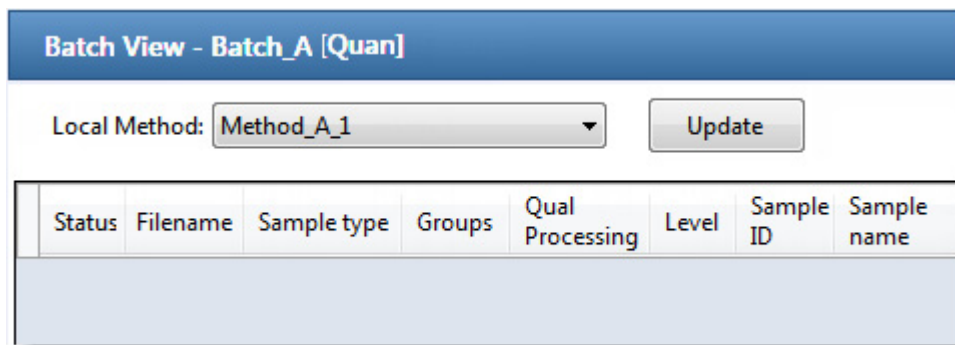
Figure 161. Quantitative peak with a reference peak




❖ To specify a chromatogram reference peak

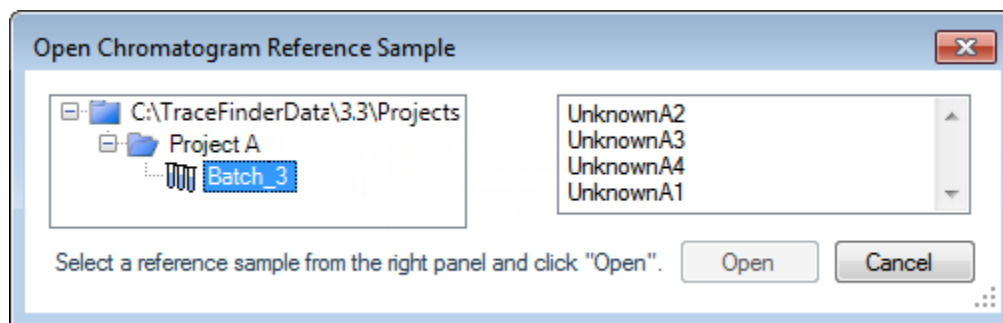
1. In the Batch View task pane, click **Reference Sample**.

An empty reference sample table opens.



2. Click the **Add Reference Sample** icon, , or right-click and choose **Add Reference Sample** from the shortcut menu.

The Open Chromatogram Reference Sample dialog box opens.



Note If you are creating a new method, you will not see any reference samples here. You must create and save a batch using the current 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 application displays only batches that were created using the current master method.

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

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

7. Click **Open**.

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

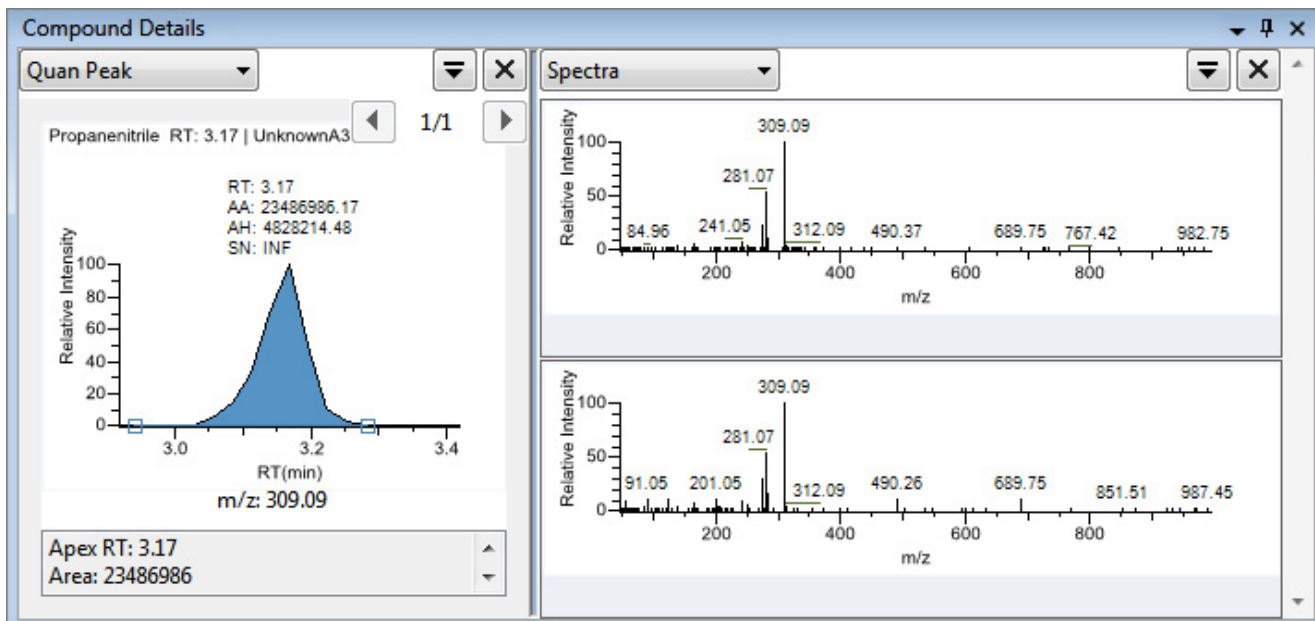
Tip To clear the reference sample from the master method, select **None** in the Set Chromatogram Reference Samples pane.

Spectra

The Spectra pane displays a comparison of the spectra found in the data and the method reference.

Note For compounds with an analog detection type, the application displays “Not Available” in the Spectra pane.

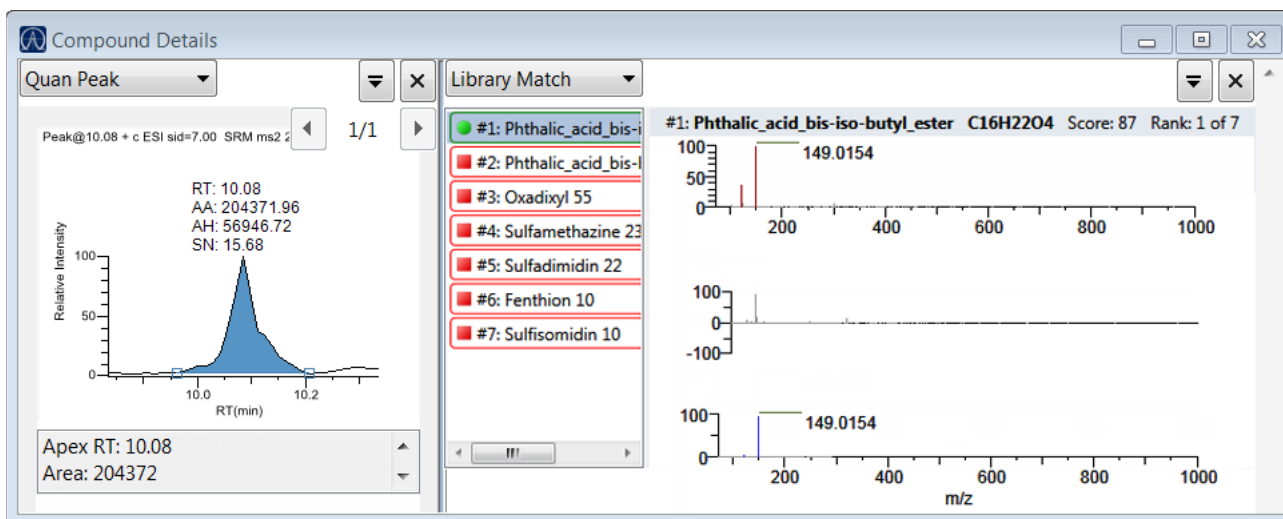
Figure 162. Quantitative peak with data and reference spectra



Library Match

The Library Match pane displays all library matches for the selected compound.

Figure 163. Library Match for selected compound



9 Using the Analysis Mode for Quantitation Batches

Working in Data Review

If you have no matches for any of your compounds, make sure you have completed all of the following:

- You installed a library.
- You selected screening libraries in the Configuration console. See [“Screening Libraries”](#) on page 59.
- You enabled Library Matching in the method. See [“To activate library matching”](#) on page 196.

Isotope

The Isotope pane displays all isotopes for the selected compound. The Isotope pane includes a shortcut menu. See [Isotopes pane shortcut menu commands](#).

Note When you select different samples, the current compound remains selected (as long as that compound is found in the sample).

The isotopes pane displays isotopic pattern results for all adducts of a compound according to the threshold and deviation parameters defined in the method.

To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

- An isotope peak is not found if its intensity, relative to the monoisotopic ion's intensity, is more than the specified intensity deviation percentage away from the theoretical relative intensity of the isotope ion.
- An isotope peak is found if its measured m/z is less than the specified mass deviation amount away from its expected m/z .

To specify isotopic criteria in a method, see [“Isotopes”](#) on page 197.

Figure 164. Isotopes for the selected compound

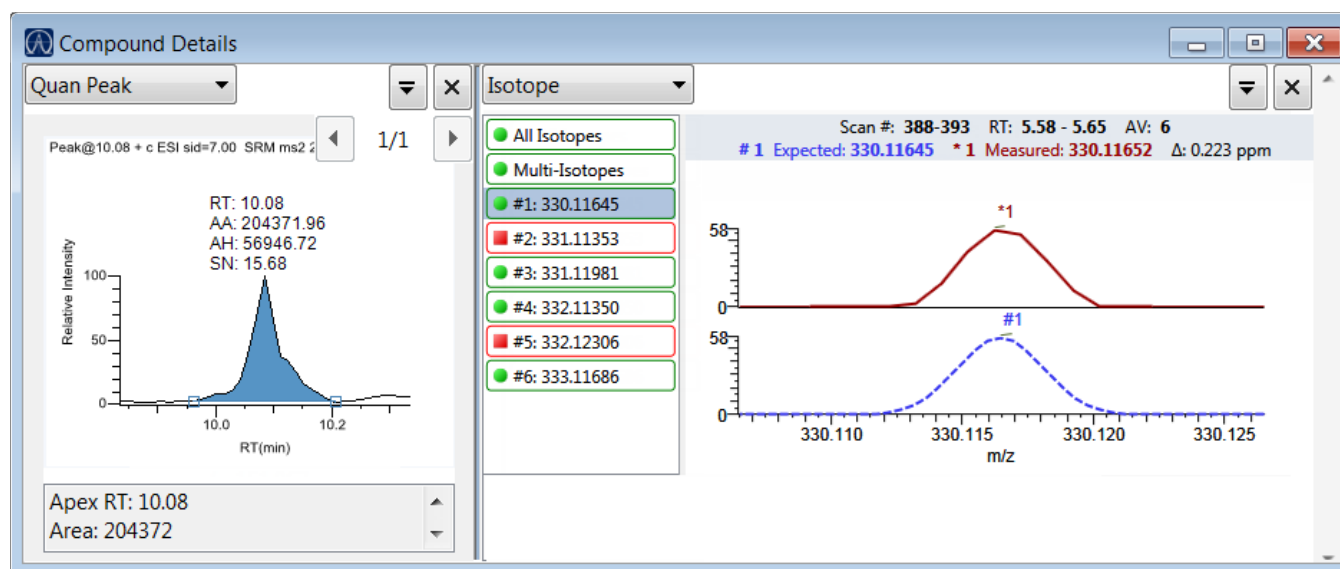
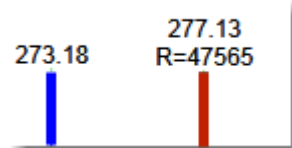
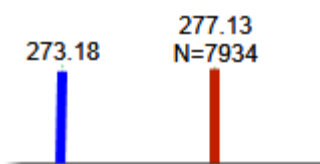


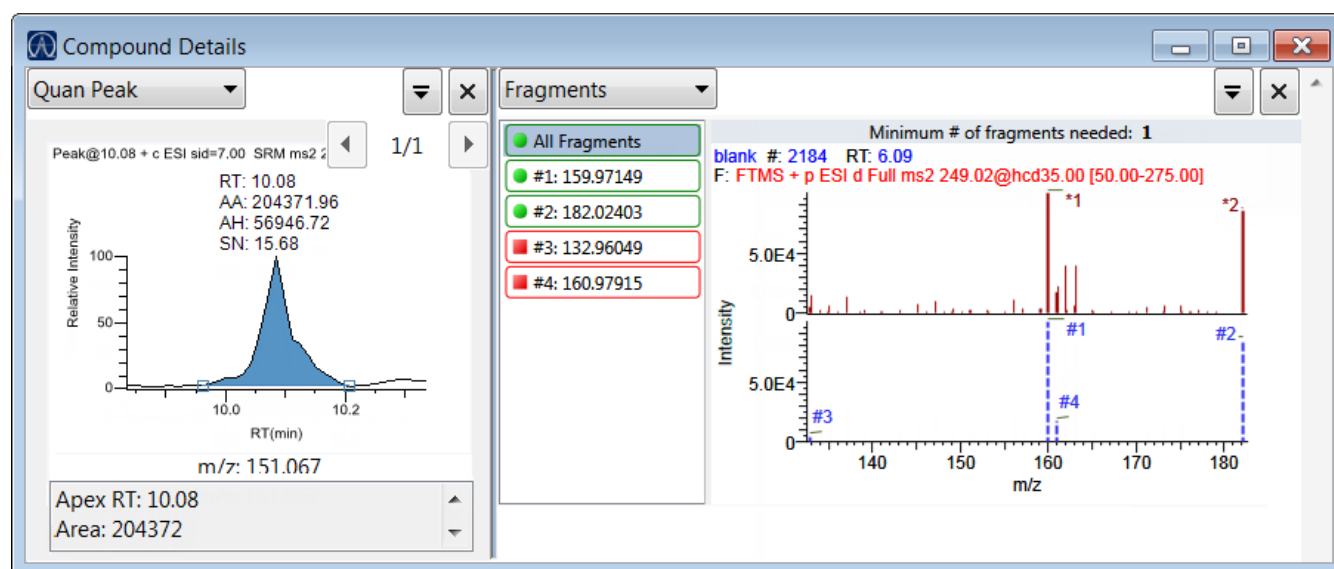
Table 119. Isotopes pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Show/Hide Noise Label	Adds a noise label to each peak. Expected isotope peaks (displayed in blue) do not display a noise label.
Show/Hide Resolution Label	Adds a resolution label to each peak. Expected isotope peaks (displayed in blue) do not display a resolution label.



Fragments

The Fragments pane displays a composite of all fragments found in the compound. The application displays the measured peak as a solid red line and displays the expected peak as a dashed blue line.

Figure 165. Fragments for the selected compound

Exporting Compounds

You can export compound data to an Excel spreadsheet, to a CSV file, to a compound database, or to a new quantitation method. These export commands are available from the File menu in the Sample View, Compound View, and Comparative View.

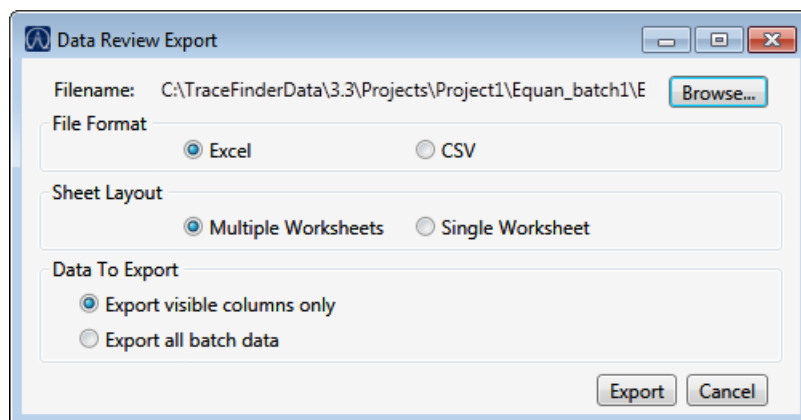
Follow these procedures:

- [To export compounds to an Excel spreadsheet](#)
- [To export compounds to a CSV file](#)

❖ To export compounds to an Excel spreadsheet

1. Choose **File > Export Data To > CSV or Excel** from the main menu.

The Data Review Export dialog box opens.



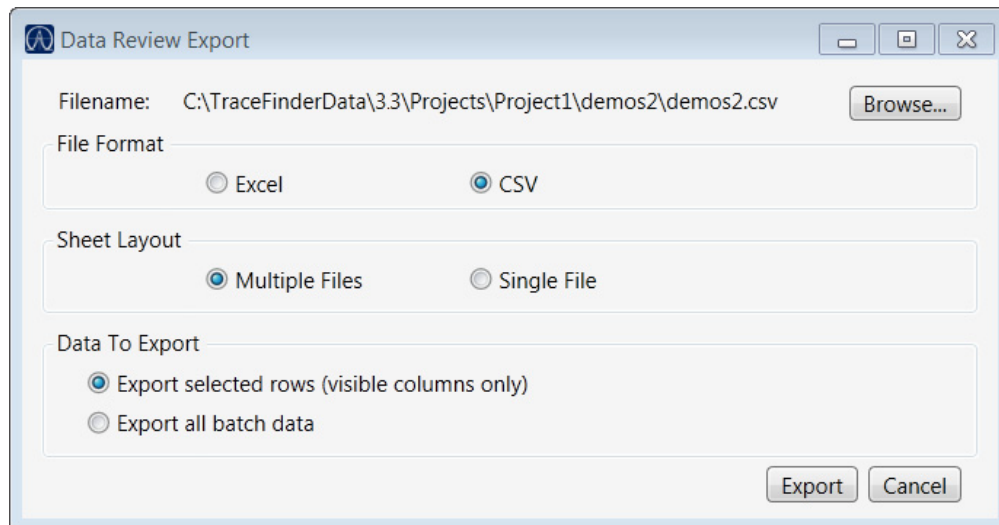
2. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.
3. Type a file name for the XLSX file and click **Save**.
4. In the File Format area, in the Data Review Export dialog box, select the **Excel** option.
5. In the Sheet Layout area, select one of the following file formats for the spreadsheet.
 - **Multiple Worksheets:** Writes one sample to each Excel worksheet tab.
 - **Single Worksheet:** Writes all samples to a single Excel worksheet tab.
6. In the Data to Export area, select one of the following sets of data to export.
 - **Export Visible Columns Only:** Writes data from only the displayed columns to the specified worksheet format.
 - **Export All Batch Data:** Writes data from all columns (displayed or hidden) of all samples to the specified worksheet format.
7. Click **Export**.

The application saves the specified compound data to an Excel spreadsheet and opens the folder where you saved the file. The application names the file *Batch.xlsx*.

❖ To export compounds to a CSV file

1. Choose **File > Export Data To > CSV or Excel** from the main menu.

The Data Review Export dialog box opens.



2. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.
3. Type a file name for the CSV file and click **Save**.
4. In the File Format area, in the Data Review Export dialog box, select the **CSV** option.
5. In the Sheet Layout area, select one of the following file formats for the spreadsheet.
 - **Multiple Files:** Writes one sample to each CSV file.
 - **Single File:** Writes all samples to a single CSV file.
6. In the Data to Export area, select one of the following sets of data to export.
 - **Export Visible Columns Only:** Writes data from only the displayed columns to the specified worksheet format.
 - **Export All Batch Data:** Writes all data from all samples in the batch to the specified worksheet format.
7. Click **Export**.

The application saves the specified compound data to a CSV spreadsheet.

When you selected to create multiple files, the application opens the folder where you saved the files. The application names each file *Batch_Compound.csv*.

When you selected to create a single file, the Excel application opens, displaying the exported data for all samples. The application names the file *Batch.csv*.

Working in the Report View

The Report View displays example reports for the current batch. You must have an open batch to use the features in the Report View.

Follow these procedures:

- To open the Report View
- To preview a report
- To generate a report as a PDF, an Excel, or a CSV file
- To print a report
- To display a generated report
- To edit a report template
- To create a new report template

❖ To open the Report View

Click **Report View** in the navigation pane.



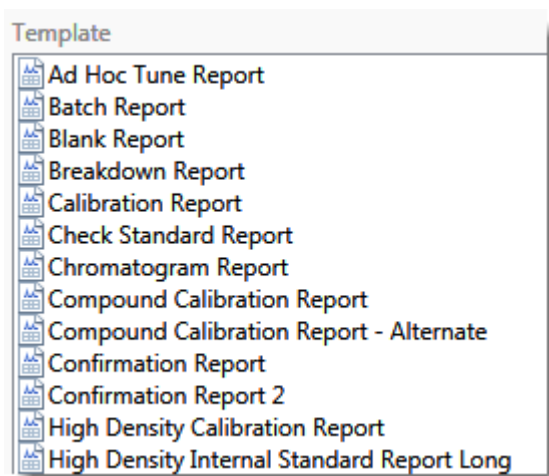
The application opens the Report View. For detailed descriptions of all parameters, see “Report View” on page 524.

❖ To preview a report

1. In the Template pane, select a report template.

The template list shows all the quantitation report templates that you configured in the Configuration console. See “Specifying the Reports” on page 71.

Figure 166. Example of a report template list

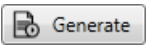


2. Click **Preview**, .

The application opens the Report Designer, showing the report information for the current batch in the selected report template format.

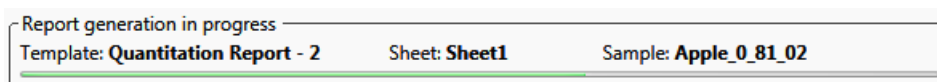
For details about using the Report Designer, see [Chapter 12, “Using the Report Designer.”](#)

❖ To generate a report as a PDF, an Excel, or a CSV file

1. In the Template pane, select a report template.
2. Select the check box for each of the file types that you want to create: **PDF**, **Excel**, or **CSV**.
3. Click **Generate**, .

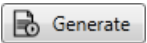
The application does the following:

- Displays a green progress bar as it generates the reports.



- Creates a report for the current batch as a PDF, an Excel, or a CSV file, using the selected report template format.
- Adds information about the generated report to the Generated Reports pane. For details about the Generated Reports pane, see [“Report View” on page 524.](#)
- Saves the report files to the ...\\TraceFinderData\\3.3\\Projects*batch*\\ReportOutput folder.

❖ To print a report

1. In the Template pane, select a report template.
2. Select the check box for the **Print** file format.
3. Click **Generate**, .

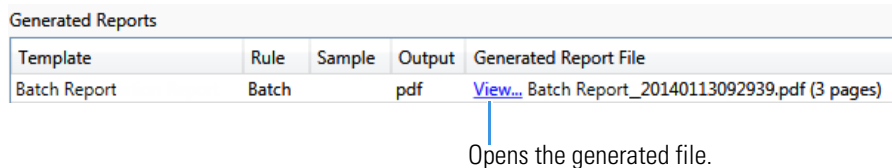
The application does the following:

- Creates a report for the current batch using the selected report template format.
- Prints the report to your default printer.
- Adds information about the generated report to the Generated Reports pane. For details about the Generated Reports pane, see [“Report View” on page 524.](#)
- Saves the report files to the ...\\TraceFinderData\\3.3\\Projects*batch*\\ReportOutput folder.

❖ To display a generated report

In the Generated Reports pane, click **View** for the report that you want to see.

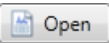
Figure 167. Generated Reports pane showing a PDF report



The application opens the output file.

❖ To edit a report template

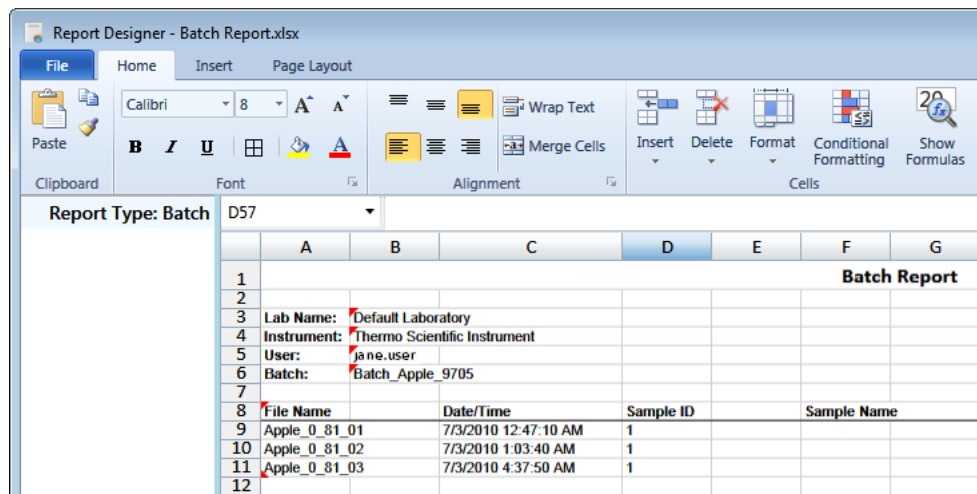
Note You cannot edit report templates that were provided with the TraceFinder application; however, you can open a TraceFinder template, make changes, and save it to a new template name.

1. In the Template pane, select a report template.
2. Click **Open**, .

The application opens the Report Designer showing the template in an Excel spreadsheet. See [Report Designer showing the template for the selected report](#).

Note When user security is activated, you must have Template Editing permission to edit report templates created by your laboratory. If the Open button is not active, user security is activated and you do not have Template Editing permission.

Figure 168. Report Designer showing the template for the selected report



3. Use the features in the Report Designer to edit the template.
See [Chapter 12, “Using the Report Designer.”](#)
4. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

❖ To create a new report template

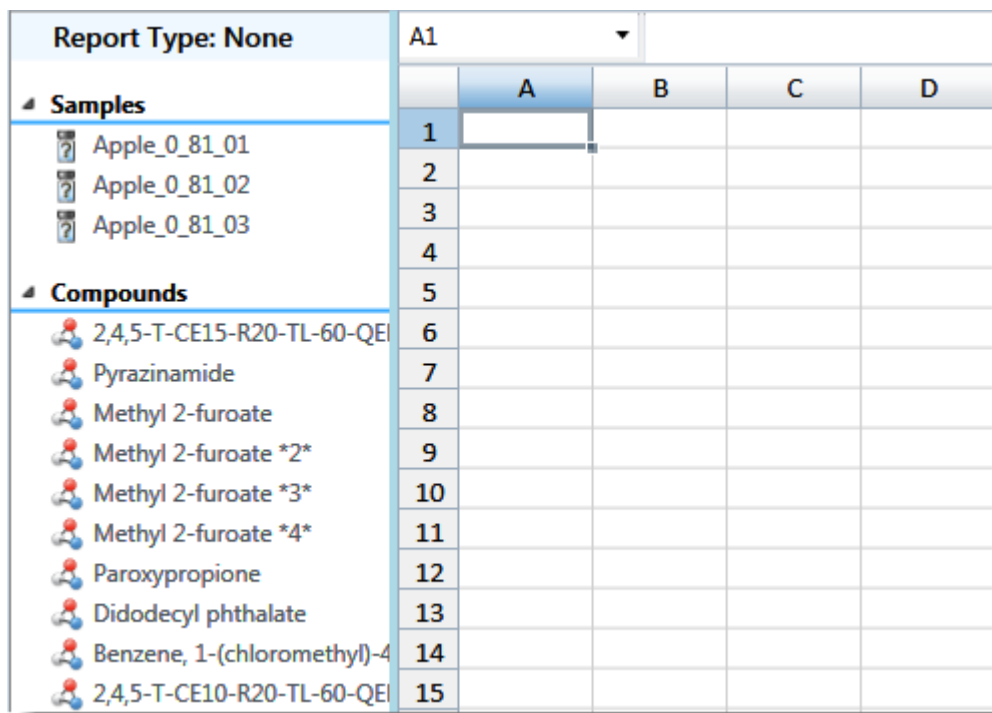
1. Click **New**, .

The application opens the Report Designer showing an empty template in an Excel spreadsheet. See [Report Designer showing a new, empty template](#).

The Report Type is None.

In the left pane, the spreadsheet lists all samples in the current batch and all compounds in the method used for the batch.

Figure 169. Report Designer showing a new, empty template



Report Type: None		A1			
Samples		A	B	C	D
?	Apple_0_81_01				
?	Apple_0_81_02				
?	Apple_0_81_03				
Compounds					
	2,4,5-T-CE15-R20-TL-60-QEI				
	Pyrazinamide				
	Methyl 2-furoate				
	Methyl 2-furoate *2*				
	Methyl 2-furoate *3*				
	Methyl 2-furoate *4*				
	Paroxypropione				
	Didodecyl phthalate				
	Benzene, 1-(chloromethyl)-4				
	2,4,5-T-CE10-R20-TL-60-QEI				

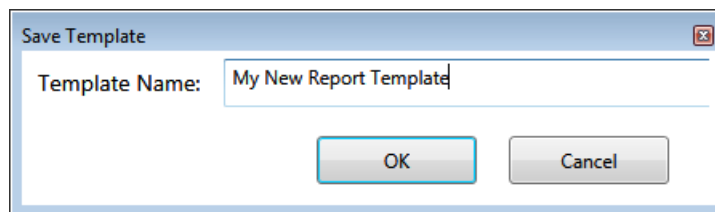
2. Use the features in the Report Designer to create the report template.

See [Chapter 12, “Using the Report Designer.”](#)

3. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

The Save Template dialog box opens.

Figure 170. Save Template dialog box



Save Template

Template Name: My New Report Template

OK Cancel

4. Type a name for the new report template and click **OK**.

Report View

Use the features in the Report View to display example reports for the current batch.

Figure 171. Report View

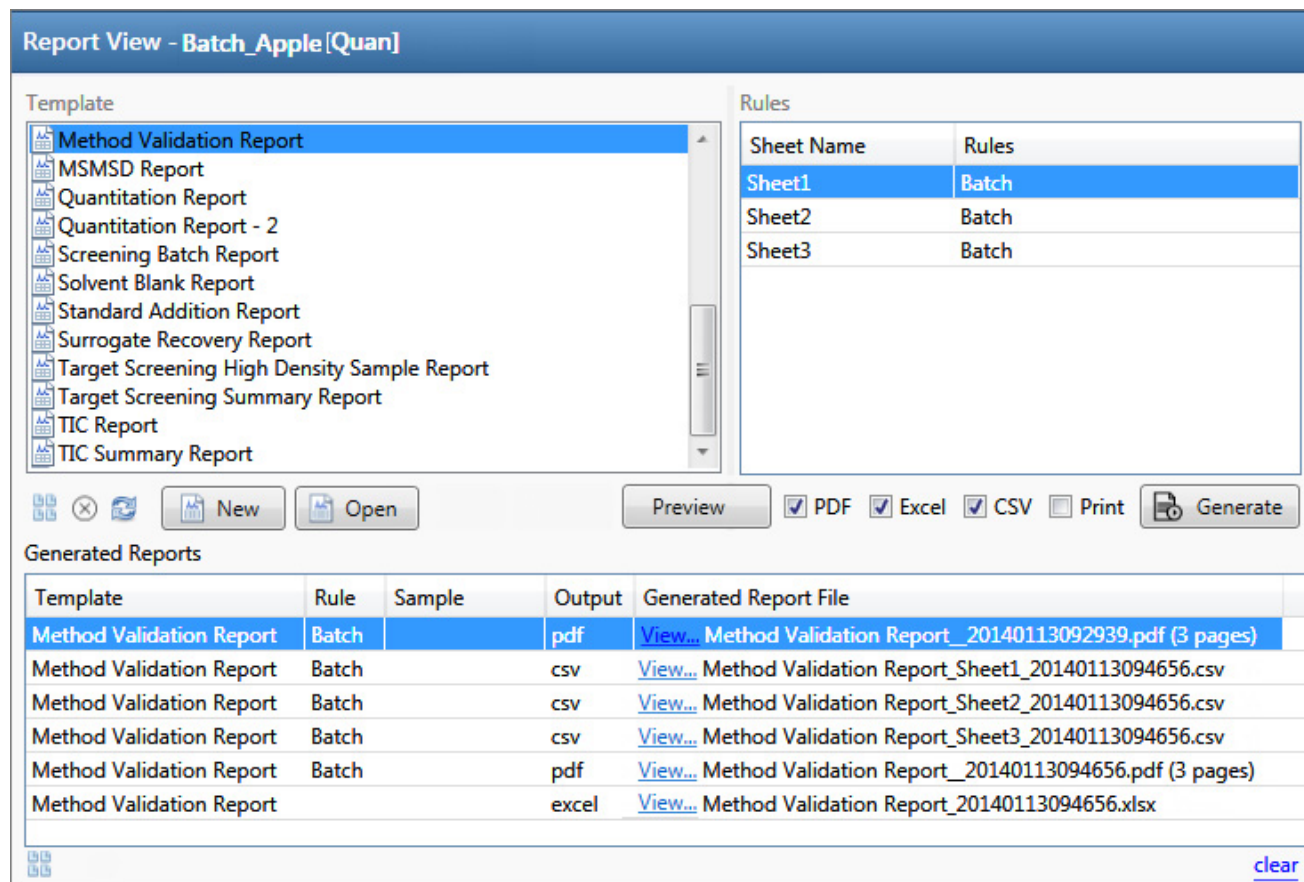

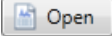

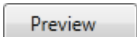
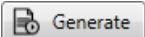



Table 120. Report View parameters (Sheet 1 of 2)

Parameter	Description
Template	
	Displays all report templates.
Rules	
Sheet Name	Specifies each sheet in the report.
Rules	Specifies the type of data used in each sheet in the selected report. <ul style="list-style-type: none"> • Batch • EachSample • SampleType: <i>SampleType</i> • CompoundType: <i>CompoundType</i> • SampleCustomFormula:

Table 120. Report View parameters (Sheet 2 of 2)

Parameter	Description
Buttons	
 View Report Templates	Displays the C:\TraceFinderData\3.3\Templates\ReportTemplates folder that contains all report templates.
 Open	Opens the selected report template in the Report Designer.
 New	Opens a blank report template in the Report Designer.
 Preview	Opens the Report Designer showing the report information for the current batch in the selected report template format.
PDF	Writes the generated report to a PDF file in the ...\\TraceFinderData\3.3\Projects\batch\ReportOutput folder.
Excel	Writes the generated report to a PDF file in the ...\\TraceFinderData\3.3\Projects\batch\ReportOutput folder.
CSV	Saves the generated report as a PDF file in the ...\\TraceFinderData\3.3\Projects\batch\ReportOutput folder. When the report contains multiple sheets, the application writes each sheet as a separate CSV file.
Print	Prints the generated report to your default printer.
 Generate	Generates the selected type of reports for the current batch using the selected report template.
Generated Reports	
Template	Report template used for the report. See “Example of a report template list” on page 520.
Rule	Type of data used in each sheet of the report. See Rules.
Sample	For sample-level reports, the name of each sample in the report.
Output	Type of output specified for the report: PDF, Excel, CSV, or Print.
Generated Report File	Lists the output file name for each report in the ...\\TraceFinderData\3.3\Projects folder.
View	Displays the generated output file.
 View Generated Reports	Displays the C:\TraceFinderData\3.3\Projects folder that contains all report outputs.
Clear	Removes all reports from the Generated Reports display. This does not delete the reports from the C:\TraceFinderData\3.3\Projects folder.

Working in the Local Method View

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.

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. Local methods are named *Batch_MasterMethod*.

❖ To open the Local Method View

1. Click **Analysis** in the navigation pane.
2. Click **Local Method**.



The Local Method view for the currently selected batch opens. See [Local Method view](#).

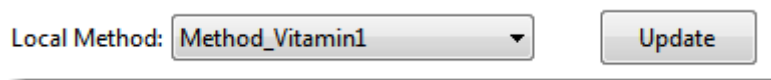
You can edit many of the method parameters in a local method. Editing the local method does not affect parameters in the master method.

For detailed descriptions of method parameters, see “[Editing a Master Method](#)” on [page 135](#).

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 172. Local Method view

The screenshot displays the 'Local Method View' for 'Equan1_408_Method_Equan_1*'. The left sidebar contains a navigation menu with 'Local Method' selected, which is further divided into 'Acquisition', 'Quantitation', 'Processing', 'Compounds', 'QAQC', 'Groups', 'Intel Seq', 'Library Settings', and 'Reports'. The main content area shows the following configuration details:

- Master method: [Method Equan 1](#)
- Lab Name: Default Laboratory
- Assay type: Assay name
- Injection Volume: 1.00
- Mass Precision: 3.00
- Ion range calc method: Level
- Use level: (empty dropdown)
- Instrument Method: Pesticides Using EQuan

At the bottom right of the configuration area are 'Edit' and 'Update' buttons. Below this is a 'Notes' section with a text input field.

Using the Analysis Mode for Target Screening Batches

This chapter includes instructions about using the features of the Analysis mode to do the following:

- Create target screening batches.
- Submit target screening batches for acquisition, processing, or report generation.
- Review target screening batches, batch data, reports, and local methods.

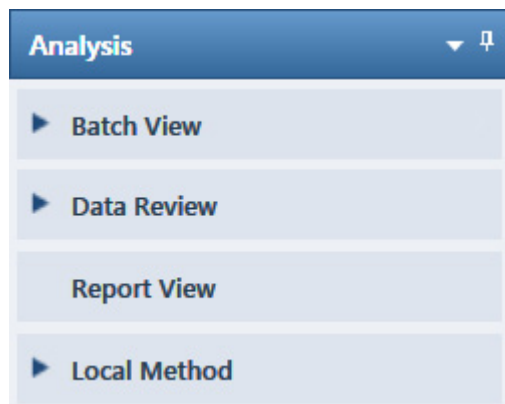
Contents

- [Working in the Batch View](#)
- [Working in Data Review](#)
- [Working in the Report View](#)
- [Working in the Local Method View](#)

❖ To access the Analysis mode

Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.



Working in the Batch View

In the Batch View, you can manually create and edit a new target screening 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.

The Analysis mode includes a toolbar:

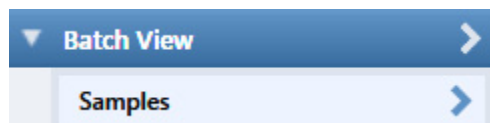


Use the toolbar or the equivalent commands in the Batch View shortcut menu to create the sample list and submit samples for acquisition. See “[Toolbar](#)” on [page 538](#) or “[Batch View Shortcut Menu](#)” on [page 541](#).

❖ To open the Batch View

1. Click **Analysis** in the navigation pane of the current mode.
2. Click **Batch View**.

The Batch View navigation pane opens.



The Batch View includes a single page of information, the Samples page.

This section contains information about the following topics:

- [Samples Page Features](#)
- [Creating a New Batch](#)
- [Editing a Batch](#)
- [Submitting a Batch](#)

Samples Page Features

The Samples page is divided into two panes:

- Samples pane

Use the samples pane to create a batch. See [Samples Pane](#).

- Compound Active Status pane

Use the Compound Active Status pane to make specific compounds active or inactive. See “[Compound Active Status Pane](#)” on page 543.

Samples pane

The screenshot shows the 'Batch View - Batch_A [Screening]' window. At the top, there is a 'Local Method' dropdown set to 'Method_Screening', an 'Update' button, an 'Instrument' dropdown set to 'Thermo Scientific Instrument', and a 'User' field. Below this is a table with columns: Status, Filename, Sample type, Groups, Blank Subtraction, Level, Sample ID, Sample name, Vial position, Injection volume, Conversion Factor, Channel, Barcode Expected, Barcode Actual, and Sample Volume. The table contains three rows of data for 'Unknown1', 'Unknown2', and 'Unknown3'. Below the table is a 'Compound Active Status' pane with a table containing two rows: one for 'FENTHION-CE20-R20-TL75-QED' at RT 1.91, and another for 'Sulfisomidine' at RT 2.72. Both have the 'Active' checkbox checked.

Status	Filename	Sample type	Groups	Blank Subtraction	Level	Sample ID	Sample name	Vial position	Injection volume	Conversion Factor	Channel	Barcode Expected	Barcode Actual	Sample Volume
▶ 1	Unknown1	Unknown		<input type="checkbox"/>					10.0	1.000	Auto			1
2	Unknown2	Unknown		<input type="checkbox"/>					10.0	1.000	Auto			1
3	Unknown3	Unknown		<input type="checkbox"/>					10.0	1.000	Auto			1

	RT	Compound	Active
▶ 1	1.91	FENTHION-CE20-R20-TL75-QED	<input checked="" type="checkbox"/>
2	2.72	Sulfisomidine	<input checked="" type="checkbox"/>

Compound Active Status pane

Tip To resize the panes, drag the separators that divide the panes.

Samples Pane

The samples pane includes the following features:

- [Column Display](#)
- [Status Indicators](#)
- [Groups](#)
- [Blank Subtraction](#)
- [Sample Weight Calculation](#)
- [Instrument Methods](#)
- [Toolbar](#)
- [Batch View Sample List](#)
- [Batch View Shortcut Menu](#)

Column Display

The sample list contains many columns of information. You can scroll to see all the columns, and you can customize which ones to display and their display order.

❖ To scroll the sample list

Use the horizontal scroll bar at the bottom of the sample list to view all the information.

When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name, while the other columns scroll right and left.

❖ To customize the column display

1. Right-click the sample list and choose **Modify Columns** from the shortcut menu.

The Modify Columns dialog box opens. See “[Modify Columns dialog box](#).”

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

These columns appear after the Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

- a. In the Displayed Columns pane, select a column name.
- b. Use **Up** or **Down** 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, and the last column in the list represents the rightmost column in the Batch View sample list.

Note The following columns are fixed: Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

- a. In the Displayed Columns pane, select the column width.

5	Sample ID	100
▶ 6	Sample name	100
7	Vial position	100

- b. Type a new value for the width.

5. Repeat [step 4](#) for all columns whose widths you want to change, and 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.

Figure 173. Modify Columns dialog box

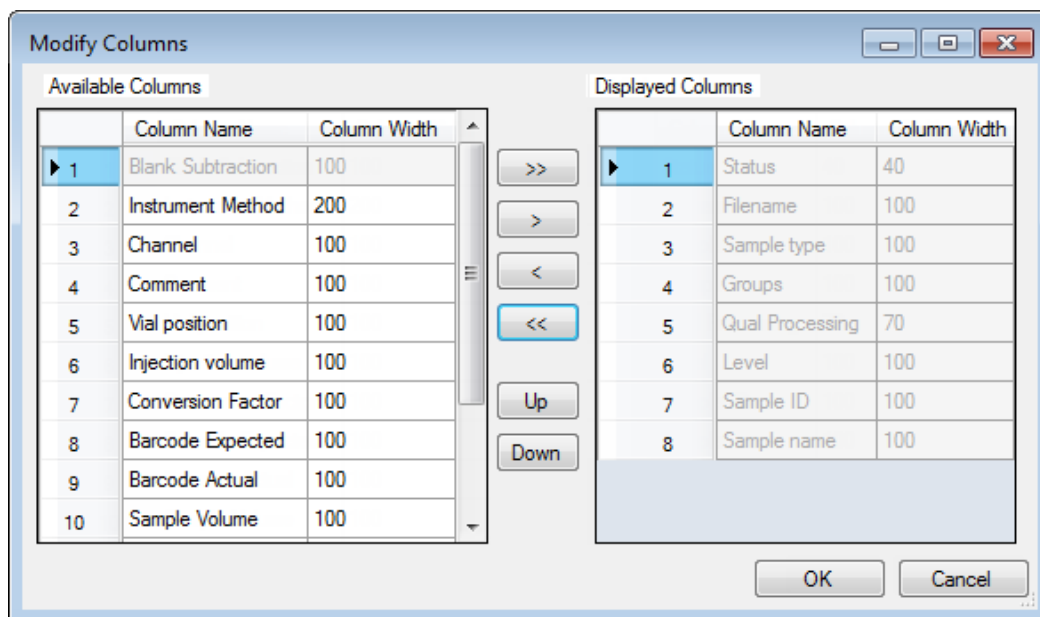












Table 121. Button descriptions for the Modify Columns dialog box




Button	Description
	Moves all columns to the Displayed Columns pane.
	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name.	
	Moves the selected column to the Available Columns pane.
	Moves all columns except fixed columns.
	Moves the selected column name in the Displayed Columns pane one row up in the column order.
	Moves the selected column name in the Displayed Columns pane one row down in the column order.

Status Indicators



Status indicators show the current status of each sample during the acquisition and processing.


-  Sample is not acquired.
-  Sample is acquired but not processed.
-  Sample is acquired and processed.
-  Sample is currently acquiring.

Local Method: Method_Screening Update

	Status	Filename	Sample type	Groups	Blank Subtraction	Sample ID	Sample name	V p
1		Solvent_A	Solvent		<input type="checkbox"/>			1
2		Cal_5	Cal Std		<input type="checkbox"/>			2
3		Unknown1	Unknown		<input type="checkbox"/>			3

Status indicators

Note When you include unknown screening features in the target screening method and you choose to process with only the target screening criteria, the Samples view shows the Status for the samples as acquired and processed () , and the Unknown Screening View shows the Status for the samples as acquired but not processed () .

Note When you include unknown screening features in the target screening method and you choose to process with only the unknown screening criteria, both the Samples view and the Unknown Screening View show the Status for the samples as acquired and processed () .




Groups

Use the Groups feature to assign samples to a group.

❖ To create a group



1. For each sample, type the name of a group in the Groups column.
Repeat this for each sample that you want to include in a group.
2. Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
	Benzo26473	groupB, groupA
	Benzo25557	groupB
	Benzo26154	groupB, groupA

Blank Subtraction

Use the Blank Subtraction feature to select which matrix blank samples you want to use for peak subtraction. The application subtracts the areas of the peaks in the selected matrix blank samples from the matching areas in the unknown samples.

Status	Filename	Sample type	Groups	Blank Subtraction
	VitWaterEquanMaxA001	Matrix Blank		<input checked="" type="checkbox"/>
	VitWaterEquanMaxA002	Unknown		<input type="checkbox"/>

When you process the batch sequence, the application subtracts the peaks in a selected matrix blank sample from all unknown samples that follow it, until it encounters another matrix blank sample.

To activate the Blank Subtraction feature, see [“Editing the Processing Page”](#) on [page 264](#).

Sample Weight Calculation

Use the sample weight features to calculate the conversion factor for a sample. The application uses different methods to calculate the conversion factor for liquid or solid calculation types.

Liquid: $SampleVolume \div DilutionFactor$

Solid: $(SampleVolume \times DilutionFactor) \div SampleWeight$

Manual: The application does not calculate the Conversion Factor. Instead, you can enter the Conversion Factor value.

Follow these procedures:

- [To display the features for calculating sample weight](#)
- [To calculate the conversion factor for a liquid sample](#)
- [To calculate the conversion factor for a solid sample](#)
- [To manually specify the conversion factor for a sample](#)

❖ To display the features for calculating sample weight

If the Conversion Factor, Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns are not visible, right-click and choose **Enable Sample Weight Calculation** from the shortcut menu.

Conversion Factor	Sample Volume	Dilution Factor	Sample Weight	Calculation Type	Final Units
1.000	1	1	1	Liquid ▼	
1.000	1	1	1	Solid ▼	
1.000	1	1	1	Manual ▼	

❖ To calculate the conversion factor for a liquid sample

Note The application uses the following formula to calculate the Conversion Factor:
 $SampleVolume \div DilutionFactor$

1. From the **Calculation Type** list, select **Liquid**.

For a liquid sample, the Sample Weight value is not editable.

2. In the Sample Volume column, type the volume in ng/mL for your sample.
3. In the Dilution Factor column, type the value for the dilution.

For example, if you have 1000 ng/mL of a substance that is too concentrated for the mass spectrometer, you can dilute it by 1000. Then your injection volume is 1, your conversion factor is 1000, and your sample amount is 1000.

4. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

❖ To calculate the conversion factor for a solid sample

Note The application uses the following formula to calculate the Conversion Factor:
 $(SampleVolume \times DilutionFactor) \div SampleWeight$

1. From the **Calculation Type** list, select **Solid**.
2. In the Sample Weight column, type the weight in ng for your sample.
3. In the Sample Volume column, type the volume in ng/ml for your sample.
4. In the Dilution Factor column, type the value for the dilution.

For example, if you have 1000 ng/ml of a substance that is too concentrated for the mass spectrometer, you can dilute it by 1000. Then your injection volume is 1, your conversion factor is 1000, and your sample amount is 1000.

5. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

❖ To manually specify the conversion factor for a sample

Note The application uses the specified conversion factor when it calculates the amount for the sample.


1. From the **Calculation Type** list, select **Manual**.
For a manually calculated sample, the only available columns are the Conversion Factor and the Final Units.
2. In the Conversion Factor column, type the conversion factor to use for your sample.
3. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

Instrument Methods

Use the Instrument Methods column to specify instrument methods for the samples.

Note By default, the Instrument Method column is not displayed in the Batch View sample list.

❖ To specify instrument methods for samples

1. Display the Instrument Method column in the sample list:
 - a. Right-click the sample list and choose **Modify Columns** from the shortcut menu.
The Modify Columns dialog box opens.
 - b. In the Available Columns pane, select **Instrument Method**.
 - c. Click  to move the Instrument Method column to the Displayed Columns pane.
 - d. Click **OK**.

The application displays the Instrument Method column, defaulting to the instrument method specified in the master method.

2. Click the Instrument Method column and select an instrument method from the list.
This list contains all the available instrument methods. Instrument methods from external sources are prefixed with “Ext:”.

You can specify a different instrument method for each sample.

When you submit the batch for acquisition, the application saves a copy of the selected instrument methods to the following folders:

External instrument methods:

... \TraceFinderData\3.3\Projects\...\batch\Methods\method\ExternalMethods

Local instrument methods:

... \TraceFinderData\3.3\Projects\...\batch\Methods\method

Toolbar

The Analysis mode includes this toolbar for creating and submitting a batch.



Table 122. Toolbar icons

Icon	Description
	Adds the specified number of new, empty samples to the end of the sample list. See the instructions “ To add samples to the list ” on page 545 .
	Inserts a new, empty sample or samples above the selected sample. See the instructions “ To insert samples into the list ” on page 546 .
	Removes the selected samples from the sample list. See the instructions “ To remove samples from the list ” on page 547 .
	Adds imported samples from a CSV, an XML, or an SLD file to the sample list. See the instructions “ To import samples into the list ” on page 546 .
	Submits only the selected samples for acquisition, processing, or report generation. See the instructions “ To submit samples in the batch ” on page 557 .
	Submits the batch for acquisition, processing, or report generation. See the instructions “ To submit samples in the batch ” on page 557 .
	Submits only the selected samples for processing. See the instructions “ To submit selected peaks for processing ” on page 556 .
	Opens the Acquisition mode where you can use a batch template to define a standard sequence composed of various sample types to be assembled into a batch of samples. See “ Working in Data Review ” on page 566 .
	Opens the Acquisition mode where you can create a batch template that contains the basic settings and sample types for your batches. See “ Using the Acquisition Mode ” on page 347 .
	Opens the Quick Acquisition window where you can quickly submit a single sample. See Appendix A , “ Using Quick Acquisition .”
	Opens the Audit Viewer where you can view audit logs. See Chapter 13 , “ Using the Audit Viewer .” Available only when you enable Auditing in the Administrator Console. Refer to the instructions in the <i>TraceFinder Administrator Console User Guide</i> .

Batch View Sample List




The sample list displays all the quantitative data for the samples of a batch.

Status indicators for each sample indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The sample list includes the following columns of information:

Figure 174. Batch View sample list





Local Method:	Method_Screening	Update	Instrument:	Thermo Scientific Instrument
---------------	------------------	--------	-------------	------------------------------

	Status	Filename	Sample type	Groups	Blank Subtraction	Level	Sample ID	Sample name	Vial position	Injection volume
1		UnknownA1	Unknown		<input type="checkbox"/>		1		CStk1-01:7	10.0
2		UnknownA2	Unknown		<input type="checkbox"/>		1		CStk1-01:7	10.0
3		UnknownA3	Unknown		<input type="checkbox"/>		1		CStk1-01:7	10.0

Calculation Type	Conversion Factor	Dilution Factor	Sample Weight	Sample Volume	Final Units
Liquid	1.000	1	1	1	
Liquid	1.000	1	1	1	
Liquid	1.000	1	1	1	

Instrument Method	Channel	Barcode Expected	Barcode Actual	Comment
Instrument1	Auto			
Instrument1	Auto			
Instrument1	Auto			

Table 123. Batch View sample list columns (Sheet 1 of 3)

Column	Description
Status	<ul style="list-style-type: none">  Sample is not acquired.  Sample is acquired but not processed.  Sample is acquired and processed.  Sample is currently acquiring.
Filename	Name of the raw data file that contains the sample data.
Sample Type	<p>Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC Std, or Unknown</p> <p>Default: Unknown</p>

10 Using the Analysis Mode for Target Screening Batches

Working in the Batch View

Table 123. Batch View sample list columns (Sheet 2 of 3)

Column	Description
Groups	Threshold group to which a sample belongs.
Blank Subtraction	Specifies a matrix blank sample to use for blank subtraction.
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.
Vial Position	The tray vial number used for an autosampler acquisition.
Injection Volume	<p>The injection volume (in microliters) of the injected sample.</p> <p>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 displayed range.</p> <p>The Injection Volume value set in the master method overwrites the value in the instrument method.</p> <p>Valid range: 0.1 through 5000 µL</p>
Calculation Type	<p>Liquid: The application calculates the Conversion Factor as</p> $\text{SampleVolume} \div \text{DilutionFactor}$ <p>Solid: The application calculates the Conversion Factor as</p> $(\text{SampleVolume} \times \text{DilutionFactor}) \div \text{SampleWeight}$ <p>Manual: Sample Volume, Dilution Factor, Sample Weight, and Final Units columns are not available, and the Conversion Factor value is editable.</p>
Conversion Factor	<p>Editable only when Calculation Type is Manual.</p> <p>Default: 1</p>
Sample Volume	Default: 1
Dilution Factor	Default: 1
Sample Weight	<p>Available only when Calculation Type is Solid.</p> <p>Default: 1</p>
Final Units	<p>Specifies the calculated amount in the Data Review view or in reports.</p> <p>Default: 1</p>
Instrument Method	Specifies the instrument to use for the acquisition. This column is hidden by default. To display this column, see “To customize the column display” on page 532.

Table 123. Batch View sample list columns (Sheet 3 of 3)

Column	Description
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. The Channel column is available only when you have activated multiplexing in the Configuration console. See “ Multiplexing ” on page 61 .
Barcode Expected	A user-entered barcode for the vial.
Barcode Actual	An actual barcode for the vial. This value is not editable.
Comment	A user-defined comment for the sample.

Batch View Shortcut Menu

The Batch View includes a shortcut menu for creating a batch.

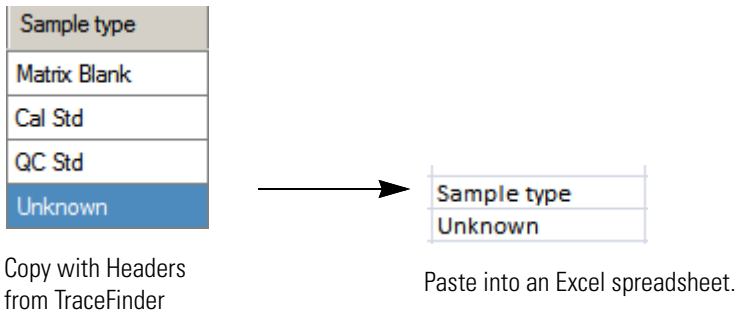
Table 124. Batch View shortcut menu commands (Sheet 1 of 2)

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 546 .
Browse in Raw File (Move)	Opens a dialog box where you can select a raw data file to use for the selected sample row. The application removes the raw data file from the source location.
Browse in Raw File (Copy)	Opens a dialog box where you can select a raw data file to use for the selected sample row. The application copies the raw data file from the source location.
Map Raw Files to Samples	Opens a dialog box where you can select multiple raw data files to use for the selected 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 532 .
Enable/Disable Sample Weight Calculation	Displays or hides the Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns.

10 Using the Analysis Mode for Target Screening Batches

Working in the Batch View

Table 124. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information into a text editor or spreadsheet application. You cannot paste this data back into the Batch View 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 into another text editor or spreadsheet application. You cannot paste this data back into the sample list. For example  <p>Copy with Headers from TraceFinder</p> <p>Paste into an Excel spreadsheet.</p>
Paste	Pastes a single column of copied data from another text editor or spreadsheet application 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.
Edit Instrument Method	Opens the Instrument Setup window where you can edit the parameters of the instrument method. <ul style="list-style-type: none">• When you edit an external method, the application updates the method in the ...\\Xcalibur\\methods folder.• When you edit an internal method, the application updates the method in the ...\\TraceFinderData\\3.3\\Projects\\...\\batch\\Methods\\method folder. <p>For detailed information about editing instrument methods, see “Working with Instrument Methods” on page 108.</p>

Compound Active Status Pane

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 sample list, select a sample.

All compounds in the selected sample are listed in the Compound Active Status pane.

Compound Active Status

	RT	Compound	Active
▶ 1	1.91	FENTHION-CE20-R20-TL75-QED	<input checked="" type="checkbox"/>
2	2.72	Sulfisomidine	<input checked="" type="checkbox"/>

The default active/inactive status is determined by the identification settings in the local method. For information about setting the identification parameters, see “[Identification](#)” on [page 152](#).

- To display compounds alphabetically, right-click and choose **Sort by Compound Name** from the shortcut menu.
 - To display compounds from shorter to longer retention times, right-click and choose **Sort by Retention Time** from the shortcut menu.
2. Select or clear the **Active** check box for the compound.

Compound Active/Inactive Status

You can specify which compounds are active or inactive in the [Local Method View](#) or the [Batch View](#).

Figure 175. Active and inactive compounds in the Local Method View

Local Method View - Batch_2_Method_Vitamin1						
Master method: Method Vitamin1						
Acquisition List	Identification	Detection	Calibration	Calibration levels	Chk Std levels	Real Time View
	RT	Compound	Compound type	Active	CAS No	
1	5.88	1-Butanol, 4-(butylnitrosoamino)-	Target Compound	<input type="checkbox"/>	3817116	
2	16.68	3,3'-Diaminodiphenylmethane	Target Compound	<input checked="" type="checkbox"/>	19471126	

For details about setting the status on the Identification page, see “[Identification](#)” on [page 152](#).

Figure 176. Active and inactive compounds in the Batch View

Batch View - Batch_2 [Screening]							
Local Method:		Method_Screening			Update		
	Status	Filename	Sample type	Groups	Blank Subtraction	Level	Sample ID
▶ 1		VitWaterEquanMaxA001	Unknown		<input type="checkbox"/>		CStk1-01:3
2		VitWaterEquanMaxA002	Unknown		<input type="checkbox"/>		CStk1-01:4

Compound Active Status			
	RT	Compound	Active
▶ 1	5.88	1-Butanol, 4-(butylnitrosoami...	<input type="checkbox"/>
2	16.68	3,3'-Diaminodiphenylmethane	<input checked="" type="checkbox"/>
3	2.91	4-Methyl-2,6,7-trioxa-1-phosp...	<input checked="" type="checkbox"/>

For details about setting the status in the Batch View, see “Compound Active Status Pane” on page 543.

Creating a New Batch

In the Batch View, you can create a new batch.

Follow these procedures:

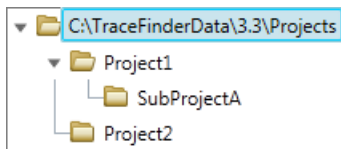
- [To create a new batch](#)
- [To add samples to the list](#)
- [To insert samples into the list](#)
- [To import samples into the list](#)
- [To remove samples from the list](#)
- [To copy a sample](#)
- [To reinject a sample](#)
- [To edit sample values](#)
- [To browse in raw data files](#)
- [To customize the column display](#)

❖ To create a new batch

1. Choose **File > New > Batch** from the main menu.

The Create New Batch dialog box opens, displaying all drives that contain projects. See “Create New Batch Dialog Box” on page 551.

2. Select a drive from the list.



Tip The application displays all configured and enabled repositories.

3. Select the folder where you want to store your batch.

Tip To activate the Create button, you must enter a unique batch name. If the Create button is not activated, you have entered a batch name that is already used.

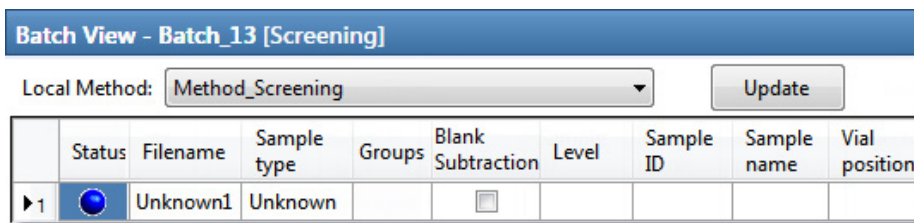
To create a new folder for the storage location, see [“Editing Folders for Batches”](#) on page 552.

4. Select **Screening** from the Type list.

The batch list displays all batches in the selected folder. The Method list displays all methods for the target screening type.


5. Select a master method from the Master Method list.
6. Click **Create**.

A new batch opens with one Unknown sample.



The batch name in the title bar indicates that you are creating a target screening batch.


❖ 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** icon,  .





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 will insert new, Unknown samples, and then 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** icon .

The application inserts the Unknown samples above the selected sample.

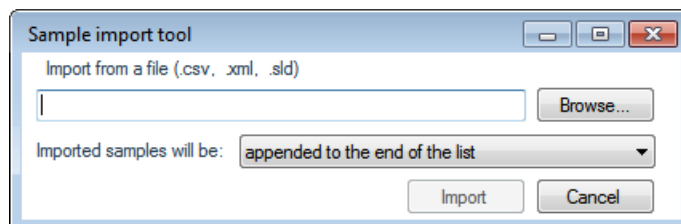
	Status	Filename	Sample type	Groups	Blank Subtraction
1		cal_std_5	Cal Std		<input type="checkbox"/>
2		Unknown2	Unknown		<input type="checkbox"/>
3		Unknown1	Unknown		<input type="checkbox"/>
4		cal_std_10	Cal Std		<input type="checkbox"/>

Inserted samples

❖ To import samples into the list

1. Choose **Batch > Import Samples** from the main menu, or click the **Import Samples** icon, .

The Sample Import Tool dialog box opens.



From this dialog box, you can import samples from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file that contains the samples 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 sample list.

When you import samples from an Xcalibur sequence file (.sld), the application makes the following column name substitutions:

Xcalibur column	TraceFinder column
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conversion Factor

When you import samples from an Xcalibur sequence file (.sld), the application makes the following sample type substitutions:

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	QC Std
Std Bracket	Cal Std

- (Optional) When using multiplexing, select a channel for each imported sample. Imported samples default to Auto.

Note The Channel column is available only when you have activated multiplexing in the Configuration console. See “Multiplexing” on page 61.

❖ To remove samples from the list

- Select the samples that you want to remove.

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

- Right-click and choose **Remove Selected Samples** from the shortcut menu.

❖ To copy a sample

- Select the sample that you want to copy.
- Right-click and choose **Insert Copy Sample** from the shortcut menu.

The application inserts the copy above the selected sample.

❖ To reinject a sample

- In the sample list, select the sample that you want to reinject.
- Right-click and choose **Reinject This Sample** from the shortcut menu.

The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

❖ To edit sample values

1. For each sample, do one of the following:

Type a new file name over the current filename.

–or–

Double-click the Filename column and locate a raw data file to use for the sample.

–or–

Right-click and choose **Browse in Raw File** from the shortcut menu, and then locate a raw data file to use for the sample.

By default, the application sets the Sample Type to Unknown.

2. For each sample, click the Sample Type column and select a sample type from the list.

Available sample types

Matrix Blank	Solvent	QC Std	Unknown
Cal Std			

3. For each Cal Std or QC Std sample, select a level from the Level list.

The sample levels are defined in the master method. If there are no levels to select in the Level list, do the following:

- a. Return to the Method Development mode.
- b. Open the method.
- c. Click the **Compounds** tab.
- d. Click the **Calibration Levels** tab.
- e. Add the levels.
- f. Save the method.
- g. Return to the Batch View in the Analysis mode, and then click **Update**.

Local Method:

The application updates the local method with the new sample levels.

For detailed instructions about specifying calibration levels, see “[Calibration Levels](#)” on [page 207](#).

4. Type a vial position in the Vial Position column for each sample.
5. Type a volume in the Injection Volume column for each sample.

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

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

Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name, while the other columns scroll right and left.

For instructions to automatically copy or fill values in these columns, see [Appendix C, “Using Copy Down and Fill Down.”](#)

❖ To browse in raw data files

1. Do one of the following:

Double-click the Filename column.


–or–

Right-click and choose **Browse in Raw File** from the shortcut menu.

The What Raw File Would You Like to Use dialog box opens.

2. Select a raw data file to use for the sample or use the CTRL key to select multiple files, and then click **Open**.

The application overwrites the selected, unacquired sample in the batch with the first “browsed in” file and adds any additional browsed in files below the selected sample.

For all browsed-in raw data files, the application sets the Status to Acquired, , and sets the Sample Type to Unknown.

Note You cannot overwrite an acquired sample. When you select a sample that is acquired, the application adds all browsed in files below the selected sample.

❖ 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. See “[Modify Columns dialog box](#)” on [page 550](#).

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

All the columns you select appear after the Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

- a. In the Displayed Columns pane, select a column name.

- b. Use **Up** or **Down** 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, and the last column in the list represents the rightmost column in the Batch View sample list.

Note The following columns are fixed: Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:
 - a. In the Displayed Columns pane, select the column width.

7	Vial position	69
▶ 8	Injection volume	100
9	Calculation Type	100

- 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.

Figure 177. Modify Columns dialog box

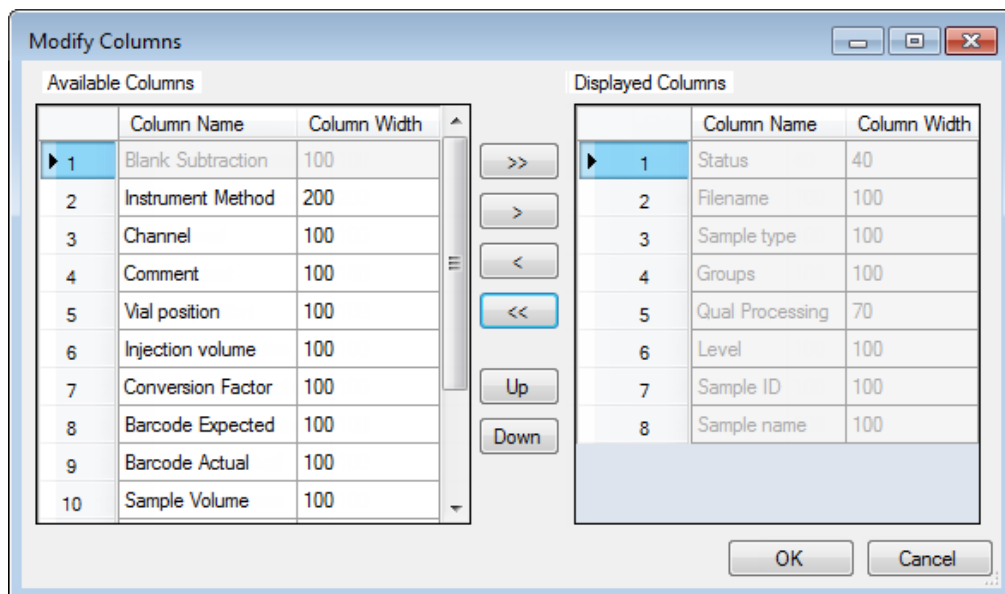






Table 125. Button descriptions for the Modify Columns dialog box (Sheet 1 of 2)

Button	Description
	Moves all columns to the Displayed Columns pane.
	Moves the selected column to the Displayed Columns pane.

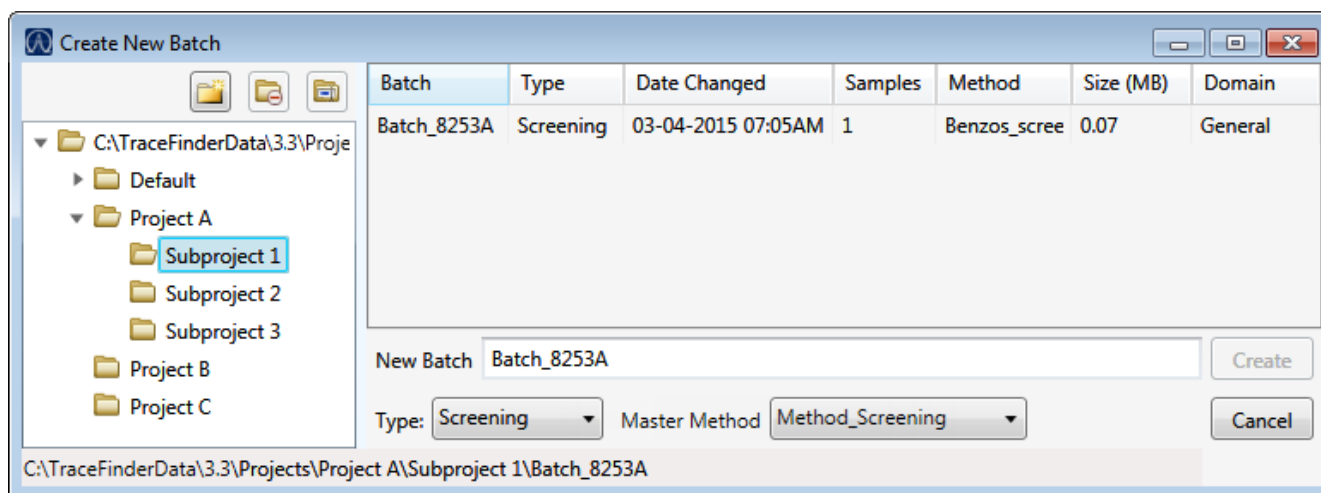
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name.



Table 125. Button descriptions for the Modify Columns dialog box (Sheet 2 of 2)

Button	Description
	Moves the selected column to the Available Columns pane.
	Moves all columns except those that are fixed.
	Moves the selected column name in the Displayed Columns pane one row up in the column order.
	Moves the selected column name in the Displayed Columns pane one row down in the column order.

Create New Batch Dialog Box

Use the Create New Batch dialog box to select a folder and method for your batch and to name the new batch.


**Table 126.** Create New Batch dialog box parameters (Sheet 1 of 2)

Parameter	Description
 Create New Folder	<p>Adds one of the following:</p> <ul style="list-style-type: none"> • When a drive is selected, adds a new project-level folder to the drive. • When a project folder is selected, adds a subproject-level folder to the selected project. • When a subproject folder is selected, adds a lower-level folder to the subproject. <p>Or, right-click and choose Create Folder from the shortcut menu.</p>
 Delete Folder	<p>With no confirmation prompt, immediately removes the selected folder.</p> <p>You cannot delete a folder that contains lower-level folders; you must delete the lower-level folders first.</p> <p>Or, right-click and choose Delete from the shortcut menu.</p>

10 Using the Analysis Mode for Target Screening Batches

Working in the Batch View

Table 126. Create New Batch dialog box parameters (Sheet 2 of 2)

Parameter	Description
	Renames the selected folder.
Rename Folder	Or, right-click and choose Rename from the shortcut menu.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
New batch parameters	
New Batch	Name of the new batch to create.
	Note If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Type	Type of batch to create: Quan, Screening, or Unknown Only.
Method	Method used to create the new batch.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is created.
Buttons	
Create	Creates the specified batch and opens the Batch View for the new batch.
Cancel	Closes the Create New Batch dialog box without creating a batch.

Editing Folders for Batches

From the Create New Batch dialog box, you can create new folders for your batches. You can also delete or rename folders.

Use these procedures:

- [To create new project folders](#)
- [To delete project folders](#)
- [To rename project folders](#)

❖ To create new project folders

1. In the Create New Batch dialog box, select the folder for which you will create a new lower-level folder.
 - You can select the main TraceFinderData\3.3\Projects folder and create a new folder under it.
 - You can select one of the existing folders and create a lower-level folder under it.

2. Click the **Create Folder** icon, .

The application adds a new lower-level folder to the selected folder.

3. Select the new folder name and type a name for the folder.

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

Note After you add a lower-level folder, you cannot rename the parent folder.

❖ To delete project folders

1. In the Create New Batch dialog box, select the folder to delete.

2. Click the **Delete Folder** icon, .

With no confirmation prompt, the application immediately removes the selected folder.

Note You cannot delete folders that contains lower-level folders; you must delete the lower-level folders first.

❖ To rename project folders

1. In the Create New Batch dialog box, select the folder to rename.

2. Click the **Rename Folder** icon, .

Note You cannot rename folders that contain lower-level folders.

3. Type a new name for the folder and press ENTER.

The application saves the new folder name.

Editing a Batch

In the Batch View, you can open a saved batch and edit the sample 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 “ready to acquire” batch.

Follow these 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 open a saved batch

1. Choose **File > Open > Batch** from the main menu.

The Open Batch dialog box opens. See [Open Batch dialog box](#) or [Open Batch dialog box parameters](#).

2. Select a project and a subproject.
3. Select **Screening** or **Any** from the Type list.

The batch list displays all batches created with Target Screening methods (or when you select Any, all methods of all types).

4. Select a batch from the list.
5. Click **Open**.

The selected batch opens in the Batch View.

Figure 178. Open Batch dialog box

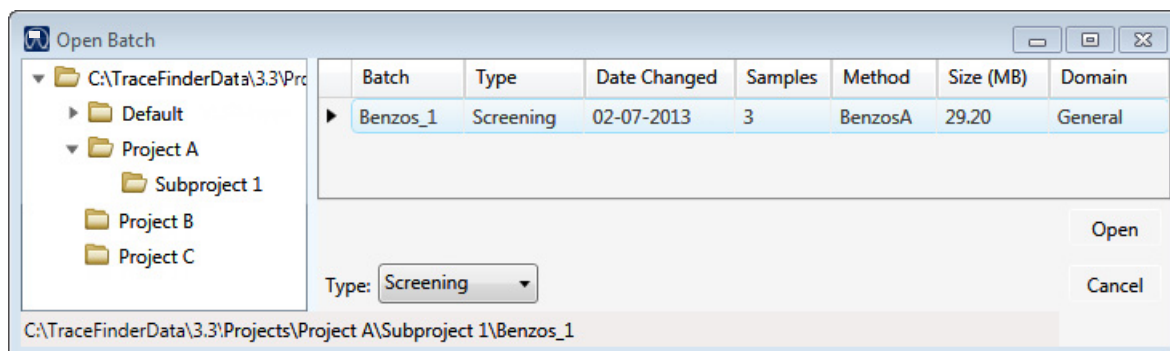
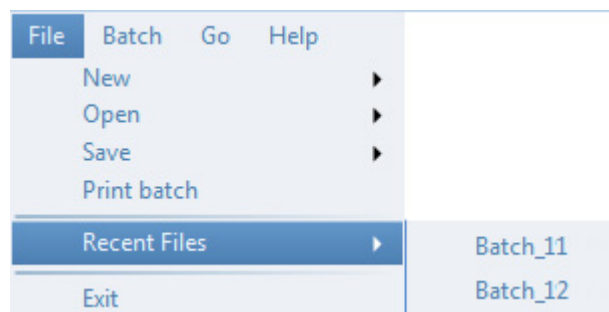


Table 127. Open Batch dialog box parameters

Parameter	Description
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is stored.
Buttons	
Type	Type of batch to display in the Batch list: Quan, Screening, Unknown Only, or Any.
Open	Opens the Batch View for the selected batch.
Cancel	Closes the Open Batch dialog box without opening a batch.

❖ To open a recent batch

Choose **File > Recent Files > *batch*** from the main menu.



The selected batch opens in the Batch View.

❖ To edit samples in a batch

Use the commands described in “[Working in the Batch View](#)” on page 530.





You can add new samples, edit samples, or delete samples.

❖ To reinject a sample from a previously acquired batch

1. In the sample list, select the sample that you want to reinject.
2. Right-click and choose **Reinject This Sample** from the shortcut menu.

The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The 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	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

When you submit all samples in this batch, the application acquires all samples (including previously acquired samples).

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 prepared batch that is ready to submit. You can open this batch from the Reinject Samples page in the Acquisition mode and submit the batch. The application acquires only the samples that have not been previously acquired.

Submitting a Batch


In the 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 559](#).

For a description of commands in the shortcut menu, see “[Batch View shortcut menu commands](#)” on [page 541](#).

Follow these procedures:

- [To submit selected peaks for processing](#)
- [To submit samples in the batch](#)
- [To view the output files](#)


❖ To submit selected peaks for processing


1. In the Peak List, select the **Selected** check box for the peaks that you want to process.
2. Click the **Submit ... for Processing** icon, .

The application processes the selected peaks and updates the data in the Peak Identifications pane.

❖ To submit samples in the batch

1. Do one of the following:

- To submit all samples in the batch, click the **Submit Batch** icon, .
- To submit specific samples, select the samples and click the **Submit Selected**

Samples icon, .

The Submit Options dialog box opens. See “[Submit Options dialog box](#)” on [page 559](#).

Note You can also submit only selected peaks for processing. See “[To submit selected peaks for processing](#)” on [page 556](#).

2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.

- When all submitted samples have been previously acquired, this option is (by default) not selected.
- When one or more samples in the batch have not been acquired, this option is (by default) selected.

Tip You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

3. To process the submitted samples, select the **Process Data** check box.

The application displays processing options for the Target Screening method.

If the method includes unknown screening features, the application also displays unknown screening options. For specifying processing data for batches that also use unknown screening features, see “[To submit samples in the batch](#)” on [page 633](#) of [Chapter 11, “Using the Analysis Mode for Unknown Screening Batches.”](#)

4. Select the check box for the options that you want to use.

Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

Identify and Confirm: Performs both identification and confirmation.

5. (Optional) Select the **Create Reports** check box.

6. (Optional with multiplexing activated) 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 activated) 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.

Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.
 - a. Select the **Use** check box for the device that you want to use for this acquisition.
 - b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

This is usually the autosampler.
 - c. 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.
 - d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.
9. To start the selected processes, click **OK**.

The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Analysis mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT When your batch also uses unknown screening features, after the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages for the unknown screening features (“[Editing the Processing Pages](#)” on [page 311](#)) and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Figure 179. Submit Options dialog box

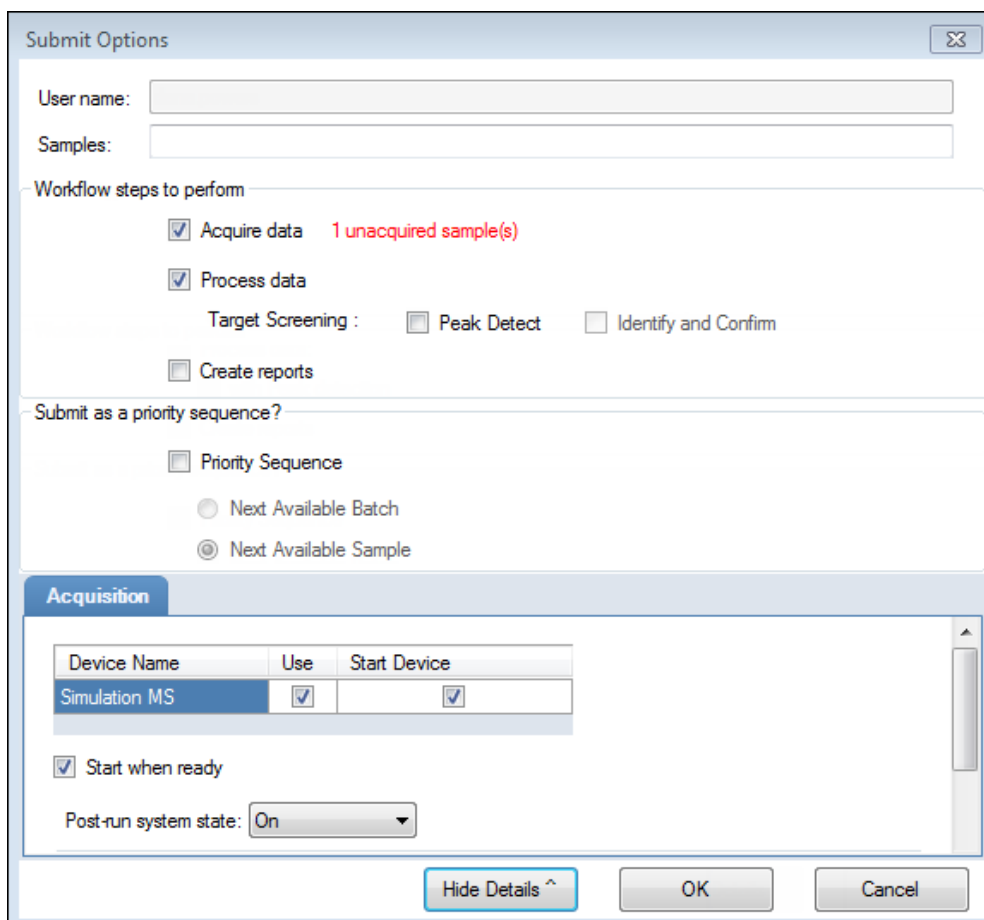


Table 128. Submit Options dialog box parameters (Sheet 1 of 3)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Workflow Steps to Perform	
Acquire Data	Submits the current batch to acquisition. <ul style="list-style-type: none"> When all submitted samples have been previously acquired, this option is (by default) not selected. When one or more samples in the batch have not been acquired, this option is (by default) selected.

Table 128. Submit Options dialog box parameters (Sheet 2 of 3)

Parameter	Description
Process Data	<p>Processes the data for the current batch using any of the following options:</p> <p>Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.</p> <p>Identify and Confirm: Performs both identification and confirmation.</p> <p>Note Target Screening methods can include unknown screening features. For specifying processing data for batches that also use unknown screening features, see “To submit samples in the batch” on page 633.</p>
Create Reports	Creates reports for the current batch.
Submit as a Priority Sequence?	
Priority Sequence	<p>With multiplexing activated, places the batch immediately after the currently acquiring batch.</p> <p>Without multiplexing activated, specifies one of the following priority options to place the batch in the queue:</p> <p>Next Available Batch: Places the batch immediately after the currently acquiring batch.</p> <p>Next Available Sample: Places the batch immediately after the currently acquiring sample.</p> <p>Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.</p>
Acquisition pane	
Device Name	<p>Lists all configured instruments.</p> <p>If the instrument that 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.</p> <p>Available only when you select the Acquire Data check box.</p>
Use	<p>Specifies the instruments used for this acquisition.</p> <p>Available only when you select the Acquire Data check box.</p>

Table 128. Submit Options dialog box parameters (Sheet 3 of 3)

Parameter	Description
Start Device	Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler. Available only when you select the Acquire Data check box.
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.
Post-run System State	Specifies the system state after it acquires the last batch: On (default), Standby, or Off.
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.

❖ To view the output files

Locate the files to view from the following directories:

The application writes saved batches to the project folder:

```
... \TraceFinderData\3.3\Projects\...
```

For each acquired sample, the application writes an RSX file to the batch Data folder:

```
... \TraceFinderData\3.3\Projects\...\Data
```

The application saves method information to the batch Methods folder:

```
... \TraceFinderData\3.3\Projects\...\Methods
```

The application writes the reports to the batch Reports folder:

```
... \TraceFinderData\3.3\Projects\... \batch\Reports
```

Saving a Batch to a New Location

You can move the current batch to a different project folder, or you can make a copy of the current batch and save the copy to a different project folder.

Follow these procedures:

- [To save a batch to another project folder](#)
- [To move a batch to another folder](#)
- [To create a new project folder](#)
- [To delete project folders](#)
- [To rename project folders](#)

❖ To save a batch to another project folder

1. Choose **File > Save > Save Batch As** from the Batch View main menu in the Analysis mode.

The Save Batch As dialog box opens. See [“Save Batch As Dialog Box” on page 564](#).

2. Select a storage location.

The default storage location is C:\TraceFinderData\3.3\Projects.

3. Select or create a project folder.

4. Type a name for the new batch.

If you are saving the batch to a different folder, you must give it a unique name. You cannot overwrite an existing batch in a folder.

5. Click **Save**.

When you save the batch to a different folder, the reports reflect the original project folders and the application does not save the calibration history.

❖ To move a batch to another folder

1. Choose **File > Save > Move Batch** from the Batch View main menu in the Analysis mode.

The Save Batch As dialog box opens. See [“Save Batch As Dialog Box” on page 564](#).

2. Select a storage location.

The default storage location is C:\TraceFinderData\3.3\Projects.

3. Select or create a project folder.


4. Type a name for the new batch.

You must give the batch a unique name in the new subproject folder. You cannot overwrite an existing batch.

5. Click **Save**.

When you move the batch, the reports reflect the original project and subproject folders and the application does not save the calibration history.

❖ To create a new project folder

1. In the Save Batch As dialog box, select the folder for which you will create a new lower-level folder.
 - You can select the main TraceFinderData\3.3\Projects folder and create a new folder under it.
 - You can select one of the existing folders and create a lower-level folder under it.
2. Click the **Create Folder** icon, .


The application adds a new lower-level folder to the selected folder.

3. Select the new folder name and type a name for the folder.

Folder names can contain spaces and special characters, except for the following special characters: \ / : + ? " < >

Note After you add a lower-level folder, you cannot rename the parent folder.


❖ To delete project folders

1. In the Save Batch As dialog box, select the folder to delete.
2. Click the **Delete Folder** icon, .

With no confirmation prompt, the application immediately removes the selected folder.

Note This feature is not available for folders that contain lower-level project or batch folders; you must first delete the lower-level project or batch folders.

❖ To rename project folders

1. In the Save Batch As dialog box, select the folder to rename.
2. Click the **Rename Folder** icon, .

Note This feature is not available for folders that contain lower-level project or batch folders; you must first delete the lower-level project or batch folders.

3. Type a new name for the folder and press ENTER.

The application saves the new folder name.

Save Batch As Dialog Box

Use the features in the Save Batch As dialog box to save a batch to a new name or to move a batch to a different project folder.

Figure 180. Save Batch As dialog box

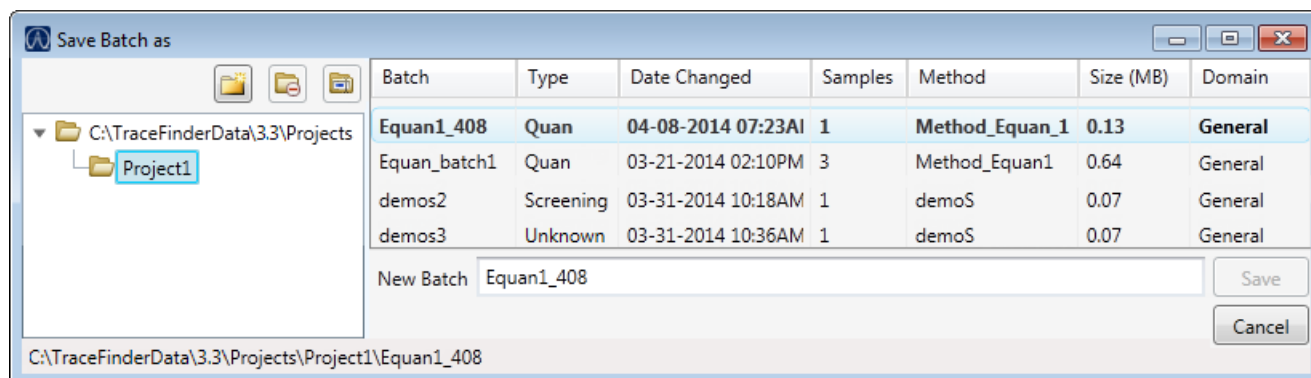


Table 129. Save Batch As dialog box parameters (Sheet 1 of 2)




Parameter	Description
 Create New Folder	Adds one of the following: <ul style="list-style-type: none"> When a drive is selected, adds a new project-level folder to the drive. When a project folder is selected, adds a subproject-level folder to the selected project. When a subproject folder is selected, adds a lower-level folder to the subproject. Or, right-click and choose Create Folder from the shortcut menu.
 Delete Folder	With no confirmation prompt, immediately removes the selected folder. You cannot delete a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders. Or, right-click and choose Delete from the shortcut menu.
 Rename Folder	Renames the selected folder. You cannot rename a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders. Or, right-click and choose Rename from the shortcut menu.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.

Table 129. Save Batch As dialog box parameters (Sheet 2 of 2)

Parameter	Description
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
New batch parameters	
New Batch	Name of the new batch to create. Note If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is created.
Buttons	
Save	Saves the batch to the specified name and folder and opens the Batch View for the new batch.
Cancel	Closes the Save Batch As dialog box without saving the batch.
Shortcut menu commands	
Create Folder	Adds one of the following: <ul style="list-style-type: none"> • When a drive is selected, adds a new project-level folder to the drive. • When a project folder is selected, adds a subproject-level folder to the selected project. • When a subproject folder is selected, adds a lower-level folder to the subproject.
Delete Folder	Immediately removes the selected folder. There is no prompt to confirm that you want to delete the selected folder. You cannot delete a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders.
Rename Folder	Renames the selected folder. You cannot rename a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders.
Expand Child Nodes	Expands all project and subproject folders in the Project tree.
Collapse Child Nodes	Collapses all project and subproject folders in the Project tree.

Working in Data Review

The Data Review view displays the data generated by the master method. Use Data Review to verify the data for a compound before you generate reports.

Follow these procedures:

- [To open the Data Review view](#)
- [To display or hide a pane on the Target Screening page](#)
- [To move, dock, or float Data Review panes](#)
- [To restore the default layout](#)

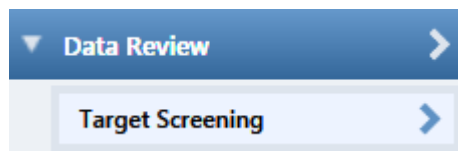
❖ To open the Data Review view

1. Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.

2. Click **Data Review**.

The Data Review navigation pane opens.

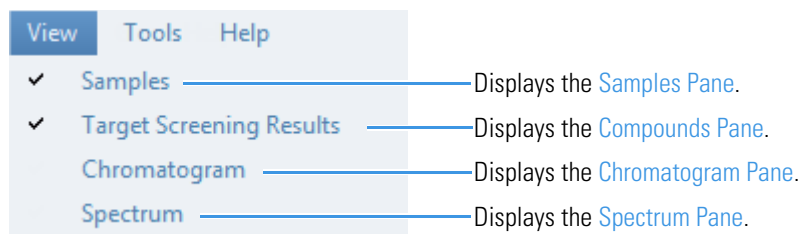


On the Target Screening page, the panes show the following:

- A list of all samples in the current batch
- The compound results for all compounds in the method
- Chromatogram and spectrum plots for all compounds found in the currently selected sample

❖ To display or hide a pane on the Target Screening page

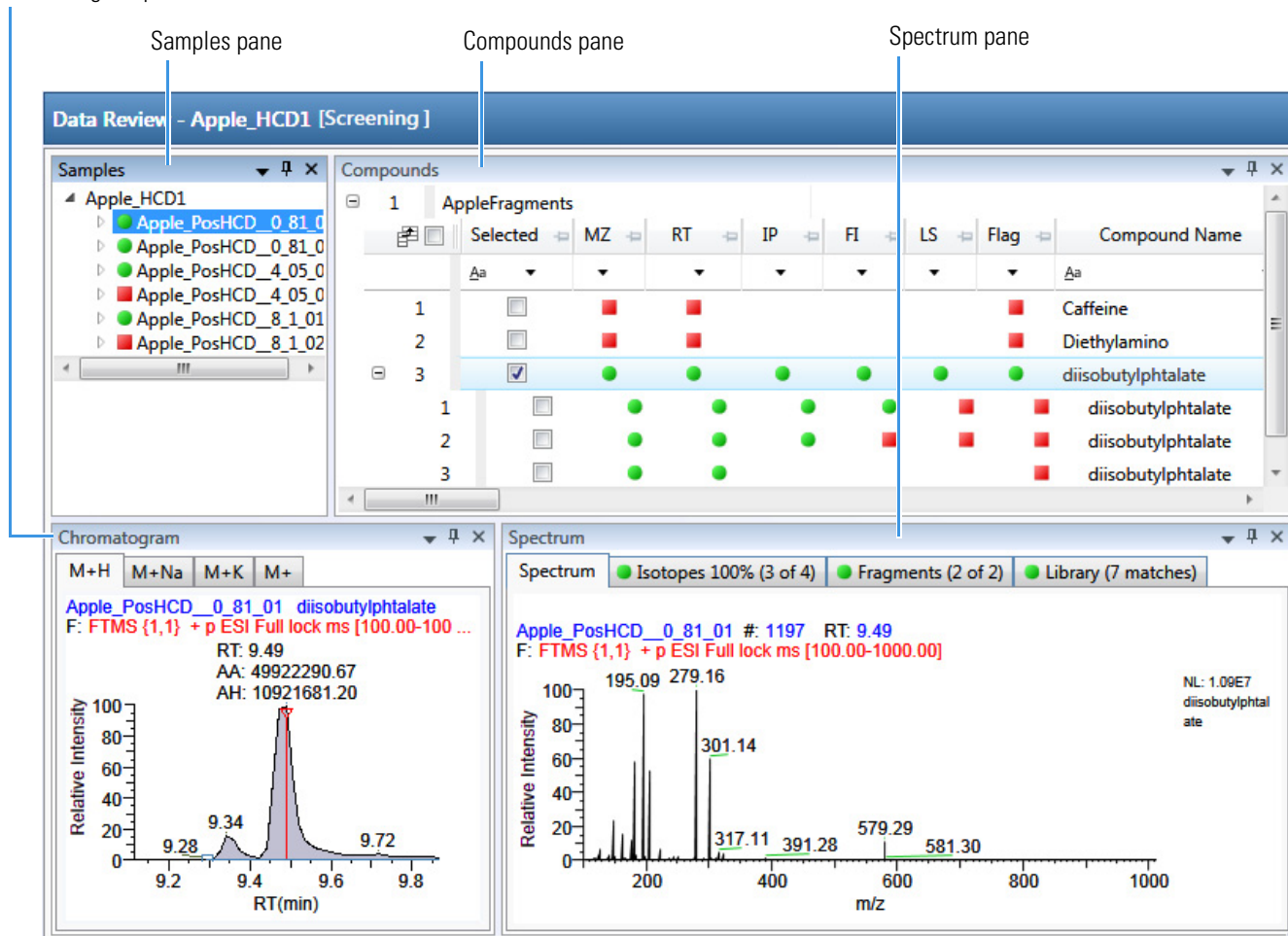
From the View menu, choose to display—indicated with a check mark—or hide the following panes:



See [Target Screening panes](#).

Figure 181. Target Screening panes

Chromatogram pane



When you select a sample in the Samples pane, the associated Compounds pane flags any compound with errors in the selected sample. The associated Chromatogram pane displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the selected sample. The Spectrum pane highlights the compound selected in the Compounds pane. You can display, hide, or move any of these panes.

❖ **To move, dock, or float Data Review panes**

Follow the instructions in [Appendix D, “Moving Data Review Panes.”](#)

❖ **To restore the default layout**

Choose **View > Restore Default Layout**.

The Target Screening view displays the default panes in their default locations.

Samples Pane

Use the Samples pane to select a specific sample in the batch. The associated [Compounds Pane](#) displays all compounds in the method and flags any compound with errors in the selected sample.

Flags in the Samples pane indicate one of the following:

- A green circle means that the sample/compound/peak combination is identified and fully confirmed.
- ▲ A yellow triangle means that the sample/compound/peak combination is identified but not fully confirmed.
- A red square means that the sample/compound/peak combination is not identified.

Figure 182. Samples pane

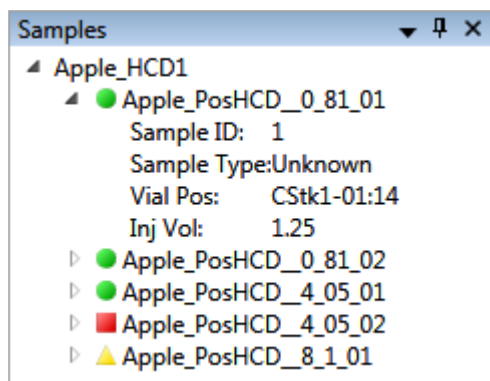


Table 130. Samples pane shortcut menu commands

Command	Description
Sort by Alphabetical	Sorts the samples alphabetically by sample name.
Sort by Import Order	Sorts the samples in the order they were processed.

Compounds Pane

The Compounds pane displays all found peaks in the selected sample and flags any compound with errors. The compounds table reflects the identified compounds found in the compound database and the results of the method processing criteria. See “[Compounds Pane Columns](#)” on [page 576](#).

Color Coding for Measured or Calculated Values

The Compounds pane uses color-coded text to indicate the following:

- Green—Indicates that the measured value of scoring and confirmations pass the criteria specified in the method.
- Red—Indicates that the measured or calculated value does not pass the criteria specified in the method.

Measured Area	Library Score (%)
3.1312E04	12
1.9131E05	10
6.7147E04	10
1.4341E05	11

Displaying Multiple Adducts

When the application finds multiple adducts at the same retention time in a sample, the Compounds pane displays the adducts on separate rows in the table.

3	<input checked="" type="checkbox"/>	●	●	●	●	●	●	diisobutylphtalate	diisobutylphtalate@RT 9.49	C16H22O4	M+H	
1	<input type="checkbox"/>	●	●	●	●	●	■	■	diisobutylphtalate	diisobutylphtalate@RT 9.49	C16H22O4	M+Na
2	<input type="checkbox"/>	●	●	●	■	■	■	■	diisobutylphtalate	diisobutylphtalate@RT 9.49	C16H22O4	M+K
3	<input type="checkbox"/>	●	●				■	■	diisobutylphtalate	diisobutylphtalate@RT 9.49	C16H22O4	M+

Exporting Compounds

Use the commands in the File menu to export data to an Excel spreadsheet, a CSV file, a compound database, or a new quantitation method.

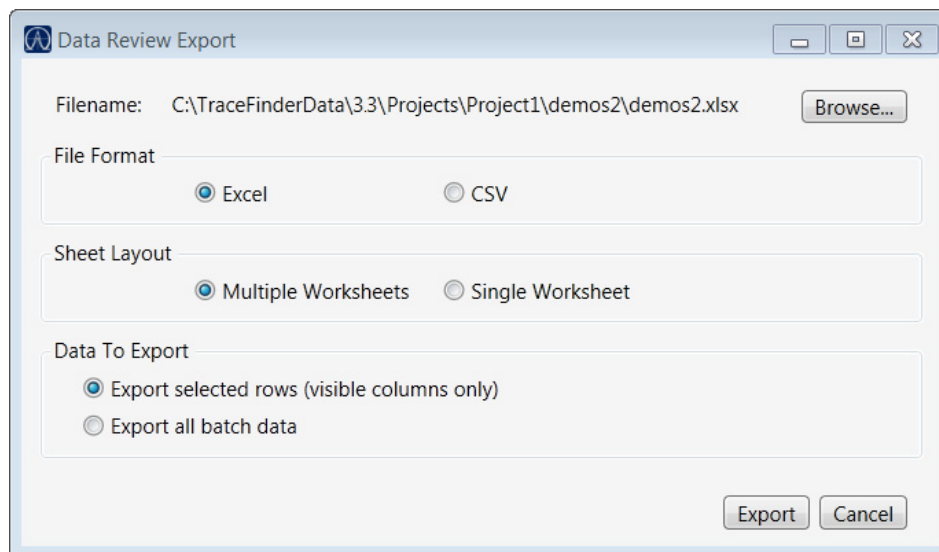
Follow these procedures:

- [To export compounds to an Excel spreadsheet](#)
- [To export compounds to a CSV file](#)
- [To export compounds to a compound database](#)
- [To create a new quantitation method with the selected compounds](#)
- [To create a new quantitation method and update the compound database](#)

❖ To export compounds to an Excel spreadsheet

1. For each compound that you want to export to an Excel spreadsheet, select the check box in the Selected column.
2. Choose **File > Export Data To > CSV or Excel** from the main menu

The Data Review Export dialog box opens.



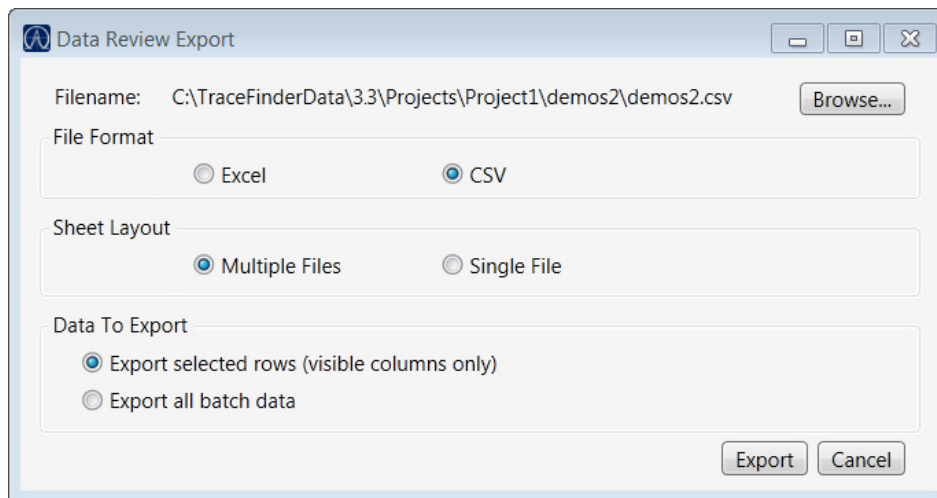
3. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.
4. Type a file name for the XLSX file and click **Save**.
5. In the File Format area, select the **Excel** option.
6. In the Sheet Layout area, select one of the following file formats for the spreadsheet.
 - **Multiple Worksheets:** Writes one sample to each Excel worksheet tab.
 - **Single Worksheet:** Writes all samples to a single Excel worksheet tab.
7. In the Data to Export area, select one of the following sets of data to export.
 - **Export Filtered and Selected Rows (Visible Columns Only):** Writes data from the displayed columns of selected samples to the specified worksheet format.
 - **Export All Batch Data:** Writes data from all columns (displayed or hidden) of all samples to the specified worksheet format.
8. Click **Export**.

The application saves the specified compound data to an Excel spreadsheet and opens the folder where you saved the file.

❖ To export compounds to a CSV file

1. For each compound that you want to export to a CSV file, select the check box in the Selected column.
2. Choose **File > Export Data > To CSV or Excel** from the main menu.

The Data Review Export dialog box opens.



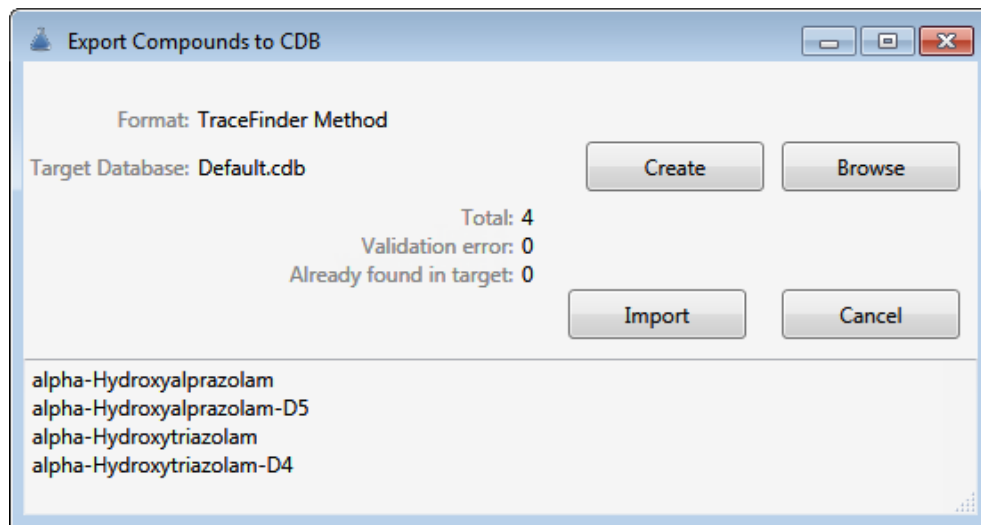
3. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.
4. Type a file name for the CSV file and click **Save**.
5. In the File Format area, select the **CSV** option.
6. In the Sheet Layout area, select one of the following file formats for the spreadsheet.
 - **Multiple Files:** Writes one sample to each CSV file.
 - **Single File:** Writes all samples to a single CSV file.
7. In the Data to Export area, select one of the following sets of data to export.
 - **Export Filtered and Selected Data Only:** Writes data from the selected compounds to the specified worksheet format.
 - **Export All Batch Data:** Writes all data from all samples in the batch to the specified worksheet format.
8. Click **Export**.

The application saves the specified compound data to an CSV spreadsheet and opens the folder where you saved the file.

❖ To export compounds to a compound database

1. For each compound that you want to export to a compound database, select the check box in the Selected column, including any adducts that you want to export.
2. Choose **File > Export Data To > Compound Database** from the main menu.

The Export Compounds to CDB dialog box opens.



3. Do one of the following:
 - Accept the default target database.
 - Click **Create** and type the name for a new compound database.
 - Click **Browse** and select from the list of compound databases.
4. Click **Import**.
 - When you export compounds to a database that already contains these compounds, the application updates the retention times in the database.
 - When you add compounds to a database that does not contain these compounds, the application adds all the compound data to the database.

When you export only one adduct for a compound, the application uses the selected adduct as the peak in the updated or new compound database. When you export multiple adducts for export, the application uses the adducts in the order of intensity.

The application uses the measured retention time value for the compound in the updated or new compound database.

The application uses the expected *m/z* value for the compound in the updated or new compound database.

The application exports all found fragments to the updated or new compound database.

❖ **To create a new quantitation method with the selected compounds**

1. For each compound that you want to export to a new quantitation method, select the check box in the Selected column including any adducts that you want to export.
2. Choose **File > Export Data To > New Quantitation Method** from the main menu.

The Acquisition page of a new quantitation method opens.

3. From the Instrument Method list, select a method (.meth) file to use for acquiring the data.
4. Choose **File > Save** from the main menu.
5. In the Save Master Method dialog box, type a name for the method and click **OK**.
6. Click **Compounds** in the Method View navigation pane.

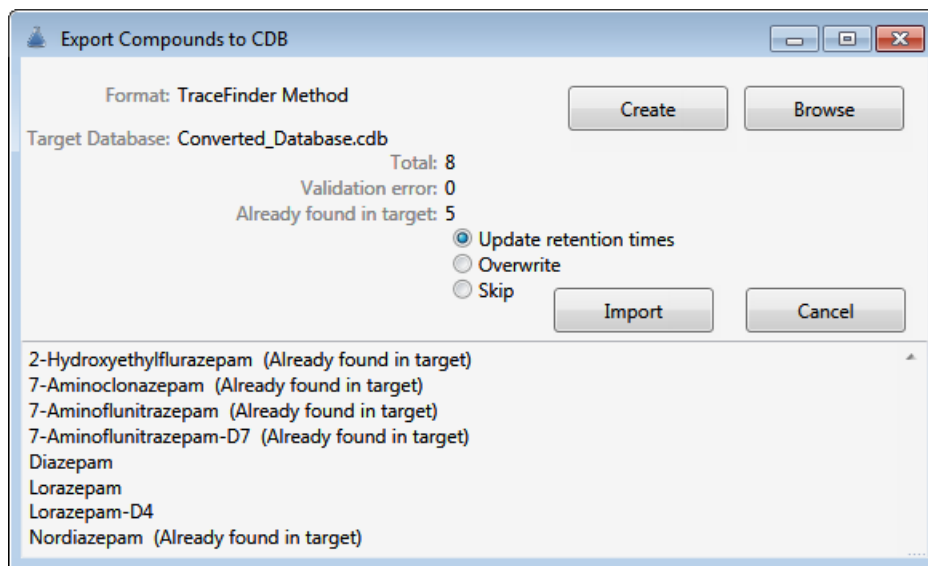
The application exports the selected compounds from the target screening method to the new quantitation method and uses data from the selected compounds as follows:

- Exports quantitation peaks in the order of intensity.
- Exports measured retention time value for the compounds in the new method.
- Exports expected m/z value for the compounds in the new method.
- Exports all found fragments to the new method.
- Adds a filter for both quantitative peaks and confirming ions.

❖ **To create a new quantitation method and update the compound database**

1. For each compound that you want to export, select the check box in the Selected column, including any adducts that you want to export.
2. Choose **File > Export Data > Update Compound Database and Create New Quantitation Method** from the main menu.

The Import Compounds to CDB dialog box opens.



The dialog box lists all compounds selected in the screening batch.

3. Do one of the following:
 - Accept the default target database.
 - Click **Create** and type the name for a new target database.
 - Click **Browse** and select from the list of compound databases.

The compounds list indicates which compounds already exist in the target compound database and which do not.

4. When any of the compounds already exist in the target database, choose one of the following options:
 - **Update Retention Times:** Updates only the retention times for the duplicate compounds in the target database.
 - **Overwrite:** Overwrites all compound data for the duplicate compounds in the target database.
 - **Skip:** Does not write any data from the duplicate compounds to the target database.

5. Click **Import**.

The Acquisition page of a new quantitation method opens.

The screenshot shows a dialog box titled "Method View - Unnamed*" with a subtitle "Calibration file last used:". The dialog contains the following fields and controls:

- Lab Name: Default Laboratory
- Assay type: Assay name
- Injection Volume: 1.00
- Mass Precision: 2.00
- Ion range calc method: Manual
- Instrument Method: (empty dropdown)
- Buttons: Edit, Update


6. From the Instrument Method list, select a method (.meth) file to use for acquiring the data.
7. Choose **File > Save** from the main menu.
8. In the Save Master Method dialog box, type a name for the method and click **OK**.
9. Click **Compounds** in the Method View navigation pane.

The application exports the selected compounds (with the specified options) from the target screening method to the new quantitation method.

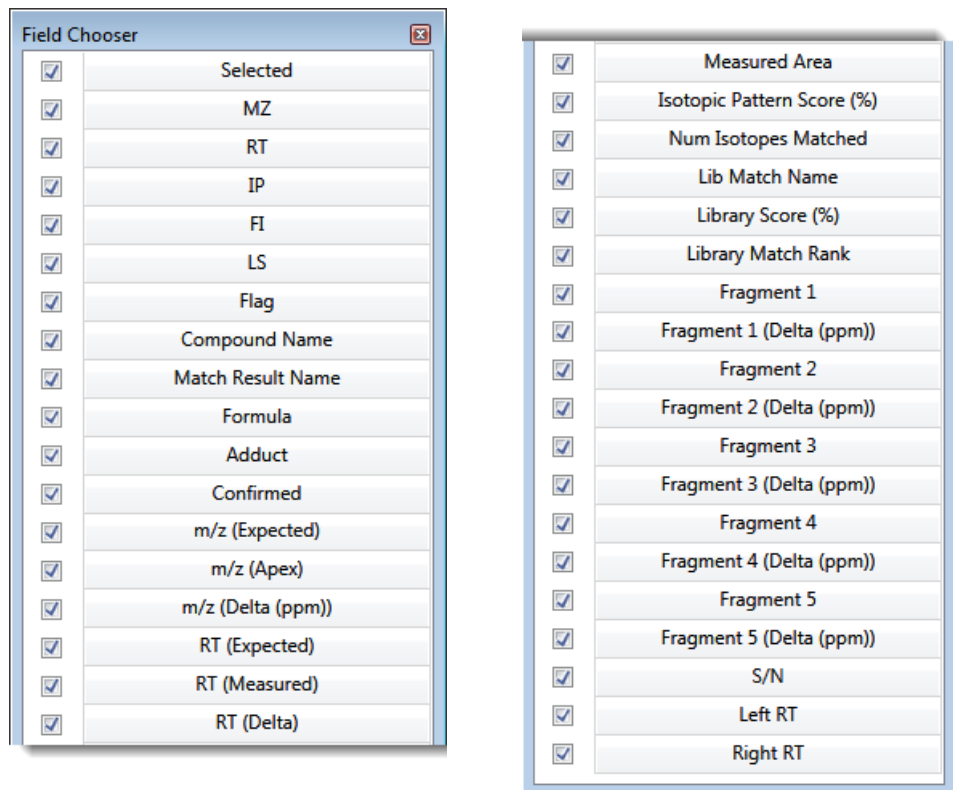
Compounds Pane Columns

The columns of data in the Compounds pane display all parameter values associated with each compound in the selected sample. See [Compounds Pane Parameters](#).

❖ To hide or display columns in the Compounds pane


1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Compounds pane.



2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

The application immediately displays or hides the column in the Compounds pane.

3. When you are finished modifying the column display, click  to close the Field Chooser.

Compounds Pane Parameters

The Compounds pane displays all parameter values associated with each compound in the selected sample.

Figure 183. Compounds pane

	Selected	MZ	RT	IP	FI	LS	Flag	Compound Name	Match Result Name	Formula
1	<input type="checkbox"/>	●	●	●	●	●	●	2-Hydroxyethylflurazepam	2-Hydroxyethylflurazepam@RT 0.19	C17H14ClFN2O2
2	<input type="checkbox"/>	●	●	●	●	●	●	2-Hydroxyethylflurazepam	2-Hydroxyethylflurazepam@RT 1.42	C17H14ClFN2O2
3	<input type="checkbox"/>	●	■	●	●	■	▲	2-Hydroxyethylflurazepam	2-Hydroxyethylflurazepam@RT 1.71	C17H14ClFN2O2
4	<input type="checkbox"/>	●	■	●	●	■	▲	2-Hydroxyethylflurazepam	2-Hydroxyethylflurazepam@RT 1.96	C17H14ClFN2O2
5	<input type="checkbox"/>	●	●	●	●	●	●	2-Hydroxyethylflurazepam	2-Hydroxyethylflurazepam@RT 2.35	C17H14ClFN2O2

Table 131. Compounds pane parameters (Sheet 1 of 6)

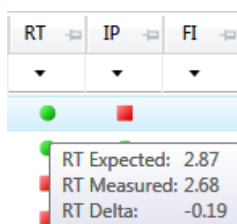
Column	Description
	<p>Displays the current compound database. When you have multiple screening databases, the application lists the results for each database separately.</p> <p> Expand the list of found compounds in the screening database.</p>
<p>Selected</p>	<p>Identifies individual compounds for export. To select all compounds for export, select the check box in the first column.</p> <p> Selects all compounds in the Compounds pane.</p> <p> Selects the compound for export.</p>
<p>MZ</p>	<p>Mass-to-charge ratio flag. The application displays one of these indicators:</p> <ul style="list-style-type: none"> • A green circle (pass) when the measured m/z value is within the specified threshold. • A red square (fail) when the measured m/z value is not within the specified threshold. • A blank when the mass-to-charge value is unavailable. <p>To display the expected, measured, and delta m/z, hold your cursor over the indicator.</p> <p></p>

Table 131. Compounds pane parameters (Sheet 2 of 6)

Column	Description
RT	<p>Retention Time flag. The application displays one of these indicators:</p> <ul style="list-style-type: none"> A green circle (pass) when the measured retention time value is within the RT Window value specified in the compound database. A red square (fail) when the measured retention time value is not within the RT Window value specified in the compound database. In turn, this results in a failure flag for the m/z value because the application cannot identify an m/z value that meets the retention time. A blank when the retention time value is unavailable. When the retention time is selected as “confirm” and the m/z is not detected, there is no flag.

Or, you can set a different retention time window in the method. See [“Editing the Processing Page”](#) on page 264.

To display the expected, measured, and delta retention times, hold your cursor over the indicator.



IP	<p>Isotopic Pattern flag. The application displays one of these indicators:</p> <ul style="list-style-type: none"> A green circle (pass) when the score percentage is higher than the specified fit threshold percentage. A red square (fail) when the score percentage is lower than the specified fit threshold percentage. A blank when the parameter is not scored.
----	--

To display the score of matched isotopes, hold your cursor over the indicator.

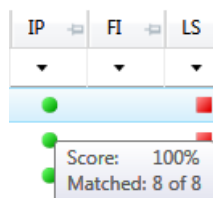


Table 131. Compounds pane parameters (Sheet 3 of 6)

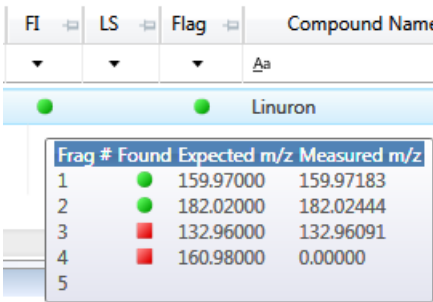
Column	Description																								
FI	<p>Fragment Ions flag. The application displays one of these indicators:</p> <ul style="list-style-type: none"> • A green circle (pass) when the measured m/z value of any of the fragments is within the mass tolerance specified in the method. On the Isotopes page in the Spectrum pane, the All Isotopes and Multi-Isotopes flags are also green. • A red square (fail) when the measured m/z value of none of the fragments is within the mass tolerance specified in the method. On the Isotopes page in the Spectrum pane, the All Isotopes and Multi-Isotopes flags are also red. • A blank when there are no fragments detected. <p>To display a list of fragments and their pass/fail status, hold your cursor over the indicator.</p>  <table border="1" data-bbox="519 861 901 1018"> <thead> <tr> <th>Frag #</th> <th>Found</th> <th>Expected m/z</th> <th>Measured m/z</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>●</td> <td>159.97000</td> <td>159.97183</td> </tr> <tr> <td>2</td> <td>●</td> <td>182.02000</td> <td>182.02444</td> </tr> <tr> <td>3</td> <td>■</td> <td>132.96000</td> <td>132.96091</td> </tr> <tr> <td>4</td> <td>■</td> <td>160.98000</td> <td>0.00000</td> </tr> <tr> <td>5</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>	Frag #	Found	Expected m/z	Measured m/z	1	●	159.97000	159.97183	2	●	182.02000	182.02444	3	■	132.96000	132.96091	4	■	160.98000	0.00000	5			
Frag #	Found	Expected m/z	Measured m/z																						
1	●	159.97000	159.97183																						
2	●	182.02000	182.02444																						
3	■	132.96000	132.96091																						
4	■	160.98000	0.00000																						
5																									
LS	<p>Library Search flag. The application displays one of these flags:</p> <ul style="list-style-type: none"> • A green circle when the library search is successful. • A red square when the library search is not successful. 																								
Flag	<p>Indicates the status of the identification and confirmation criteria.</p> <ul style="list-style-type: none"> • A green circle when the sample/compound/peak combination is identified and fully confirmed. • A yellow triangle when the sample/compound/peak combination is identified but not fully confirmed. • A red square when the sample/compound/peak combination is not identified. 																								
Compound Name	The compound name match in the compound database.																								
Match Result Name	The compound name match in the compound database and the retention time.																								
Formula	The formula for the peak as specified in the compound database.																								
Adduct	The most intense adduct for the retention time for a compound.																								
Confirmed	The number of criteria confirmed out of the total number specified in the method.																								

Table 131. Compounds pane parameters (Sheet 4 of 6)

Column	Description
<i>m/z</i> (Expected)	<p>Mass-to-charge ratio from the compound database. Assumes the charge is 1.</p> <ul style="list-style-type: none"> When an adduct is found, the application displays the neutral mass value for the compound (calculated from the neutral formula) ± the mass of the most intense adduct ion found for the compound. When no adduct is found, the application displays the neutral mass value for the compound ± the mass of the first adduct entered in the compound database. <p>For details about defining adducts for the compound database, see “Specifying Adducts” on page 53.</p> <p>For details about adding adducts to compounds, see “Editing Compounds in the Database” on page 84.</p> <p>Note When the adduct is a gain, the adduct mass is a positive number. When the adduct is a loss, the adduct mass is a negative number. The resulting mass value after adding or subtracting the adduct mass is always a positive number.</p>
<i>m/z</i> (Apex)	<p>Mass-to-charge ratio found in the spectra for the peak. Assumes the charge is 1.</p> <p>When the application successfully integrates the peak, this column displays the charged <i>m/z</i> value for the compound, which is the highest intensity in the apex scan.</p> <p>When the application cannot successfully integrate the peak, this column displays “N/F” (not found).</p>
<i>m/z</i> (Delta)	<p>Difference between the <i>m/z</i> (Expected) and <i>m/z</i> (Apex). Assumes the charge is 1.</p> <p>When the <i>m/z</i> (Apex) column displays <i>m/z</i> value for the compound, this column displays the delta <i>m/z</i> corresponding to the highest intensity in the apex scan.</p> <ul style="list-style-type: none"> When the mass tolerance is specified in ppm in the master method, then $m/z \text{ (Delta)} = 1\,000\,000 \times ([m/z \text{ (Apex)} - m/z \text{ (Expected)}] \times m/z \text{ (Expected)})$. When the mass tolerance is specified in mmu in the master method, then $m/z \text{ (Delta)} = 1000 \times m/z \text{ (Apex)} - m/z \text{ (Expected)}$.
RT (Expected)	The retention time for the peak as specified in the compound database.
RT (Measured)	The found retention time for the peak apex.
RT (Delta)	Difference between the expected and measured retention time for the peak.
Measured Area	The AA value from the chromatogram pane.
Isotopic Pattern Score (%)	The percentage of the number of total isotopes to the number of matched isotopes.

Table 131. Compounds pane parameters (Sheet 5 of 6)

Column	Description
Num Isotopes Matched	<p>The number of isotopes matched in the expected calculated isotope spectra relative to the total number of isotopes used in the score calculation, in the format “x of y”, where</p> <ul style="list-style-type: none"> • x = the number of isotopes matching the elemental composition used for the Isotopic Pattern Score calculation. • y = the total number of isotopes considered in the Isotopic Pattern Score calculation. This is the number of isotope peaks expected to be above the spectral noise.
Lib Match Name	<p>The name of the best matching compound in the library search. When the application finds a match in the library, this column displays the matching library entry with the highest score.</p> <ul style="list-style-type: none"> • When the application does not perform a library search, this column displays “N/A” in black text. • When the application does not perform an MS/MS scan, this column displays “N/A” in red text.
Library Score (%)	<p>The score from the library fit. When the application finds a match in the library, this column displays the highest score associated with the Lib Match Name parameter.</p> <p>When the application performs both a library search and an MS/MS scan and both the library entry and the formula match the target compound:</p> <ul style="list-style-type: none"> • A library score that is higher than or equal to the score threshold meets the criteria, and the values in this column appear in green. • A library score that is lower than the score threshold fails to meet the criteria, and the values in this column appear in red. <p>When the application does not perform a library search, this column displays “N/A” in black text.</p> <p>When the application does not perform an MS/MS scan, this column displays “N/A” in red text.</p> <p>Valid range: 1 through 100%</p>

Table 131. Compounds pane parameters (Sheet 6 of 6)

Column	Description
Library Match Rank	<p>Displays the ranking of the library match. When the application finds a match in the library, this column displays the library entry's relative rank, in the format "x of y", where</p> <ul style="list-style-type: none"> x = the rank of the highest scoring library match. y = the total number of library matches from the list of matches for a particular adduct that contains the highest scoring match. <p>When the application performs both a library search and an MS/MS scan and both the library entry and the formula match the target compound:</p> <ul style="list-style-type: none"> A library score that is higher than or equal to the score threshold meets the criteria, and the values in this column appear in green. A library score that is lower than the score threshold fails to meet the criteria, and the values in this column appear in red. <p>When the application does not perform a library search, this column displays "N/A" in black text.</p> <p>When the application does not perform an MS/MS scan, this column displays "N/A" in red text.</p>
Fragment <i>n</i>	<p>Displays the measured <i>m/z</i> for the fragment ion. The application displays a separate column for each found fragment.</p> <ul style="list-style-type: none"> For each fragment found in the compound database that passes the filter in the method, the Compounds table displays the <i>m/z</i> value in green text. For each fragment found in the compound database that does not pass the filter in the method, the Compounds table displays the <i>m/z</i> value in red text. For each fragment that is not found in the compound database, the Compounds table displays N/S (none specified). <div style="border: 1px solid black; padding: 5px; margin: 10px 0;"> <p>Fragment 1</p> <p>Aa</p> <p>N/S</p> <p>187.06</p> <p>159.97</p> </div> <ul style="list-style-type: none"> — Fragment not found in the compound database — Fragment found but does not meet method parameters — Fragment found and meets method parameters
<p>Note Compounds can have a maximum of five fragments, and the Compounds table has a maximum of five Fragment columns. When a compound contains fewer than five fragments, all remaining Fragment columns display N/S.</p>	
Fragment <i>n</i> (Delta (ppm/mmu))	<p>The difference between the expected fragment ion <i>m/z</i> from the compound database and the measured fragment ion <i>m/z</i>.</p> <p>The application displays a separate delta column for each identified fragment.</p>
S/N	The signal-to-noise ratio calculated for the found peak.
Left RT	The time point of the left leading edge of the integrated peak.
Right RT	The time point of the right trailing edge of the integrated peak.

Chromatogram Pane

Use the Chromatogram pane to display all extracted chromatograms of all adducts of the selected compound.

The first tab displays the most intense target adduct for the peak result. Additional (optional) tabs display extracted ion chromatograms for other adducts for the target compound at the same retention time in order of intensity. If no signal exists for an adduct, it displays the XIC of the expected m/z within the specified retention and chromatogram windows. When you do not specify a retention time or window, the application displays the full time range.

For each adduct, the Spectrum pane displays the spectrum, isotopes, fragments, and library matches. See [Spectrum Pane](#).

Figure 184. Chromatogram pane

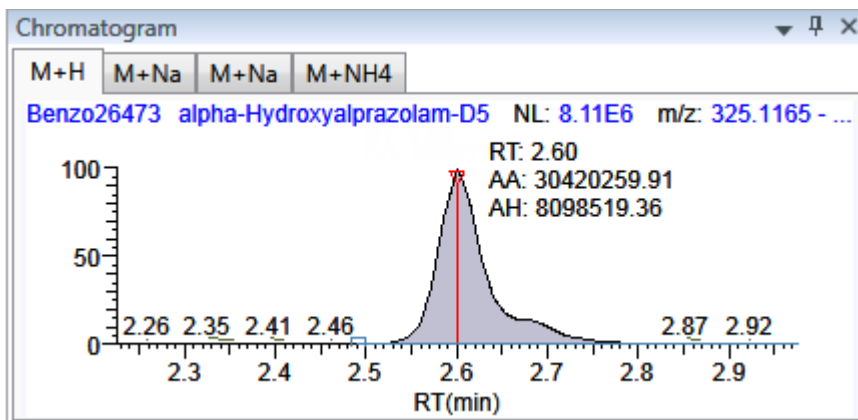


Table 132. Chromatogram pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Spectrum Pane

Use the Spectrum pane to display the spectrum, isotopes, fragments, and library search information for the selected adduct in the Chromatogram pane. The Spectrum pane displays only the identification and confirmation criteria specified in the method. The confirmations are based only on the most intense adduct. See “Editing the Processing Page” on page 264.

The Spectrum pane includes the following pages of information (when available) for each selected sample/compound/peak combination:

- [Spectrum](#)
- [Isotopes](#)
- [Fragments](#)
- [Library](#)

Spectrum

The application displays the neutral loss (NL) and compound/peak name information on the right side of the Spectrum page. When data is available, the plot width is the full mass range in the raw data file. Otherwise, the application scales the width to the scan range.

Figure 185. Spectrum page

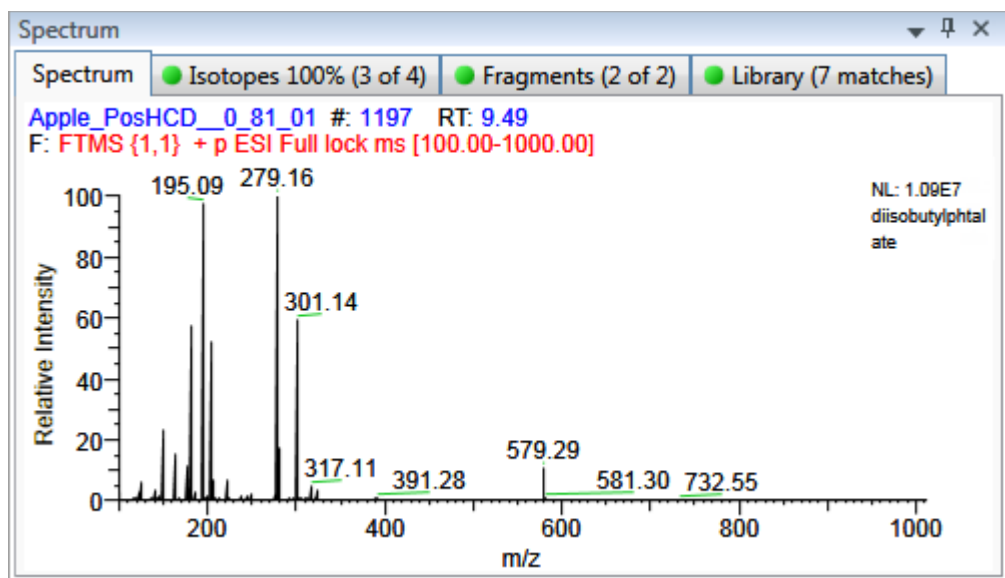


Table 133. Spectrum page shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Isotopes

The isotopes page displays isotopic pattern results for all adducts of a compound according to the threshold and deviation parameters defined in the screening method.

To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

- An isotope peak is not found if its intensity, relative to the monoisotopic ion's intensity, is more than the specified intensity deviation percentage away from the theoretical relative intensity of the isotope ion.
- An isotope peak is found if its measured m/z is less than the specified mass deviation amount away from its expected m/z .

To specify threshold and deviation parameters, see “[Editing the Processing Page](#)” on [page 264](#).

The Isotopes page displays the isotopes in one of three ways:

- [All Isotopes](#)
- [Multi-Isotopes](#)
- [Individual Isotopes](#)

All isotopes pages use a shortcut menu so that you can specify how to display the data. See “[Isotopes Page Shortcut Menu](#)” on [page 590](#).

All Isotopes

The All Isotopes view displays a composite of all isotopes found in the compound. The application scales the window with respect to the most intense isotope. The most intense isotope is usually the first isotope unless you are using halogenated compounds. The application displays the measured peak as a solid red line; the application displays the expected peak as a dashed blue line.

The application displays these headers for the All Isotopes view:

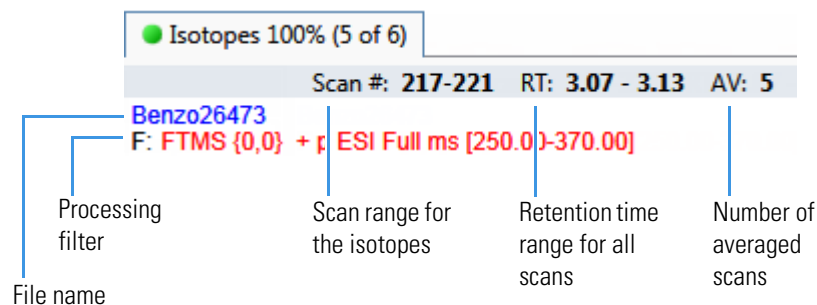


Figure 186. Isotopes page with stacked spectra for all isotopes

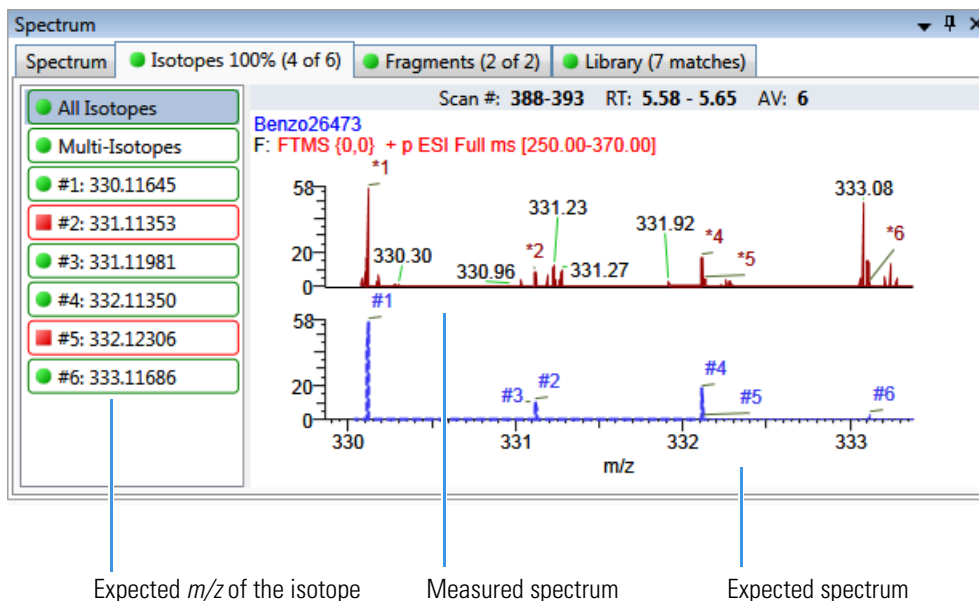
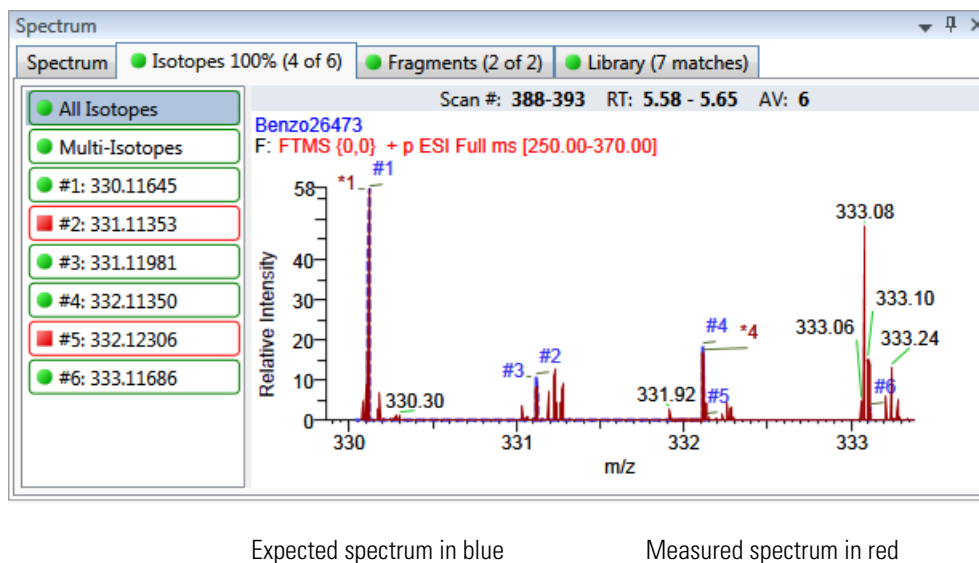


Figure 187. Isotopes page with overlaid spectra for all isotopes



Multi-Isotopes

The Multi-Isotopes view displays individual plots for each isotope. You can individually stack or overlay the plots for each isotope.

The application displays these headers for the Multi-Isotopes view:

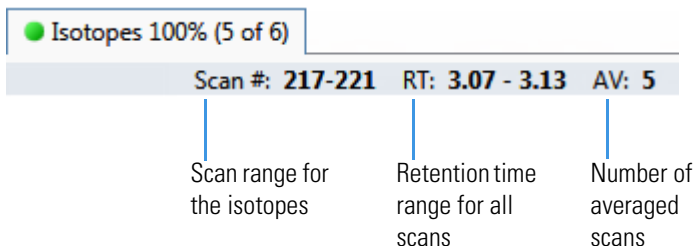
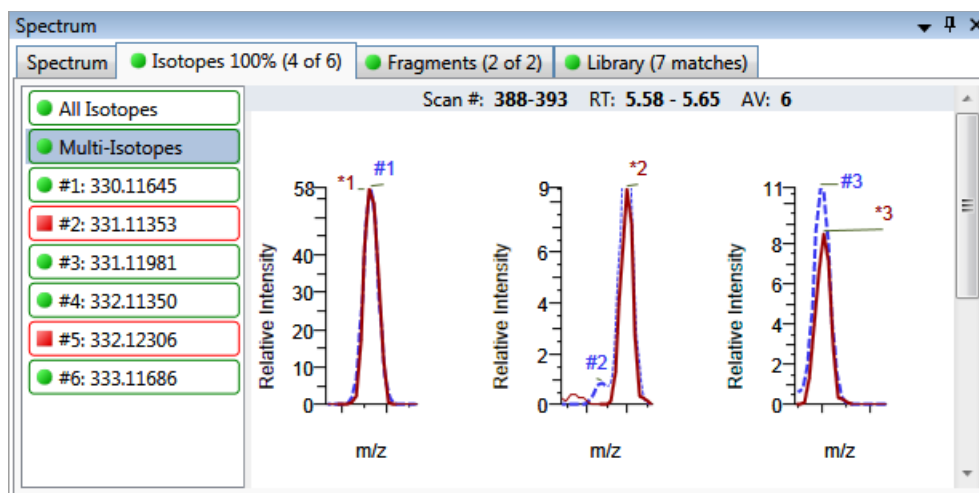


Figure 188. Isotopes page with overlaid spectra for multi-isotopes



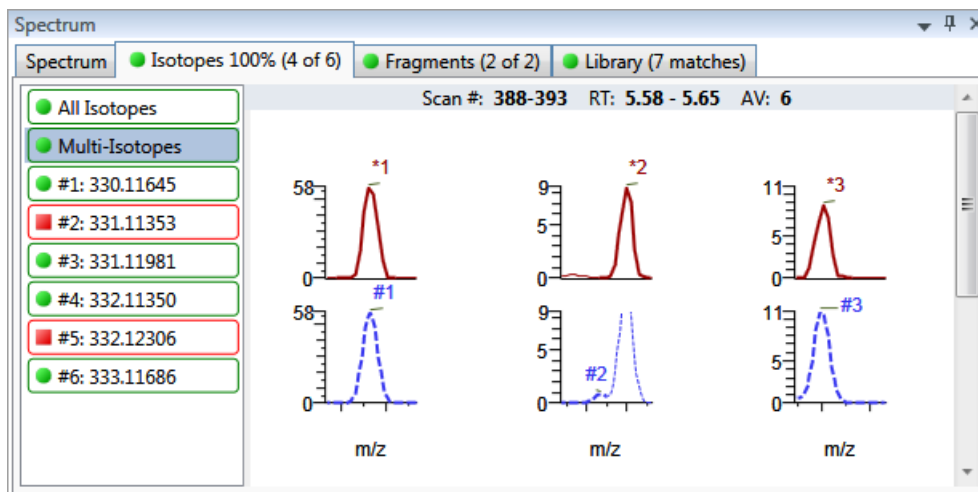
Expected spectrum in blue

Measured spectrum in red

10 Using the Analysis Mode for Target Screening Batches

Working in Data Review

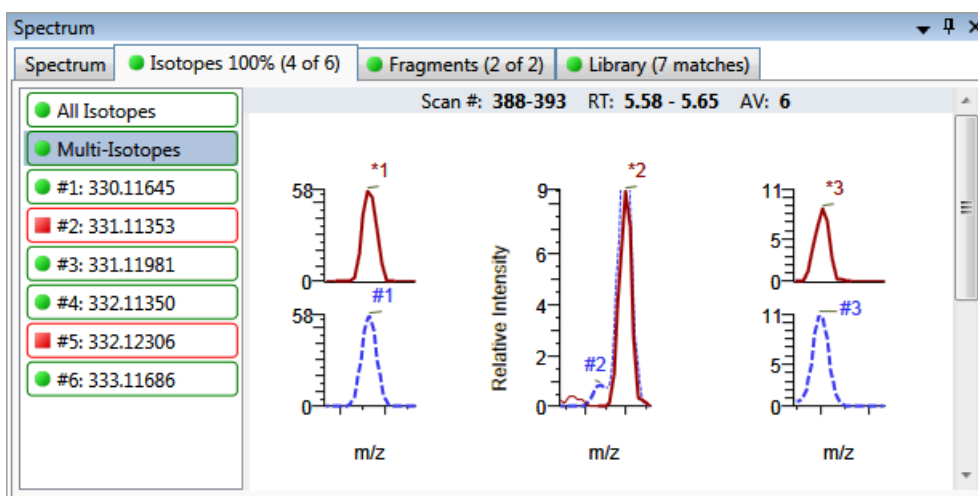
Figure 189. Isotopes page with stacked spectra for multi-isotopes



Expected spectrum in blue

Measured spectrum in red

Figure 190. Isotopes page with stacked and overlaid spectra for multi-isotopes



Expected spectrum in blue

Measured spectrum in red

Individual Isotopes

The individual isotopes view displays the expected and measured peaks for a single isotope.

The application displays these headers for the individual isotopes view:

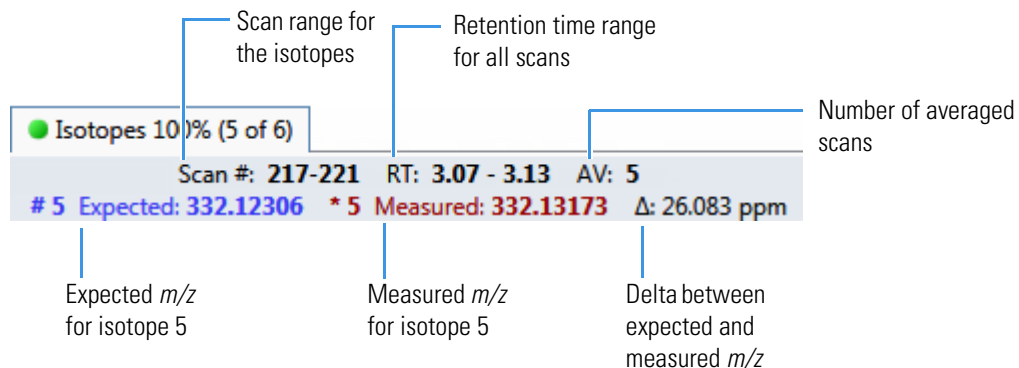
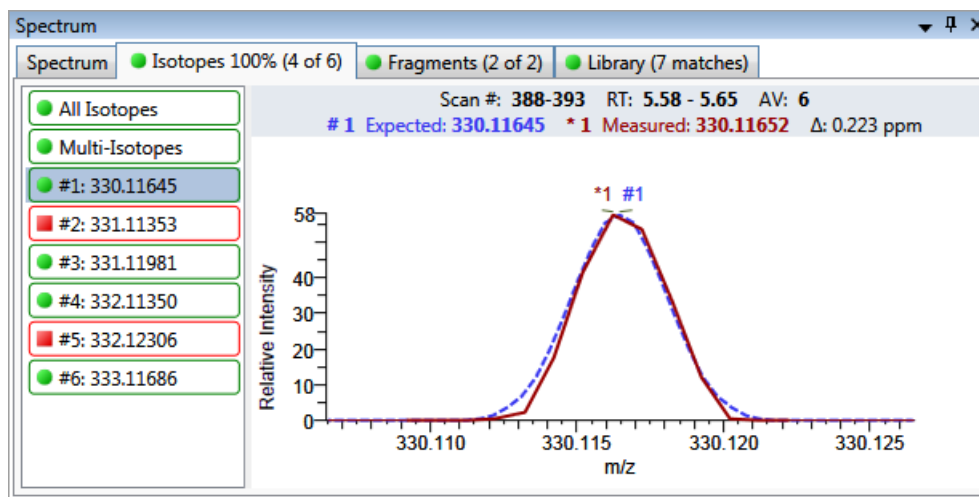


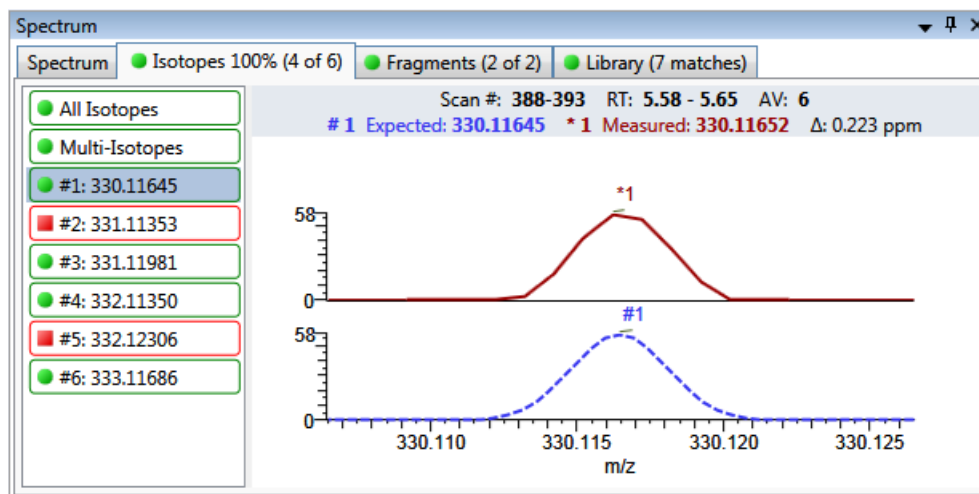
Figure 191. Isotopes page with overlaid spectra for a single isotope



Expected spectrum in blue

Measured spectrum in red

Figure 192. Isotopes page with stacked spectra for a single isotope



Expected spectrum in blue

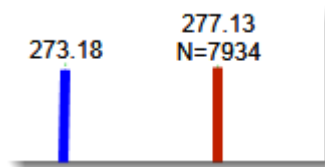
Measured spectrum in red

Isotopes Page Shortcut Menu

Use the commands in the shortcut menu to specify how you want the data displayed.

Table 134. Isotopes page shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Show/Hide Noise Label	Adds a noise label to each peak. Expected isotope peaks (displayed in blue) do not display a noise label.



Show/Hide Resolution Label
 Adds a resolution label to each peak. Expected isotope peaks (displayed in blue) do not display a resolution label.



Fragments

The Fragments page displays the maximum number of fragments as specified in the screening method. See “Editing the Processing Page” on page 264.

If there are no fragments defined in the screening library for the compound, you can add fragments to the screening library. See “To add a fragment to a target peak” on page 90.

The Fragments page displays the fragments in one of two ways:

- All Fragments
- Individual Fragments

All fragments pages use a shortcut menu so that you can specify how to display the data. See “Fragments Page Shortcut Menu” on page 593.

All Fragments

The All Fragments view displays a composite of all fragments found in the compound. The application displays the measured peak as a solid red line; the application displays the expected peak as a dashed blue line.

The application displays these headers for the All Fragments view:

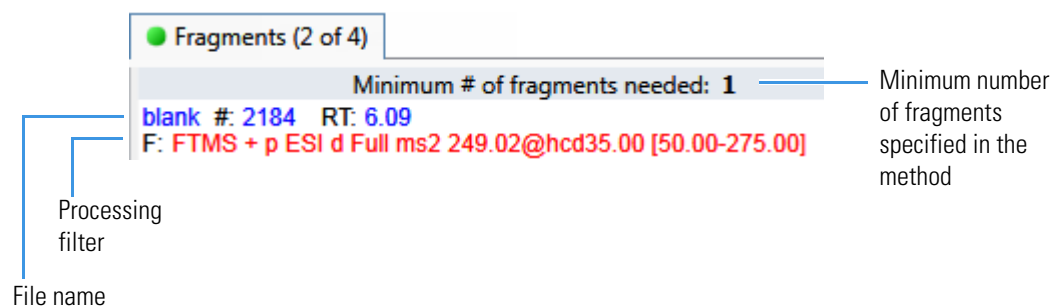


Figure 193. Fragments page with overlaid spectra for all fragments

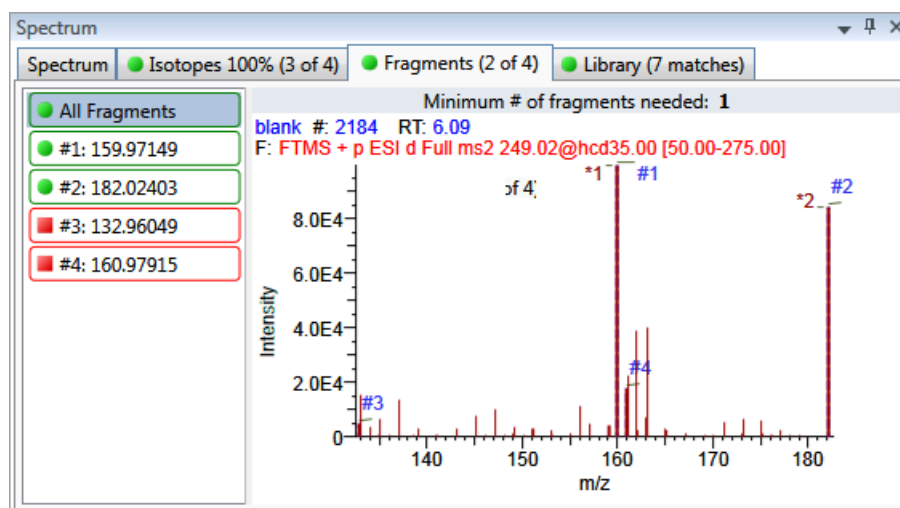
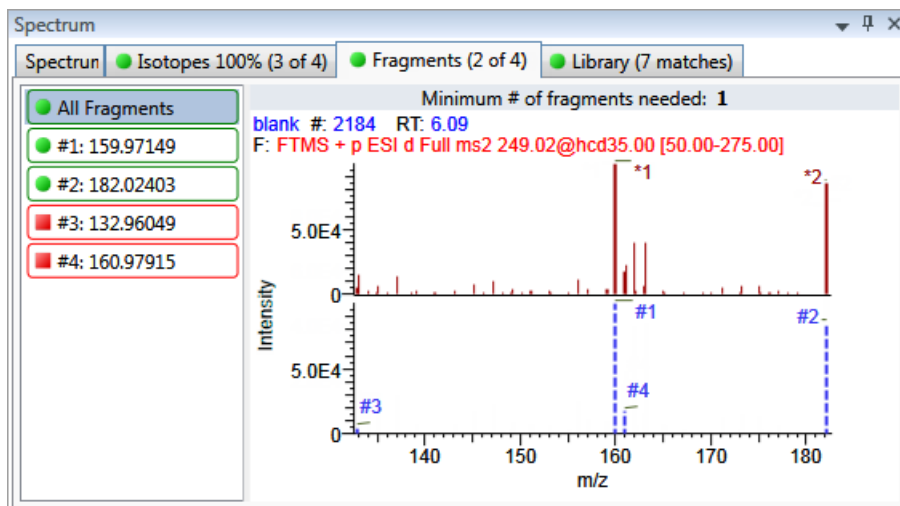


Figure 194. Fragments page with stacked spectra for all fragments



Individual Fragments

The individual fragments view displays the expected and measured peaks for a single fragment.

The application displays these headers for the individual fragments view:

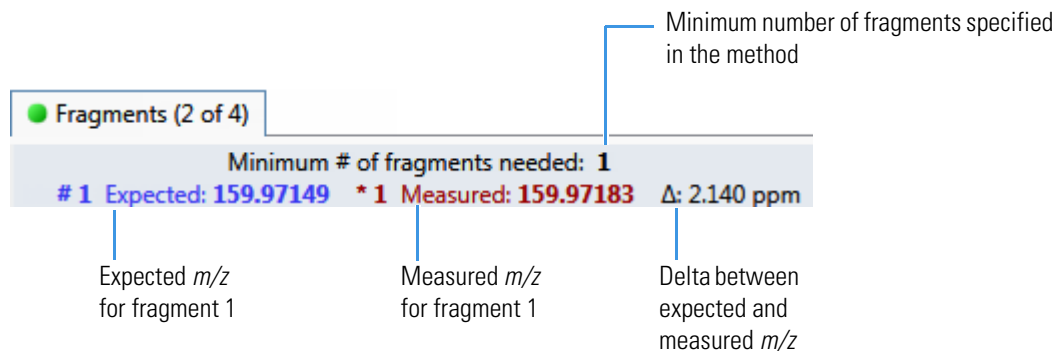
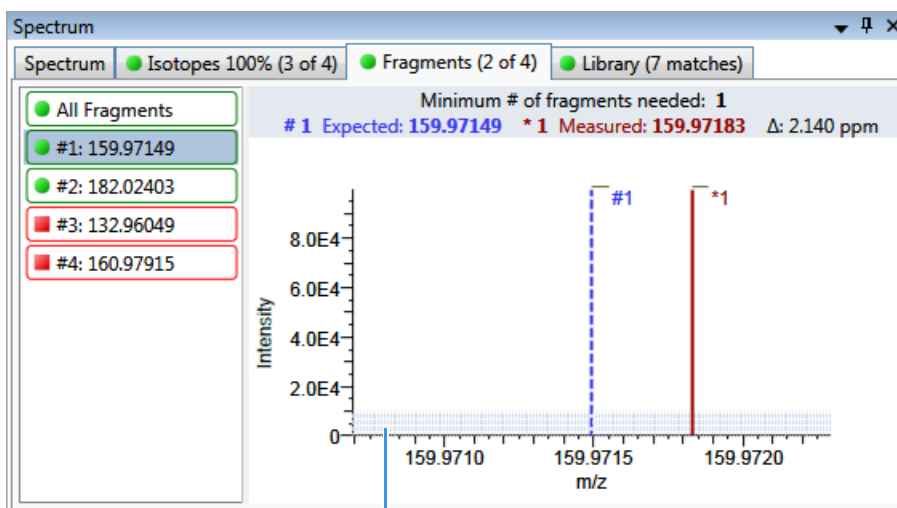
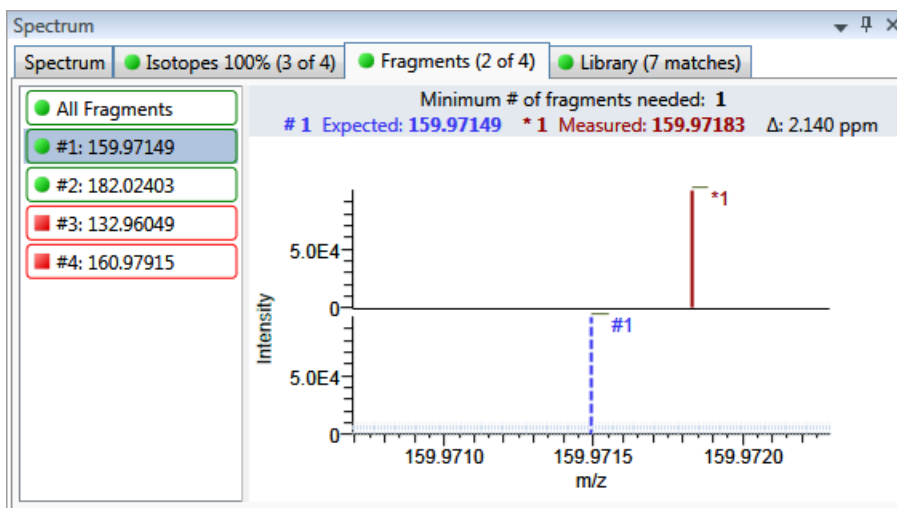


Figure 195. Fragments page with overlaid spectra for a single fragment



Intensity threshold specified in the method

Figure 196. Fragments page with stacked spectra for a single fragment



Fragments Page Shortcut Menu

Use the commands in the shortcut menu to specify how you want the data displayed.

Table 135. Fragments page shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Display Stack Spectra	

Library

The Library page displays the matching library spectrum (in blue) and the experimental spectrum (in black). The resulting score percentage from a library search match must be higher than your specified threshold value to identify or confirm the presence of a compound. See “[Editing the Processing Page](#)” on [page 264](#).

The application scales both the matched library spectrum and the highest peak in the experimental spectra at 100 percent intensity and displays the resulting neutral loss (NL) value for the matched library entry name on the right of the plot.

The application displays these headers for the individual adducts:

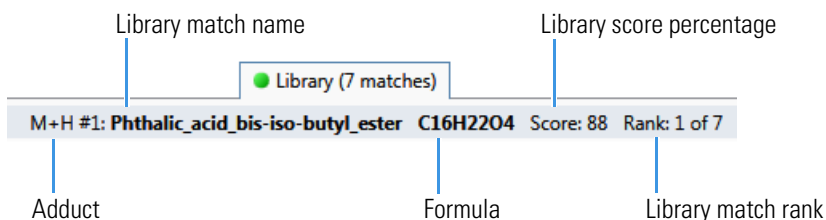


Figure 197. Library page with stacked spectra

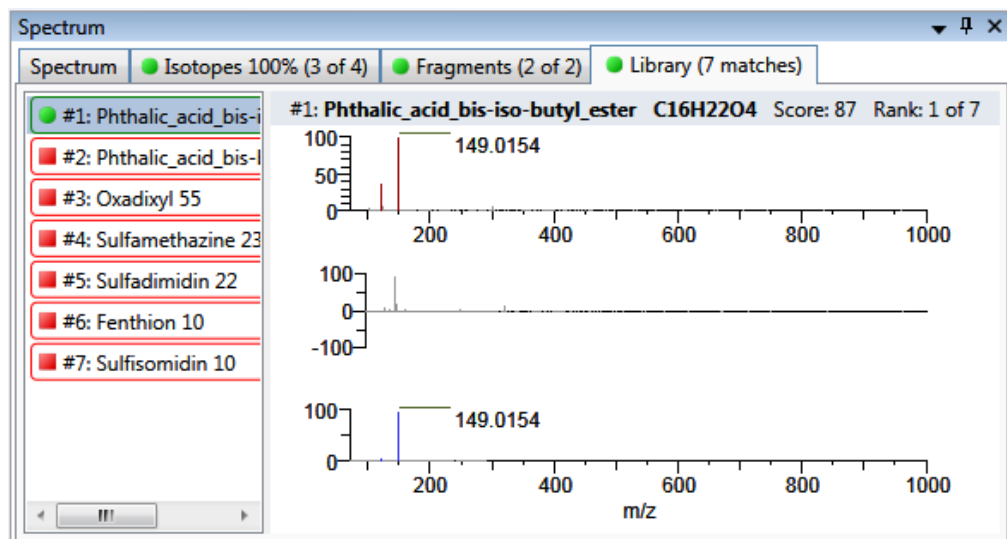
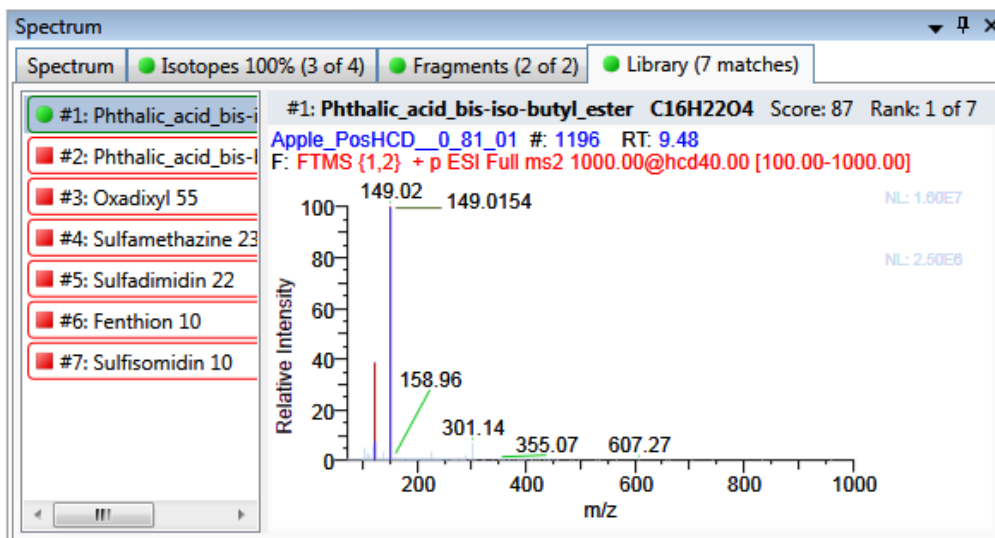


Figure 198. Library page with overlaid spectra



Library Page Shortcut Menu

Use the commands in the shortcut menu to specify how you want the data displayed.

Table 136. Library page shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Display Stack Spectra	

Working in the Report View

The Report View displays example reports for the current batch. You must have an open batch to use the features in the Report View.

Follow these procedures:

- [To open the Report View](#)
- [To preview a report](#)
- [To generate a report as a PDF, an Excel, or a CSV file](#)
- [To print a report](#)
- [To display a generated report](#)
- [To edit a report template](#)
- [To create a new report template](#)

❖ To open the Report View

Click **Report View** in the navigation pane.



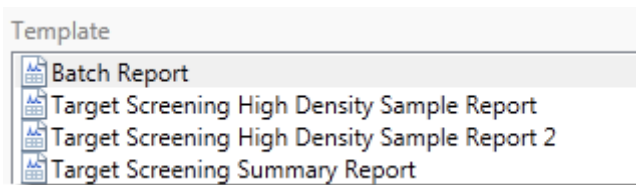
The application opens the Report View. For detailed descriptions of all parameters, see [“Report View”](#) on [page 600](#).

❖ To preview a report

1. In the Template pane, select a report template.

The template list shows all the report templates that you configured in the Configuration console. See [“Specifying the Reports”](#) on [page 71](#).

Figure 199. Example of a report template list




2. Click **Preview**, .

The application opens the Report Designer, showing the report information for the current batch in the selected report template format.

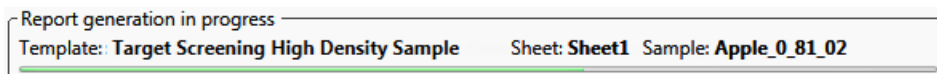
For details about using the Report Designer, see [Chapter 12, “Using the Report Designer.”](#)

❖ To generate a report as a PDF, an Excel, or a CSV file

1. In the Template pane, select a report template.
2. Select the check box for each of the file types that you want to create: **PDF**, **Excel**, or **CSV**.
3. Click **Generate**,  **Generate**.


The application does the following:

- Displays a green progress bar as it generates the reports.



- Creates a report for the current batch as a PDF, an Excel, or a CSV file, using the selected report template format.
- Adds information about the generated report to the Generated Reports pane.
For details about the Generated Reports pane, see “[Report View](#)” on [page 600](#).
- Saves the report files to the ...\\TraceFinderData\\3.3\\Projects*batch*\\ReportOutput folder.

❖ To print a report

1. In the Template pane, select a report template.
2. Select the check box for the **Print** file format.
3. Click **Generate**,  **Generate**.

The application does the following:

- Creates a report for the current batch using the selected report template format.
- Prints the report to your default printer.
- Adds information about the generated report to the Generated Reports pane.
For details about the Generated Reports pane, see “[Report View](#)” on [page 600](#).
- Saves the report files to the ...\\TraceFinderData\\3.3\\Projects*batch*\\ReportOutput folder.

❖ To display a generated report

In the Generated Reports pane, click **View** for the report that you want to see.


Generated Reports				
Template	Rule	Sample	Output	Generated Report File
Batch Report	Batch		pdf	View... Batch Report_20140113092939.pdf (3 pages)

Opens the generated file.

The application opens the output file.

❖ **To edit a report template**

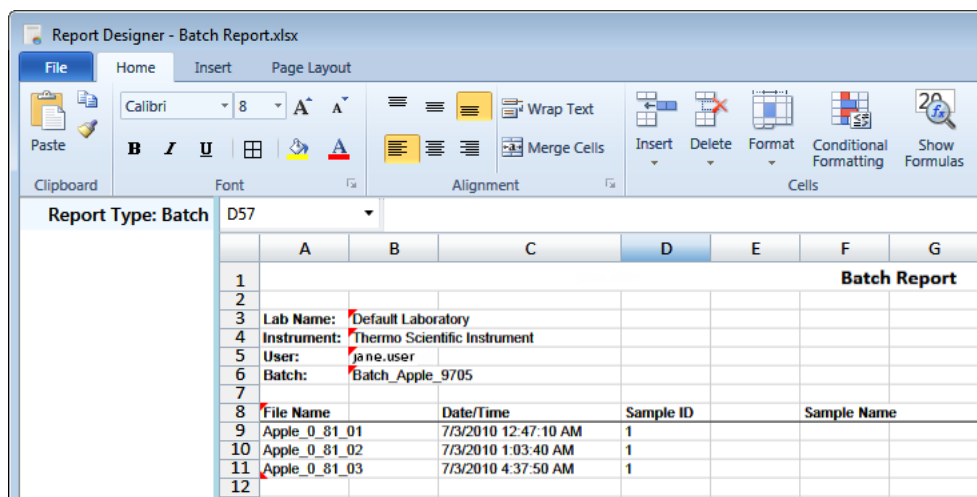
Note You cannot edit report templates that were provided with the TraceFinder application; however, you can open a TraceFinder template, make changes, and save it to a new template name.

1. In the Template pane, select a report template.
2. Click **Open**, .

The application opens the Report Designer showing the template in an Excel spreadsheet. See [Report Designer showing the template for the selected report](#).

Note When user security is activated, you must have Template Editing permission to edit report templates created by your laboratory. If the Open button is not active, user security is activated and you do not have Template Editing permission.

Figure 200. Report Designer showing the template for the selected report



3. Use the features in the Report Designer to edit the template.
See [Chapter 12, “Using the Report Designer.”](#)
4. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

❖ **To create a new report template**

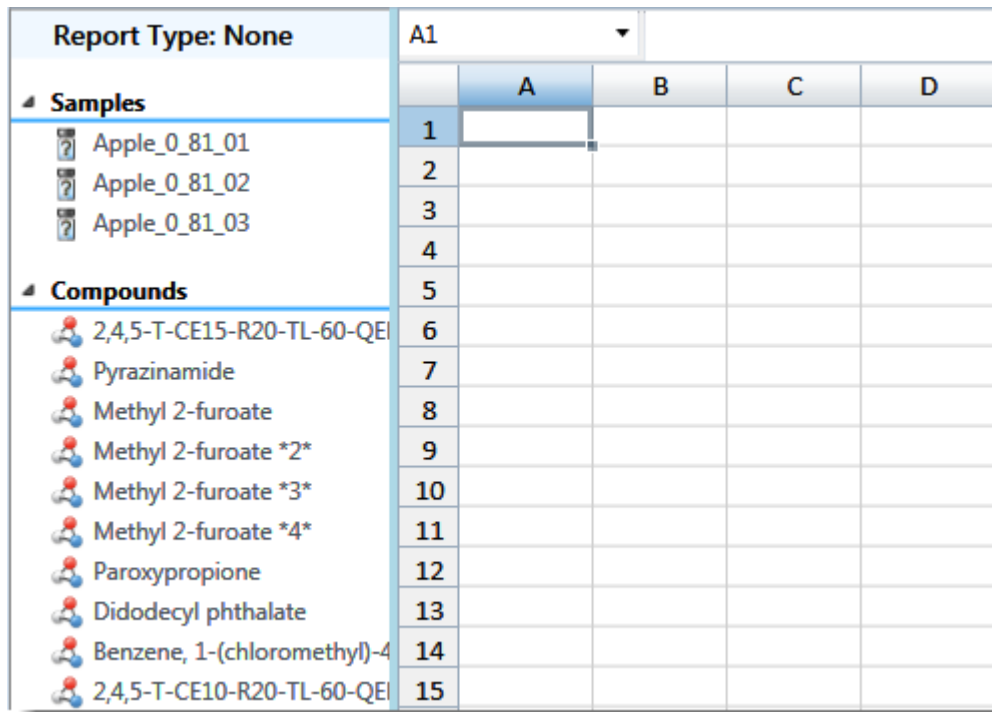
1. Click **New**, .

The application opens the Report Designer showing an empty template in an Excel spreadsheet. See [Report Designer showing a new, empty template](#).

The Report Type is None.

In the left pane, the spreadsheet lists all samples in the current batch and all compounds in the method used for the batch.

Figure 201. Report Designer showing a new, empty template



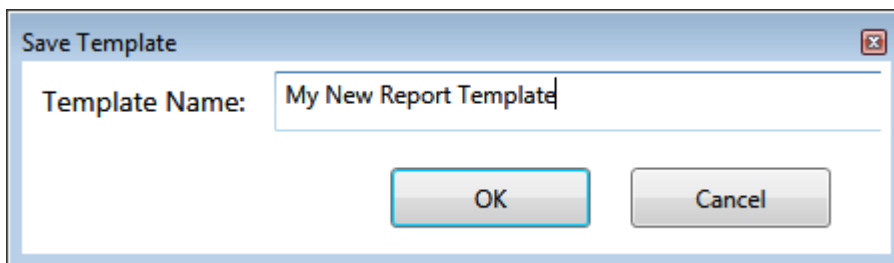
2. Use the features in the Report Designer to create the report template.

See [Chapter 12, “Using the Report Designer.”](#)

3. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

The Save Template dialog box opens.

Figure 202. Save Template dialog box



4. Type a name for the new report template and click **OK**.

10 Using the Analysis Mode for Target Screening Batches

Working in the Report View

Report View

Use the features in the Report View to display example reports for the current batch.

Figure 203. Report View

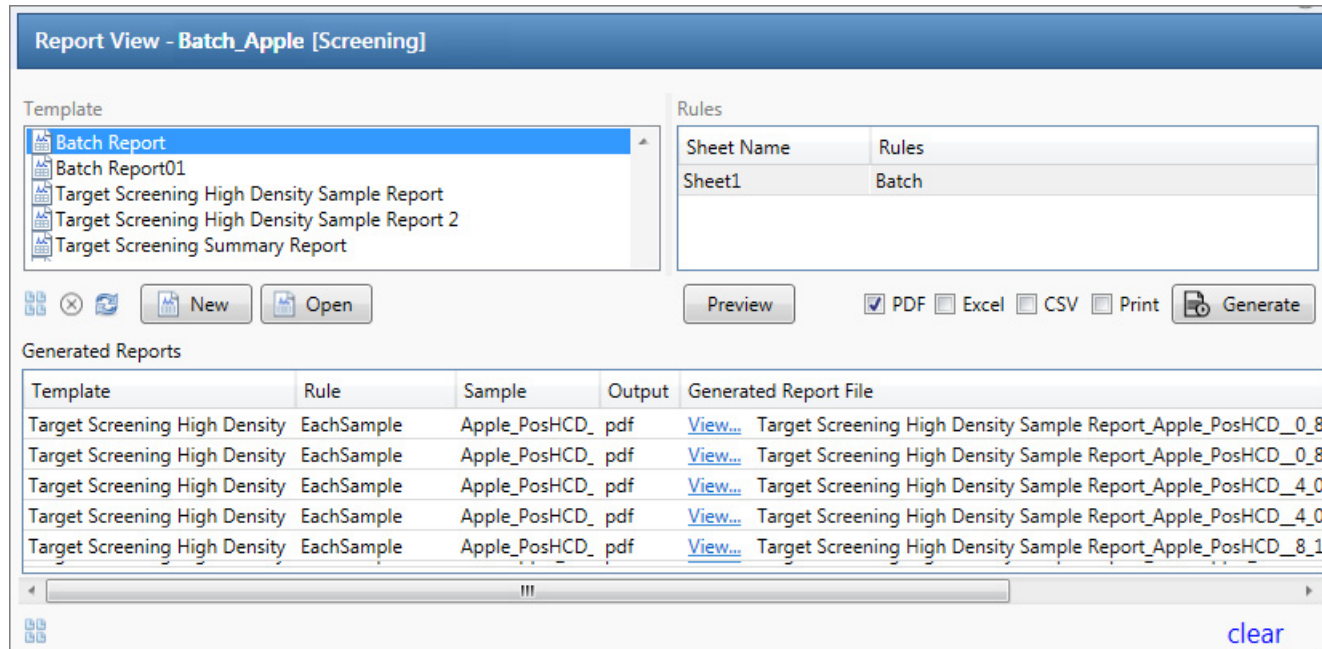
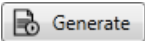



Table 137. Report View parameters (Sheet 1 of 2)

Parameter	Description
Template	
	Displays all report templates.
Rules	
Sheet Name	Specifies each sheet in the report.
Rules	Specifies the type of data used in each sheet in the selected report. <ul style="list-style-type: none">• Batch• EachSample• SampleType: <i>SampleType</i>• CompoundType: <i>CompoundType</i>• SampleCustomFormula:
Buttons	
View Report Templates	Displays the C:\TraceFinderData\3.3\Templates\ReportTemplates folder that contains all report templates.
Open	Opens the selected report template in the Report Designer.
New	Opens a blank report template in the Report Designer.
Preview	Opens the Report Designer showing the report information for the current batch in the selected report template format.

Table 137. Report View parameters (Sheet 2 of 2)

Parameter	Description
PDF	Writes the generated report to a PDF file in the ...\\TraceFinderData\3.3\Projects\batch\ReportOutput folder.
Excel	Writes the generated report to a PDF file in the ...\\TraceFinderData\3.3\Projects\batch\ReportOutput folder.
CSV	Saves the generated report as a PDF file in the ...\\TraceFinderData\3.3\Projects\batch\ReportOutput folder. When the report contains multiple sheets, the application writes each sheet as a separate CSV file.
Print	Prints the generated report to your default printer.
 Generate	Generates the selected type of reports for the current batch using the selected report template.
Generated Reports	
Template	Report template used for the report. See “Example of a report template list” on page 596 .
Rule	Type of data used in each sheet of the report. See Rules .
Sample	For sample-level reports, the name of each sample in the report.
Output	Type of output specified for the report: PDF, Excel, CSV, or Print.
Generated Report File	Lists the output file name for each report in the ...\\TraceFinderData\3.3\Projects folder.
View	Displays the generated output file.
 View Generated Reports	Displays the C:\TraceFinderData\3.3\Projects folder that contains all report outputs.
Clear	Removes all reports from the Generated Reports display. This does not delete the reports from the C:\TraceFinderData\3.3\Projects folder.

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 *Batch_MasterMethod*.

❖ To open the Local Method View

1. Click **Analysis** in the navigation pane.
2. Click **Local Method**.



The Local Method view for the currently selected batch opens. See [Local Method View](#).

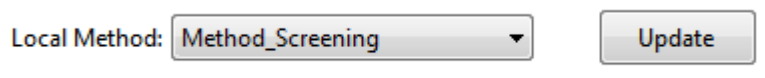
You can edit many of the method parameters in a local method. Editing the local method does not affect parameters in the master method.

For detailed descriptions of method parameters, see “[Editing a Master Method](#)” on [page 261](#).

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 204. Local Method View

The screenshot displays the 'Local Method View' for 'Batch_1_Method_Screening'. The interface is organized into a sidebar on the left and a main configuration area on the right. The sidebar includes sections for 'Batch View' (Samples), 'Data Review' (Target Screening), 'Report View', and 'Local Method' (Acquisition, Target Screening, Processing, Peak Detection, Reports). The main area shows the 'Master method: Method Screening' and various parameters: 'Lab Name' is 'Default Laboratory', 'Assay type' is 'Assay name', 'Injection Volume' is '1.00', and 'Mass Precision' is '2.00'. The 'Instrument Method' is set to 'Pesticides Using EQuan', with 'Edit' and 'Update' buttons. A 'Notes' section is present at the bottom of the main area.

Using the Analysis Mode for Unknown Screening Batches

This chapter includes instructions about using the features of the Analysis mode to do the following:

- Create unknown screening batches.
- Submit unknown screening batches for acquisition, processing, or report generation.
- Review unknown screening batches, batch data, reports, and local methods.

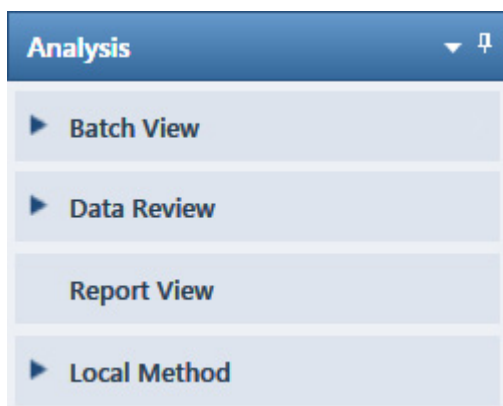
Contents

- [Working in the Batch View](#)
- [Working in Data Review](#)
- [Working in the Report View](#)
- [Working in the Local Method View](#)

❖ To access the Analysis mode

Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.



Working in the Batch View

In the Batch View, you can manually create and edit a new unknown screening 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.

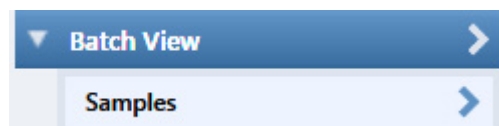
The Analysis mode includes a toolbar:



Use the toolbar or the equivalent commands in the Batch View shortcut menu to create the sample list and submit samples for acquisition. See “[Toolbar](#)” on [page 614](#) or “[Batch View Shortcut Menu](#)” on [page 618](#).

❖ To open the Samples page in the Batch View

1. Click **Analysis** in the navigation pane of the current mode.
2. Click **Batch View** or **Samples**.



The Samples page opens.

This section contains information about the following topics:

- [Samples Page Features](#)
- [Creating a New Batch](#)
- [Editing a Batch](#)
- [Submitting a Batch](#)

Samples Page Features

The Samples page (see [Samples page](#)) is divided into two panes:

- Samples pane

Use the samples pane to create a batch. See [Samples Pane](#).

- Compound Active Status pane

Use the Compound Active Status pane to make specific compounds active or inactive. See “[Compound Active Status Pane](#)” on [page 620](#).

Figure 205. Samples page

Samples pane

Batch View - Batch_A

Local Method: Instrument: User:

	Status	Filename	Sample type	Groups	Level	Sample ID	Sample name	Vial position	Injection volume	Conversion Factor	Channel	Barcode Expected	Barcode Actual	Sample Volume
▶ 1	<input checked="" type="radio"/>	Unknown1	Unknown						10.0	1.000	Auto			1
2	<input checked="" type="radio"/>	Unknown2	Unknown						10.0	1.000	Auto			1
3	<input checked="" type="radio"/>	Unknown3	Unknown						10.0	1.000	Auto			1

Compound Active Status

	RT	Compound	Active
▶ 1	1.91	FENTHION-CE20-R20-TL75-QED	<input checked="" type="checkbox"/>
2	2.72	Sulfisomidine	<input checked="" type="checkbox"/>

Compound Active Status pane

Tip To resize the panes, drag the separators that divide the panes.

Samples Pane

The samples pane includes the following features:

- [Column Display](#)
- [Status Indicators](#)
- [Groups](#)
- [Sample Weight Calculation](#)
- [Instrument Methods](#)
- [Toolbar](#)
- [Batch View Sample List](#)
- [Batch View Shortcut Menu](#)

Column Display

The sample list contains many columns of information. You can scroll to see all the columns, and you can customize which ones to display and their display order.

❖ To scroll the sample list

Use the horizontal scroll bar at the bottom of the sample list to view all the information.

When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name, while the other columns scroll right and left.

❖ To customize the column display

1. Right-click the sample list and choose **Modify Columns** from the shortcut menu.

The Modify Columns dialog box opens. See “[Modify Columns dialog box.](#)”

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

These columns appear after the Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

- a. In the Displayed Columns pane, select a column name.
- b. Use **Up** or **Down** 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, and the last column in the list represents the rightmost column in the Batch View sample list.

Note The following columns are fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

- a. In the Displayed Columns pane, select the column width.

5	Sample ID	100
▶ 6	Sample name	100
7	Vial position	100

- b. Type a new value for the width.

5. Repeat [step 4](#) for all columns whose widths you want to change, and 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.

Figure 206. Modify Columns dialog box

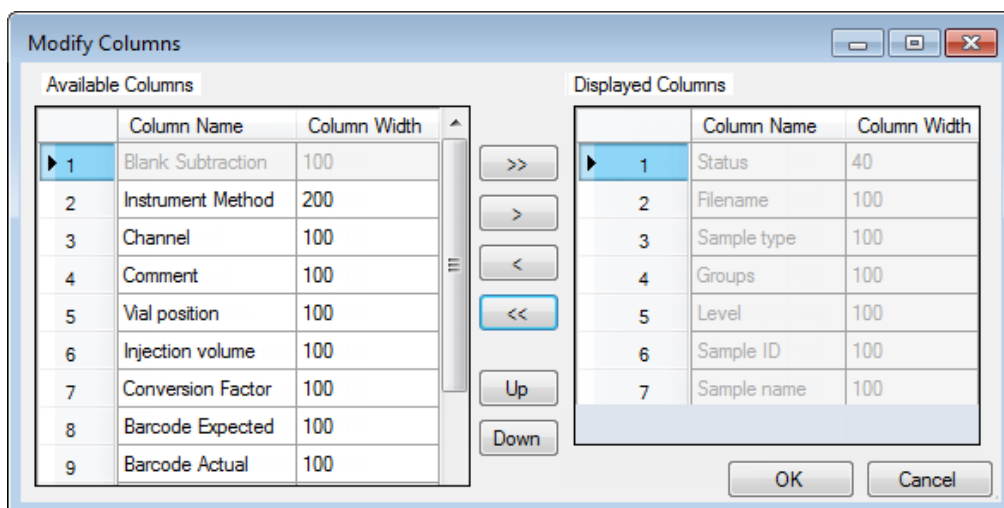












Table 138. Button descriptions for the Modify Columns dialog box




Button	Description
	Moves all columns to the Displayed Columns pane.
	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name.	
	Moves the selected column to the Available Columns pane.
	Moves all columns except fixed columns.
	Moves the selected column name in the Displayed Columns pane one row up in the column order.
	Moves the selected column name in the Displayed Columns pane one row down in the column order.

Status Indicators

Status indicators show the current status of each sample during the acquisition and processing.

-  Sample is not acquired.
-  Sample is acquired but not processed.
-  Sample is acquired and processed.
-  Sample is currently acquiring.

Local Method: Method_Alprazolam Update

	Status	Filename	Sample type	Groups	Sample ID	Sample name	Vi pc
1		Solvent_A	Solvent				1
2		Cal_5	Cal Std				2
3		Unknown1	Unknown				3

Status indicators




Groups

Use the Groups feature to assign samples to a group.

❖ To create a group

1. For each sample, type the name of a group in the Groups column.
Repeat this for each sample that you want to include in a group.
2. Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
	Benzo26473	groupB, groupA
	Benzo25557	groupB
	Benzo26154	groupB, groupA

The application uses the first group listed for the Maximum Fold analysis and in the Group Averages pane.

You can create a control group (specify the group name as Control) to use for group averages in Data Review.

For information about group averages, see [“Group Averages Pane” on page 656](#). For information about maximum fold analysis, see [“Cross Sample Peak List Pane” on page 643](#).

Sample Weight Calculation

Use the sample weight features to calculate the conversion factor for a sample. The application uses different methods to calculate the conversion factor for liquid or solid calculation types.

Liquid: $SampleVolume \div DilutionFactor$

Solid: $(SampleVolume \times DilutionFactor) \div SampleWeight$

Manual: The application does not calculate the Conversion Factor. Instead, you can enter the Conversion Factor value.

Follow these procedures:

- To display the features for calculating sample weight
- To calculate the conversion factor for a liquid sample
- To calculate the conversion factor for a solid sample
- To manually specify the conversion factor for a sample

❖ To display the features for calculating sample weight

If the Conversion Factor, Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns are not visible, right-click and choose **Enable Sample Weight Calculation** from the shortcut menu.

Conversion Factor	Sample Volume	Dilution Factor	Sample Weight	Calculation Type	Final Units
1.000	1	1	1	Liquid ▼	
1.000	1	1	1	Solid ▼	
1.000	1	1	1	Manual ▼	

❖ To calculate the conversion factor for a liquid sample

Note The application uses the following formula to calculate the Conversion Factor:
 $SampleVolume \div DilutionFactor$

1. From the **Calculation Type** list, select **Liquid**.

For a liquid sample, the Sample Weight value is not editable.

2. In the Sample Volume column, type the volume in ng/mL for your sample.
3. In the Dilution Factor column, type the value for the dilution.

For example, if you have 1000 ng/mL of a substance that is too concentrated for the mass spectrometer, you can dilute it by 1000. Then your injection volume is 1, your conversion factor is 1000, and your sample amount is 1000.

4. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

❖ To calculate the conversion factor for a solid sample

Note The application uses the following formula to calculate the Conversion Factor:
 $(SampleVolume \times DilutionFactor) \div SampleWeight$

1. From the **Calculation Type** list, select **Solid**.
2. In the Sample Weight column, type the weight in ng for your sample.
3. In the Sample Volume column, type the volume in ng/ml for your sample.
4. In the Dilution Factor column, type the value for the dilution.

For example, if you have 1000 ng/ml of a substance that is too concentrated for the mass spectrometer, you can dilute it by 1000. Then your injection volume is 1, your conversion factor is 1000, and your sample amount is 1000.

5. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

❖ To manually specify the conversion factor for a sample

Note The application uses the specified conversion factor when it calculates the amount for the sample.


1. From the **Calculation Type** list, select **Manual**.
For a manually calculated sample, the only available columns are the Conversion Factor and the Final Units.
2. In the Conversion Factor column, type the conversion factor to use for your sample.
3. In the Final Units column, type the units that you want to use for the calculated amount in the Data Review view or in reports.

Instrument Methods

Use the Instrument Methods column to specify instrument methods for the samples.

Note By default, the Instrument Method column is not displayed in the Batch View sample list.

❖ To specify instrument methods for samples

1. Display the Instrument Method column in the sample list:
 - a. Right-click the sample list and choose **Modify Columns** from the shortcut menu.
The Modify Columns dialog box opens.
 - b. In the Available Columns pane, select **Instrument Method**.
 - c. Click  to move the Instrument Method column to the Displayed Columns pane.

d. Click **OK**.

The application displays the Instrument Method column, defaulting to the instrument method specified in the master method.

2. Click the Instrument Method column and select an instrument method from the list.

This list contains all the available instrument methods. Instrument methods from external sources are prefixed with “Ext:”.

You can specify a different instrument method for each sample.

When you submit the batch for acquisition, the application saves a copy of the selected instrument methods to the following folders:

External instrument methods:

...\\TraceFinderData\\3.3\\Projects\\...*batch*\\Methods*method**ExternalMethods*

Local instrument methods:

...\\TraceFinderData\\3.3\\Projects\\...*batch*\\Methods*method*

Toolbar

The Analysis mode includes this toolbar for creating and submitting a batch.



Table 139. Toolbar icons

Icon	Description
	Adds the specified number of new, empty samples to the end of the sample list. See the instructions “ To add samples to the list ” on page 622 .
	Inserts a new, empty sample or samples above the selected sample. See the instructions “ To insert samples into the list ” on page 623 .
	Removes the selected samples from the sample list. See the instructions “ To remove samples from the list ” on page 624 .
	Adds imported samples from a CSV, an XML, or an SLD file to the sample list. See the instructions “ To import samples into the list ” on page 623 .
	Submits only the selected samples for acquisition, processing, or report generation. See the instructions “ To submit samples in the batch ” on page 633 .
	Submits the batch for acquisition, processing, or report generation. See the instructions “ To submit samples in the batch ” on page 633 .
	Submits only the selected samples for processing. See the instructions “ To submit selected peaks for processing ” on page 633 .
	Opens the Acquisition mode where you can use a batch template to define a standard sequence composed of various sample types to be assembled into a batch of samples. See “ Working in Data Review ” on page 642 .
	Opens the Acquisition mode where you can create a batch template that contains the basic settings and sample types for your batches. See “ Using the Acquisition Mode ” on page 347 .
	Opens the Quick Acquisition window where you can quickly submit a single sample. See Appendix A, “Using Quick Acquisition.”
	Opens the Audit Viewer where you can view audit logs. See Chapter 13, “Using the Audit Viewer.” Available only when you enable Auditing in the Administrator Console. Refer to the instructions in the <i>TraceFinder Administrator Console User Guide</i> .

Batch View Sample List

The sample list displays all the quantitative data for the samples of a batch.

Status indicators for each sample indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The sample list includes the following columns of information:

Figure 207. Batch View sample list

Local Method:	Method_Unknown ▼	Update	Instrument:	Thermo Scientific Instrument
---------------	------------------	--------	-------------	------------------------------

	Status	Filename	Sample type	Groups	Level	Sample ID	Sample name	Vial position	Injection volume
1	●	UnknownA1	Unknown			1		CStk1-01:7	10.0
2	●	UnknownA2	Unknown			1		CStk1-01:7	10.0
3	●	UnknownA3	Unknown			1		CStk1-01:7	10.0

Calculation Type	Conversion Factor	Dilution Factor	Sample Weight	Sample Volume	Final Units
Liquid ▼	1.000	1	1	1	
Liquid ▼	1.000	1	1	1	
Liquid ▼	1.000	1	1	1	

Instrument Method	Channel	Barcode Expected	Barcode Actual	Comment
Instrument1 ▼	Auto			
Instrument1 ▼	Auto			
Instrument1 ▼	Auto			

11 Using the Analysis Mode for Unknown Screening Batches

Working in the Batch View

Table 140. Batch View sample list columns (Sheet 1 of 2)







Column	Description
Status	<ul style="list-style-type: none"> Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring. <p>Note When you include unknown screening features in a quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed ().</p> <p>Note When you include unknown screening features in a target screening method and you choose to process with only the unknown screening criteria, both the Samples view and the Unknown Screening View show the Status for the samples as acquired and processed (.</p>
Groups	Threshold group to which a sample belongs.
Filename	Name of the raw data file that contains the sample data.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC Std, or Unknown Default: Unknown
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.
Vial Position	The tray vial number used for an autosampler acquisition.
Injection Volume	The injection volume (in microliters) of the injected sample. 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 displayed range. The Injection Volume value set in the master method overwrites the value in the instrument method. Valid range: 0.1 through 5000 µL

Table 140. Batch View sample list columns (Sheet 2 of 2)

Column	Description
Calculation Type	<p>Liquid: The application calculates the Conversion Factor as</p> $\text{SampleVolume} \div \text{DilutionFactor}$ <p>Solid: The application calculates the Conversion Factor as</p> $(\text{SampleVolume} \times \text{DilutionFactor}) \div \text{SampleWeight}$ <p>Manual: Sample Volume, Dilution Factor, Sample Weight, and Final Units columns are not available, and the Conversion Factor value is editable.</p>
Conversion Factor	<p>Editable only when Calculation Type is Manual.</p> <p>Default: 1</p>
Sample Volume	Default: 1
Dilution Factor	Default: 1
Sample Weight	<p>Available only when Calculation Type is Solid.</p> <p>Default: 1</p>
Final Units	<p>Specifies the calculated amount in the Data Review view or in reports.</p> <p>Default: 1</p>
Instrument Method	Specifies the instrument to use for the acquisition. This column is hidden by default. To display this column, see “To customize the column display” on page 608.
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. The Channel column is available only when you have activated multiplexing in the Configuration console. See “Multiplexing” on page 61.
Barcode Expected	A user-entered barcode for the vial.
Barcode Actual	An actual barcode for the vial. This value is not editable.
Comment	A user-defined comment for the sample.

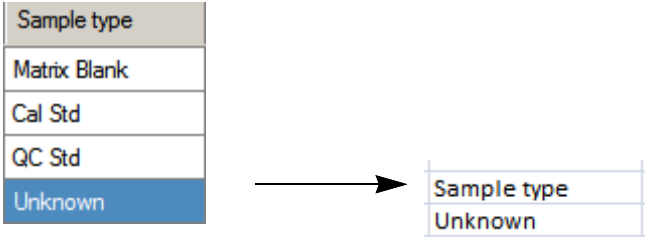
Batch View Shortcut Menu

The Batch View includes a shortcut menu for creating a batch.

Table 141. 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 623.
Browse in Raw File (Move)	Opens a dialog box where you can select a raw data file to use for the selected sample row. The application removes the raw data file from the source location.
Browse in Raw File (Copy)	Opens a dialog box where you can select a raw data file to use for the selected sample row. The application copies the raw data file from the source location.
Map Raw Files to Samples	Opens a dialog box where you can select multiple raw data files to use for the selected 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 607.
Enable/Disable Sample Weight Calculation	Displays or hides the Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information into a text editor or spreadsheet application. You cannot paste this data back into the Batch View sample list.

Table 141. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
Copy with Headers	<p>Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information into another text editor or spreadsheet application. You cannot paste this data back into the sample list.</p> <p>For example</p>  <p>Copy with Headers from TraceFinder</p> <p>Paste into an Excel spreadsheet.</p>
Paste	Pastes a single column of copied data from another text editor or spreadsheet application 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.
Edit Instrument Method	<p>Opens the Instrument Setup window where you can edit the parameters of the instrument method.</p> <ul style="list-style-type: none"> • When you edit an external method, the application updates the method in the ... \Xcalibur\methods folder. • When you edit an internal method, the application updates the method in the ... \TraceFinderData\3.3\Projects\...\batch\Methods\method folder. <p>For detailed information about editing instrument methods, see “Working with Instrument Methods” on page 108.</p>

Compound Active Status Pane

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 sample list, select a sample.

All compounds in the selected sample are listed in the Compound Active Status pane.

Compound Active Status

	RT	Compound	Active
▶ 1	1.91	FENTHION-CE20-R20-TL75-QED	<input checked="" type="checkbox"/>
2	2.72	Sulfisomidine	<input checked="" type="checkbox"/>

The default active/inactive status is determined by the identification settings in the local method. For information about setting the identification parameters, see [“Identification”](#) on [page 152](#).

- To display compounds alphabetically, right-click and choose **Sort by Compound Name** from the shortcut menu.
 - To display compounds from shorter to longer retention times, right-click and choose **Sort by Retention Time** from the shortcut menu.
2. Select or clear the **Active** check box for the compound.

Compound Active/Inactive Status

You can specify which compounds are active or inactive in the Local Method View or the Batch View.

Figure 208. Active and inactive compounds in the Local Method View

Local Method View - Batch_2_Method_Unknown [Unknown]						
Master method: Method Vitamin1						
Acquisition List	Identification	Detection	Calibration	Calibration levels	Chk Std levels	Real Time View
	RT	Compound	Compound type	Active	CAS No	
1	5.88	1-Butanol, 4-(butylnitrosoamino)-	Target Compound	<input type="checkbox"/>	3817116	
2	16.68	3,3'-Diaminodiphenylmethane	Target Compound	<input checked="" type="checkbox"/>	19471126	

For details about setting the status on the Identification page, see [“Identification”](#) on [page 152](#).

Figure 209. Active and inactive compounds in the Batch View

Batch View - Batch_2 [Unknown]

Local Method:

	Status	Filename	Sample type	Groups	Level	Sample ID
▶ 1		VitWaterEquanMaxA001	Unknown			CStk1-01:3
2		VitWaterEquanMaxA002	Unknown			CStk1-01:4

Compound Active Status

	RT	Compound	Active
▶ 1	5.88	1-Butanol, 4-(butylnitrosoami...	<input type="checkbox"/>
2	16.68	3,3'-Diaminodiphenylmethane	<input checked="" type="checkbox"/>
3	2.91	4-Methyl-2,6,7-trioxa-1-phosp...	<input checked="" type="checkbox"/>

For details about setting the status in the Batch View, see “[Compound Active Status Pane](#)” on [page 620](#).

Creating a New Batch

In the Batch View, you can create a new batch.

Follow these 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 browse in raw data files](#)
- [To customize the column display](#)

❖ To create a new batch

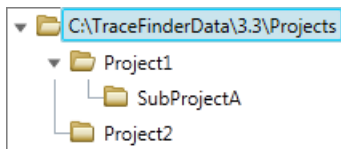
1. Choose **File > New > Batch** from the main menu.

The Create New Batch dialog box opens, displaying all drives that contain projects. See “[Create New Batch Dialog Box](#)” on [page 628](#).

11 Using the Analysis Mode for Unknown Screening Batches

Working in the Batch View

2. Select a drive from the list.



Tip The application displays all configured and enabled repositories.

3. Select the folder where you want to store your batch.

Tip To activate the Create button, you must enter a unique batch name. If the Create button is not activated, you have entered a batch name that is already used.

To create a new folder for the storage location, see “[Editing Folders for Batches](#)” on page 629.

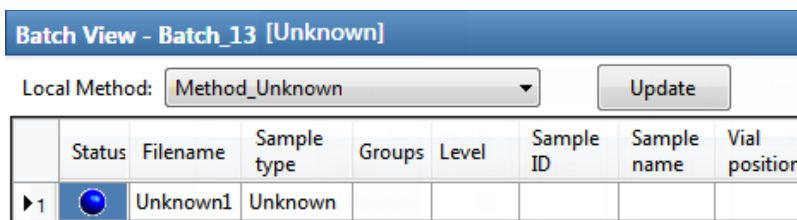
4. Select **Unknown Only** from the Type list.

The batch list displays all batches in the selected folder. The Method list displays all methods for the unknown screening type.

5. Select a master method from the Master Method list.


6. Click **Create**.

A new batch opens with one Unknown sample.



The batch name in the title bar indicates that you are creating an unknown screening batch.


❖ 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** icon, .





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 will insert new, Unknown samples, and then 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** icon  .

The application inserts the Unknown samples above the selected sample.

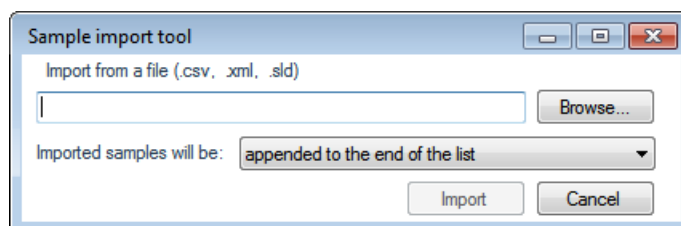
	Status	Filename	Sample type	Groups	Level
1		cal_std_5	Cal Std		
2		Unknown2	Unknown		
3		Unknown1	Unknown		
4		cal_std_10	Cal Std		

Inserted samples

❖ To import samples into the list

1. Choose **Batch > Import Samples** from the main menu, or click the **Import Samples** icon,  .

The Sample Import Tool dialog box opens.



From this dialog box, you can import samples from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file that contains the samples 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 sample list.

When you import samples from an Xcalibur sequence file (.sld), the application makes the following column name substitutions:

Xcalibur column	TraceFinder column
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conversion Factor

11 Using the Analysis Mode for Unknown Screening Batches

Working in the Batch View

When you import samples from an Xcalibur sequence file (.sld), the application makes the following sample type substitutions:

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	QC Std
Std Bracket	Cal Std

5. (Optional) When using multiplexing, select a channel for each imported sample. Imported samples default to Auto.

Note The Channel column is available only when you have activated multiplexing in the Configuration console. See “[Multiplexing](#)” on [page 61](#).

❖ To remove samples from the list

1. Select the samples that 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 copy a sample

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

The application inserts the copy above the selected sample.

❖ To reinject a sample

1. In the sample list, select the sample that you want to reinject.
2. Right-click and choose **Reinject This Sample** from the shortcut menu.

The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

❖ To edit sample values

1. For each sample, do one of the following:

Type a new file name over the current filename.

–or–

Double-click the Filename column and locate a raw data file to use for the sample.

–or–

Right-click and choose **Browse in Raw File** from the shortcut menu, and then locate a raw data file to use for the sample.

By default, the application sets the Sample Type to Unknown.

- For each sample, click the Sample Type column and select a sample type from the list.

Available sample types			
Matrix Blank	Solvent	QC Std	Unknown
Cal Std			

- For each Cal Std or QC Std sample, select a level from the Level list.

The sample levels are defined in the master method. If there are no levels to select in the Level list, do the following:

- Return to the Method Development mode.
- Open the method.
- Click the **Compounds** tab.
- Click the **Calibration Levels** tab.
- Add the levels.
- Save the method.
- Return to the Batch View in the Analysis mode, and then click **Update**.



The application updates the local method with the new sample levels.

For detailed instructions about specifying calibration levels, see [“Calibration Levels”](#) on page 207.

- Type a vial position in the Vial Position column for each sample.
- Type a volume in the Injection Volume column for each sample.

The minimum injection volume value allowed is 0.1 μ L; the maximum injection volume value allowed is 5000 μ L.

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

Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name, while the other columns scroll right and left.

For instructions to automatically copy or fill values in these columns, see [Appendix C, “Using Copy Down and Fill Down.”](#)

❖ To browse in raw data files

- Do one of the following:

Double-click the Filename column.

–or–

Right-click and choose **Browse in Raw File** from the shortcut menu.


11 Using the Analysis Mode for Unknown Screening Batches

Working in the Batch View

The What Raw File Would You Like to Use dialog box opens.

2. Select a raw data file to use for the sample or use the CTRL key to select multiple files, and then click **Open**.

The application overwrites the selected, unacquired sample in the batch with the first “browsed in” file and adds any additional browsed in files below the selected sample.

For all browsed-in raw data files, the application sets the Status to Acquired, , and sets the Sample Type to Unknown.

Note You cannot overwrite an acquired sample. When you select a sample that is acquired, the application adds all browsed in files below the selected sample.

❖ 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. See [Modify Columns dialog box](#).

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

All the columns you select appear after the Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

- a. In the Displayed Columns pane, select a column name.
- b. Use **Up** or **Down** 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, and the last column in the list represents the rightmost column in the Batch View sample list.

Note The following columns are fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

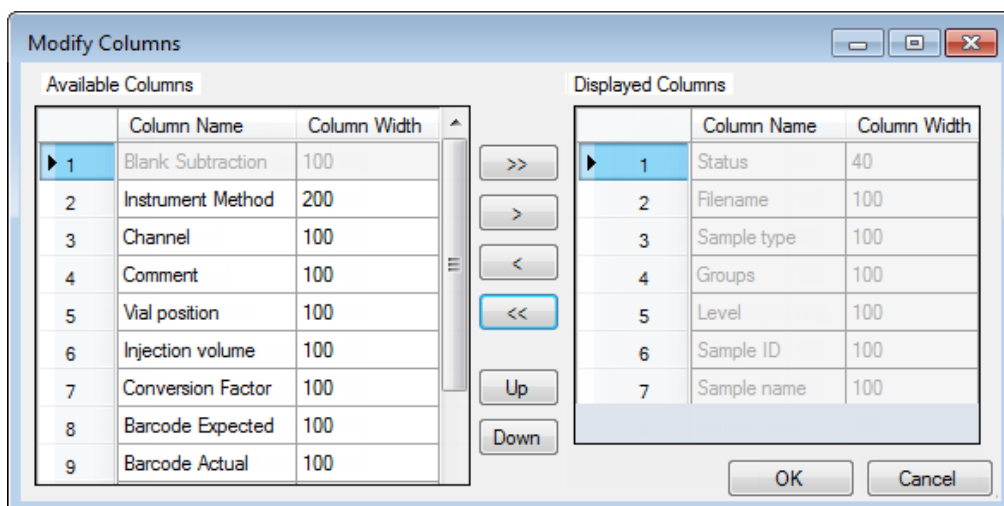
- a. In the Displayed Columns pane, select the column width.







7	Vial position	69
▶ 8	Injection volume	100
9	Calculation Type	100

- 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.

Figure 210. Modify Columns dialog box**Table 142.** Button descriptions for the Modify Columns dialog box

Button	Description
	Moves all columns to the Displayed Columns pane.
	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name.	
	Moves the selected column to the Available Columns pane.
	Moves all columns except those that are fixed.
	Moves the selected column name in the Displayed Columns pane one row up in the column order.
	Moves the selected column name in the Displayed Columns pane one row down in the column order.

11 Using the Analysis Mode for Unknown Screening Batches

Working in the Batch View

Create New Batch Dialog Box

Use the Create New Batch dialog box to select a folder and method for your batch and to name the new batch.

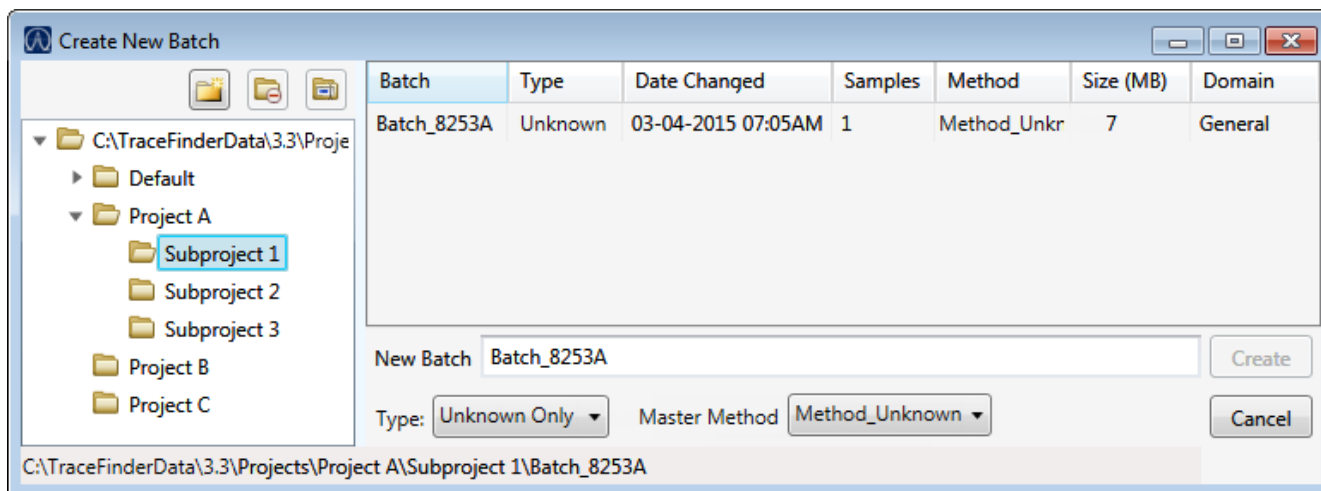


Table 143. Create New Batch dialog box parameters (Sheet 1 of 2)




Parameter	Description
 Create New Folder	Adds one of the following: <ul style="list-style-type: none">• When a drive is selected, adds a new project-level folder to the drive.• When a project folder is selected, adds a subproject-level folder to the selected project.• When a subproject folder is selected, adds a lower-level folder to the subproject. Or, right-click and choose Create Folder from the shortcut menu.
 Delete Folder	With no confirmation prompt, immediately removes the selected folder. You cannot delete a folder that contains lower-level folders; you must delete the lower-level folders first. Or, right-click and choose Delete from the shortcut menu.
 Rename Folder	Renames the selected folder. Or, right-click and choose Rename from the shortcut menu.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.

Table 143. Create New Batch dialog box parameters (Sheet 2 of 2)

Parameter	Description
Domain	TraceFinder domain in which the batch was created.
New batch parameters	
New Batch	Name of the new batch to create. Note If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Type	Type of batch to create: Quan, Screening, or Unknown Only.
Method	Method used to create the new batch.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is created.
Buttons	
Create	Creates the specified batch and opens the Batch View for the new batch.
Cancel	Closes the Create New Batch dialog box without creating a batch.


Editing Folders for Batches

From the Create New Batch dialog box, you can create new folders for your batches. You can also delete or rename folders.

Use these procedures:

- [To create new project folders](#)
- [To delete project folders](#)
- [To rename project folders](#)

❖ To create new project folders

1. In the Create New Batch dialog box, select the folder for which you will create a new lower-level folder.
 - You can select the main TraceFinderData\3.3\Projects folder and create a new folder under it.
 - You can select one of the existing folders and create a lower-level folder under it.
2. Click the **Create Folder** icon, .


The application adds a new lower-level folder to the selected folder.

3. Select the new folder name and type a name for the folder.

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

Note After you add a lower-level folder, you cannot rename the parent folder.


❖ To delete project folders

1. In the Create New Batch dialog box, select the folder to delete.
2. Click the **Delete Folder** icon, .

With no confirmation prompt, the application immediately removes the selected folder.

Note You cannot delete folders that contains lower-level folders; you must delete the lower-level folders first.

❖ To rename project folders

1. In the Create New Batch dialog box, select the folder to rename.
2. Click the **Rename Folder** icon, .

Note You cannot rename folders that contain lower-level folders.

3. Type a new name for the folder and press ENTER.

The application saves the new folder name.

Editing a Batch

In the Batch View, you can open a saved batch and edit the sample 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 “ready to acquire” batch.

Follow these 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 open a saved batch

1. Choose **File > Open > Batch** from the main menu.

The Open Batch dialog box opens. See [Open Batch dialog box](#).

2. Select a project and a subproject.
3. Select **Unknown Only** or **Any** from the Type list.

The batch list displays all batches created with Unknown methods (or all methods of all types when you select Any).

4. Select a batch from the list.
5. Click **Open**.

The selected batch opens in the Batch View.

Figure 211. Open Batch dialog box

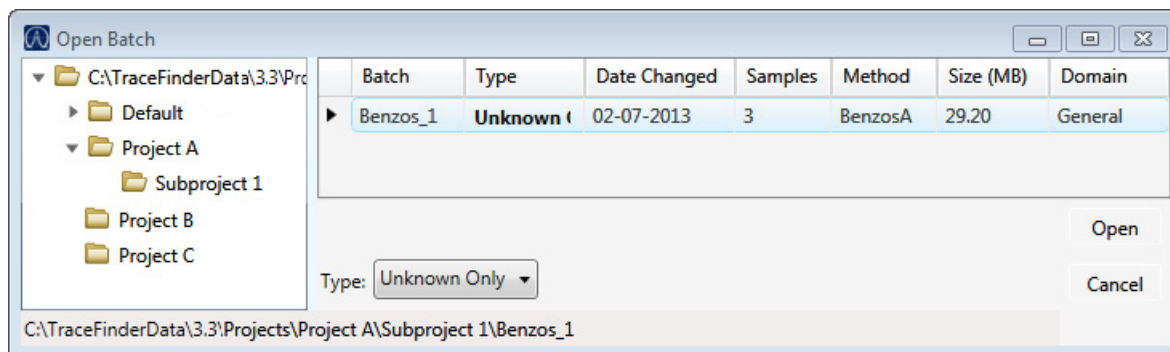
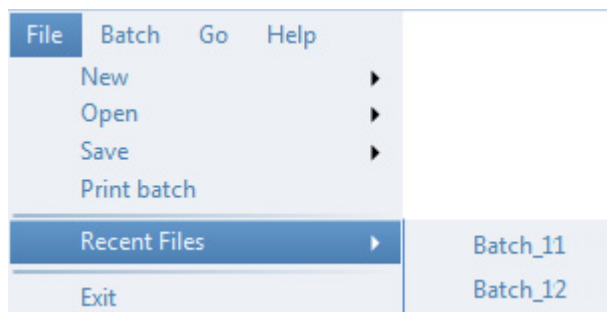


Table 144. Open Batch dialog box parameters

Parameter	Description
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is stored.
Buttons	
Type	Type of batch to display in the Batch list: Quan, Screening, Unknown Only, or Any.
Open	Opens the Batch View for the selected batch.
Cancel	Closes the Open Batch dialog box without opening a batch.

❖ To open a recent batch

Choose **File > Recent Files > *batch*** from the main menu.



The selected batch opens in the Batch View.

❖ To edit samples in a batch

Use the commands described in “[Working in the Batch View](#)” on page 606.





You can add new samples, edit samples, or delete samples.

❖ To reinject a sample from a previously acquired batch

1. In the sample list, select the sample that you want to reinject.
2. Right-click and choose **Reinject This Sample** from the shortcut menu.

The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The 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	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

When you submit all samples in this batch, the application acquires all samples (including previously acquired samples).

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 prepared batch that is ready to submit. You can open this batch from the Reinject Samples page in the Acquisition mode and submit the batch. The application acquires only the samples that have not been previously acquired.

Submitting a Batch


In the 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 635](#).

For a description of commands in the shortcut menu, see “[Batch View shortcut menu commands](#)” on [page 618](#).

Follow these procedures:



- [To submit selected peaks for processing](#)
- [To submit samples in the batch](#)
- [To view the output files](#)

❖ To submit selected peaks for processing

1. In the Peak List, select the **Selected** check box for the peaks that you want to process.
2. Click the **Submit ... for Processing** icon, .

The application processes the selected peaks and updates the data in the Peak Identifications pane.

❖ To submit samples in the batch

1. Do one of the following:
 - To submit all samples in the batch, click the **Submit Batch** icon, .
 - To submit specific samples, select the samples and click the **Submit Selected Samples** icon, .

The Submit Options dialog box opens. See “[Submit Options dialog box](#)” on [page 635](#).

Note You can also submit only selected peaks for processing. See [To submit selected peaks for processing](#).

2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.
 - When all submitted samples have been previously acquired, this option is (by default) not selected.
 - When one or more samples in the batch have not been acquired, this option is (by default) selected.

Tip You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

3. To process the submitted samples, select the **Process Data** check box.

The application displays processing options for the Unknown Screening method.

4. Select the check box for the unknown screening options that you want to use.

Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

Identify: Performs identification. This produces the peak identification data in the Unknown Screening View.

With RT Alignment: Performs retention time alignment. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.

5. (Optional) Select the **Create Reports** check box.
6. (Optional with multiplexing activated) 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 activated) 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.

Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.
 - a. Select the **Use** check box for the device that you want to use for this acquisition.
 - b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

This is usually the autosampler.
 - c. 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.
 - d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.
9. To start the selected processes, click **OK**.

The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Analysis mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT After the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages in the method (“[Editing the Processing Pages](#)” on [page 311](#)) and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Figure 212. Submit Options dialog box

The screenshot shows the 'Submit Options' dialog box. It includes fields for 'User name' and 'Samples'. Under 'Workflow steps to perform', 'Acquire data' is checked and shows '1 unacquired sample(s)'. 'Process data' is also checked. Under 'Unknown Screening', 'Peak Detect', 'Identify', and 'With RT Alignment' are unchecked. 'Create reports' is unchecked. Under 'Submit as a priority sequence?', 'Priority Sequence' is unchecked, and 'Next Available Sample' is selected. The 'Acquisition' section shows a table with 'Simulation MS' selected, 'Start when ready' checked, and 'Post-run system state' set to 'On'. Buttons for 'Hide Details ^', 'OK', and 'Cancel' are at the bottom.

Table 145. Submit Options dialog box parameters (Sheet 1 of 3)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.

Table 145. Submit Options dialog box parameters (Sheet 2 of 3)

Parameter	Description
Workflow Steps to Perform	
Acquire Data	<p>Submits the current batch to acquisition.</p> <ul style="list-style-type: none"> When all submitted samples have been previously acquired, this option is (by default) not selected. When one or more samples in the batch have not been acquired, this option is (by default) selected.
Process Data	<p>Processes the data for the current batch using any of the following options:</p> <p>Peak Detect: Performs peak detection for all method types. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.</p> <p>Identify: Performs identification for unknown screening methods.</p> <p>With RT Alignment: Performs retention time alignment for unknown screening methods. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.</p> <p>Note You can use Unknown Screening features in conjunction with Quantitation or Target Screening methods.</p> <p>For specifying processing data for batches that also use Quantitation methods, see “To submit samples in the batch” on page 433.</p> <p>For specifying processing data for batches that also use Target Screening methods, see “To submit samples in the batch” on page 557.</p>
Create Reports	Creates reports for the current batch.

Table 145. Submit Options dialog box parameters (Sheet 3 of 3)

Parameter	Description
Submit as a Priority Sequence?	
Priority Sequence	<p>With multiplexing activated, places the batch immediately after the currently acquiring batch.</p> <p>Without multiplexing activated, specifies one of the following priority options to place the batch in the queue:</p> <p>Next Available Batch: Places the batch immediately after the currently acquiring batch.</p> <p>Next Available Sample: Places the batch immediately after the currently acquiring sample.</p> <p>Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.</p>
Acquisition pane	
Device Name	<p>Lists all configured instruments.</p> <p>If the instrument that 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.</p> <p>Available only when you select the Acquire Data check box.</p>
Use	<p>Specifies the instruments used for this acquisition.</p> <p>Available only when you select the Acquire Data check box.</p>
Start Device	<p>Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler.</p> <p>Available only when you select the Acquire Data check box.</p>
Start When Ready	<p>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.</p>
Post-run System State	<p>Specifies the system state after it acquires the last batch: On (default), Standby, or Off.</p>
Buttons	
Hide/Show Details	<p>Collapses or expands the acquisition details of the Submit Options dialog box.</p>
OK	<p>Begins the selected processes.</p>
Cancel	<p>Closes the Submit Options dialog box without submitting any tasks.</p>

❖ To view the output files

Locate the files to view from the following directories:

The application writes saved batches to the project folder:

...\\TraceFinderData\\3.3\\Projects\\...

For each acquired sample, the application writes an RSX file to the batch Data folder:

...\\TraceFinderData\\3.3\\Projects\\...\\Data

The application saves method information to the batch Methods folder:

...\\TraceFinderData\\3.3\\Projects\\...\\Methods

The application writes the reports to the batch Reports folder:

...\\TraceFinderData\\3.3\\Projects\\...*batch*\\Reports

Saving a Batch to a New Location

You can move the current batch to a different project folder, or you can make a copy of the current batch and save the copy to a different project folder.

Follow these procedures:

- [To save a batch to another project folder](#)
- [To move a batch to another folder](#)
- [To create new project folder](#)
- [To delete project folders](#)
- [To rename project folders](#)

❖ To save a batch to another project folder

1. Choose **File > Save > Save Batch As** from the Batch View main menu in the Analysis mode.

The Save Batch As dialog box opens. See “[Save Batch As Dialog Box](#)” on [page 640](#).

2. Select a storage location.

The default storage location is C:\\TraceFinderData\\3.3\\Projects.

3. Select or create a project folder.

4. Type a name for the new batch.

If you are saving the batch to a different folder, you must give it a unique name. You cannot overwrite an existing batch in a folder.

5. Click **Save**.

When you save the batch to a different folder, the reports reflect the original project folders and the application does not save the calibration history.

❖ To move a batch to another folder

1. Choose **File > Save > Move Batch** from the Batch View main menu in the Analysis mode.

The Save Batch As dialog box opens. See “[Save Batch As Dialog Box](#)” on [page 640](#).

2. Select a storage location.

The default storage location is C:\TraceFinderData\3.3\Projects.

3. Select or create a project folder.

4. Type a name for the new batch.

You must give the batch a unique name in the new subproject folder. You cannot overwrite an existing batch.

5. Click **Save**.

When you move the batch, the reports reflect the original project and subproject folders and the application does not save the calibration history.

❖ To create new project folder

1. In the Save Batch As dialog box, select the folder for which you will create a new lower-level folder.

- You can select the main TraceFinderData\3.3\Projects folder and create a new folder under it.
- You can select one of the existing folders and create a lower-level folder under it.

2. Click the **Create Folder** icon, .

The application adds a new lower-level folder to the selected folder.

3. Select the new folder name and type a name for the folder.

Folder names can contain spaces and special characters, except for the following special characters: \ / : + ? ” < >

Note After you add a lower-level folder, you cannot rename the parent folder.

❖ To delete project folders


1. In the Save Batch As dialog box, select the folder to delete.

2. Click the **Delete Folder** icon, .

With no confirmation prompt, the application immediately removes the selected folder.

Note This feature is not available for folders that contain lower-level project or batch folders; you must first delete the lower-level project or batch folders.

❖ To rename project folders

1. In the Save Batch As dialog box, select the folder to rename.
2. Click the **Rename Folder** icon, .

Note This feature is not available for folders that contain lower-level project or batch folders; you must first delete the lower-level project or batch folders.

3. Type a new name for the folder and press ENTER.

The application saves the new folder name.

Save Batch As Dialog Box

Use the features in the Save Batch As dialog box to save a batch to a new name or to move a batch to a different project folder.

Figure 213. Save Batch As dialog box

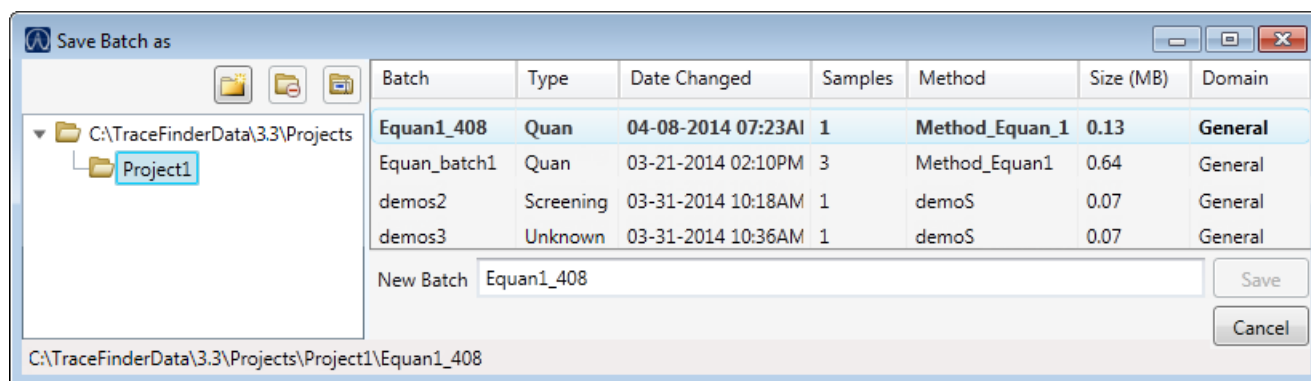


Table 146. Save Batch As dialog box parameters (Sheet 1 of 2)




Parameter	Description
 Create New Folder	Adds one of the following: <ul style="list-style-type: none"> • When a drive is selected, adds a new project-level folder to the drive. • When a project folder is selected, adds a subproject-level folder to the selected project. • When a subproject folder is selected, adds a lower-level folder to the subproject. Or, right-click and choose Create Folder from the shortcut menu.
 Delete Folder	With no confirmation prompt, immediately removes the selected folder. You cannot delete a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders. Or, right-click and choose Delete from the shortcut menu.
 Rename Folder	Renames the selected folder. You cannot rename a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders. Or, right-click and choose Rename from the shortcut menu.

Table 146. Save Batch As dialog box parameters (Sheet 2 of 2)

Parameter	Description
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
New batch parameters	
New Batch	Name of the new batch to create. Note If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
<i>Path</i>	Path to the project in the TraceFinderData\3.3\Projects folder where the batch is created.
Buttons	
Save	Saves the batch to the specified name and folder and opens the Batch View for the new batch.
Cancel	Closes the Save Batch As dialog box without saving the batch.
Shortcut menu commands	
Create Folder	Adds one of the following: <ul style="list-style-type: none"> • When a drive is selected, adds a new project-level folder to the drive. • When a project folder is selected, adds a subproject-level folder to the selected project. • When a subproject folder is selected, adds a lower-level folder to the subproject.
Delete Folder	Immediately removes the selected folder. There is no prompt to confirm that you want to delete the selected folder. You cannot delete a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders.
Rename Folder	Renames the selected folder. You cannot rename a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders.
Expand Child Nodes	Expands all project and subproject folders in the Project tree.
Collapse Child Nodes	Collapses all project and subproject folders in the Project tree.

Working in Data Review

The Data Review view displays the data generated by the master method. Use Data Review to verify the data for identified peaks before you generate reports.

When you run samples in an experiment, you can check for peaks that are not already identified in either an associated target screening or quantitation method and take appropriate steps when the application finds these peaks and proposes whether they match one or more compounds using various identification sources.

IMPORTANT When unknown screening features are associated with a quantitation or target screening method, the unknown screening results do not include any compounds (other than internal standards) that were identified by the quantitation or target screening methods.

Follow these procedures:

- [To open the Data Review view](#)
- [To display or hide a pane on the Unknown Screening View page](#)
- [To move, dock, or float Data Review panes](#)
- [To restore the default layout](#)

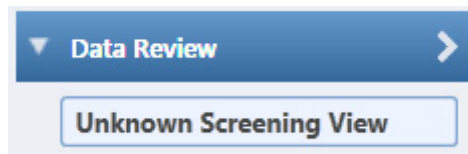
❖ To open the Data Review view

1. Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.

2. Click **Data Review**.

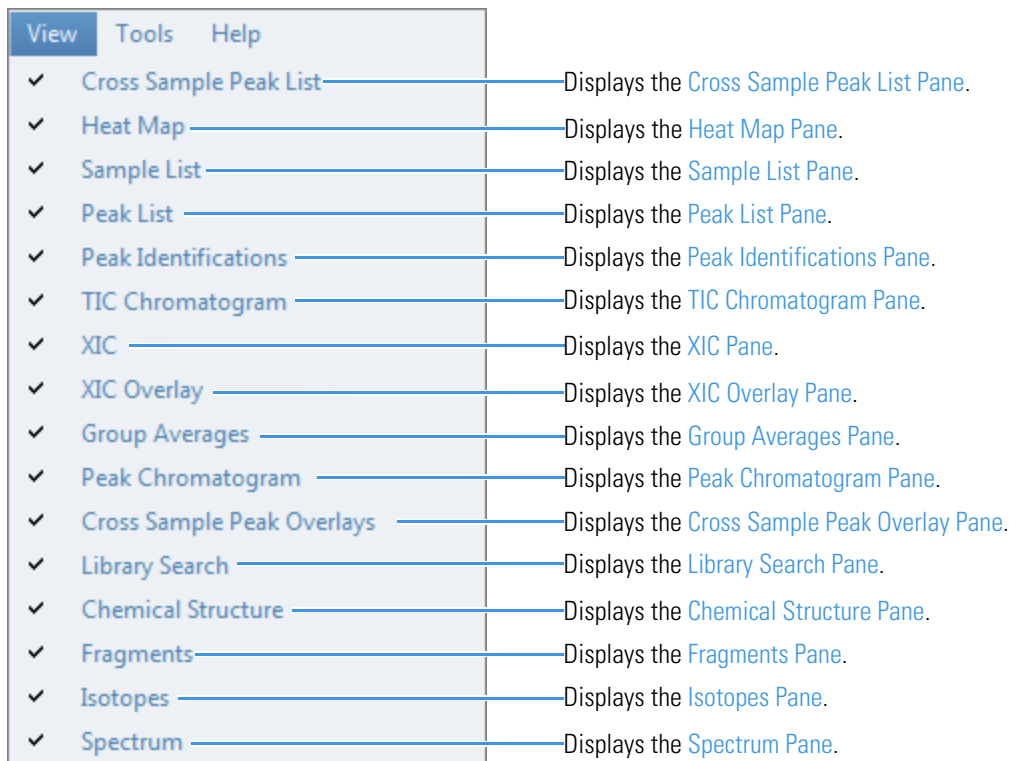
The Data Review navigation pane opens.



❖ To display or hide a pane on the Unknown Screening View page

From the View menu, choose to display or hide any of the following panes.

A check mark indicates a displayed pane.



❖ To move, dock, or float Data Review panes

Follow the instructions in [Appendix D, “Moving Data Review Panes.”](#)

❖ To restore the default layout

Choose **View > Restore Default Layout**.

The Unknown Screening View displays the default panes in their default locations.

Cross Sample Peak List Pane

Use the Cross Sample Peak List pane to compare peak values across all samples in a batch.

❖ To use the Cross Sample Peak List pane

1. In the Peak List pane, select a peak.

The application scrolls the Cross Sample Peak List pane to the specified peak and selects the peak.

2. Use the scroll bar at the bottom of the pane to scroll across the values for the selected peak in all samples and groups in the batch.

Figure 214. Cross Sample Peak List pane

The figure shows two screenshots of the software interface. The top screenshot is the 'Cross Sample Peak List' pane, which contains a table with the following data:

	Selected	Retention Time	M/Z	Mass	Mono Isotopic Mass	Maximum Fold
2	<input type="checkbox"/>	0.80	203.05	202.05	202.05	0.00
3	<input type="checkbox"/>	5.92	169.12	168.11	168.12	0.00
4	<input type="checkbox"/>	6.72	245.08	244.07	244.07	0.00

The bottom screenshot shows a detailed view of the 'Apple_I' column, with the following data:

Apple_I	MS Area	Apple_I Avg Area	Apple_I CV	Apple_I Fold
=	0.00	1.00	0.00	0.00
	0.00	1.00	0.00	0.00
	157,846.41	157,846.41	0.00	0.00

Table 147. Cross Sample Peak List pane columns (Sheet 1 of 2)


Column	Description
Selected	Identifies peaks to display when you select the Selected option in the XIC Overlay pane, or identifies which peaks to process when you click the Submit ... for Processing icon,  . Do not confuse a check mark in the Selected column with the currently selected peak. The row for a currently selected peak is highlighted in blue.
Retention Time	The time after injection when the compound elutes. The total time that the compound is retained on the column.
M/Z	Mass-to-charge ratio found in the spectra for the peak. Assumes that the charge is 1.
Mass	The uncharged mass found in the spectra for the peak.
Monoisotopic Mass	The most abundant mass in the spectra for the peak.
Maximum Fold	The maximum difference of the group average response from the control average response.
Compound Name	Displays the compound name found in the library or compound database. This column is displayed only when the peaks are aligned and you have performed a simple search. See “Editing the Peak Settings” on page 311.
Sample n MS Area	The MS peak area for each sample.
Default Average Area	The averaged response of all peak occurrences in the sample.

Table 147. Cross Sample Peak List pane columns (Sheet 2 of 2)

Column	Description
Default % CV	The coefficient of variance for each sample. The coefficient of variance is calculated as the 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.
Default Fold	The maximum difference of the sample average response from the control average response.
<i>Group n</i> Average Area	The averaged response of all peak occurrences in the group. The minimum value is 1, even when the peak never occurs in the group.
<i>Group n</i> % CV	The coefficient of variance for each sample. The coefficient of variance is calculated as the 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 all the peaks in the group of samples.
<i>Group n</i> Fold	The maximum difference of the average response of all samples in a group from the control average response.

Heat Map Pane

Use the Heat Map pane to display the response of each peak occurrence in the batch. The Heat Map pane displays all MS Area values for all peaks in all samples in the batch that are above the peak threshold value specified in the method. When you select a peak in the Heat Map pane, the application displays the associated results for the selected peak in all panes of the Unknown Screening view.

The Heat Map pane is available only when you select the Alignment and Gap Filling option in the method (see [“Editing the Peak Settings”](#) on page 311) or select the RT Alignment option when you submit the batch (see [“Submitting a Batch”](#) on page 633).

Follow these procedures:

- [To use the Heat Map pane](#)
- [To use the Heat Map pane with the TIC Chromatogram pane](#)
- [To use the Heat Map pane with the XIC chromatogram pane](#)

❖ To use the Heat Map pane

1. Click the **Heat Map** tab to display the pane.

For detailed descriptions of all parameters in the Heat Map pane, see “Heat Map pane” on page 647.

2. In the Peak List pane, select a peak.

The application scrolls the Heat Map pane to the specified peak and selects the peak.

For each found peak in the batch, the application assigns a color code indicating the relative MS area value from highest (orange) to lowest (green).

Highest	5,054,199.00
	2,041,157.25
	388,806.75
	220,048.25
	148,246.16
Lowest	102,254.38

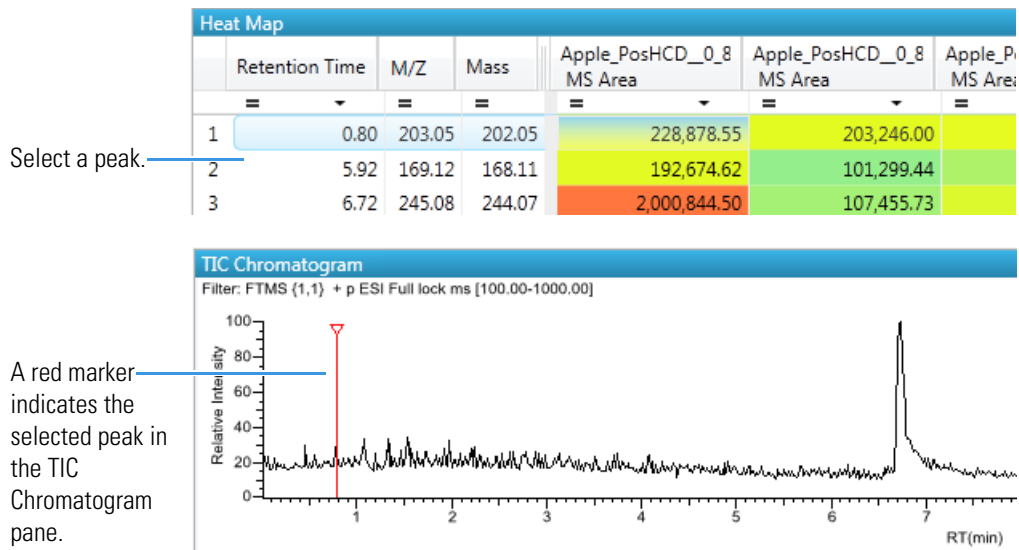
❖ To use the Heat Map pane with the TIC Chromatogram pane

1. Click the **TIC Chromatogram** tab to display the pane.

The total ion current (TIC) chromatogram pane displays the relative intensity of all found peaks in the batch.

2. In the Heat Map pane, select a peak.

The application identifies the selected peak in the TIC Chromatogram pane and indicates it with a red marker.



Or, you can select a peak in the TIC Chromatogram pane, and the application scrolls the heat map to the selected peak.

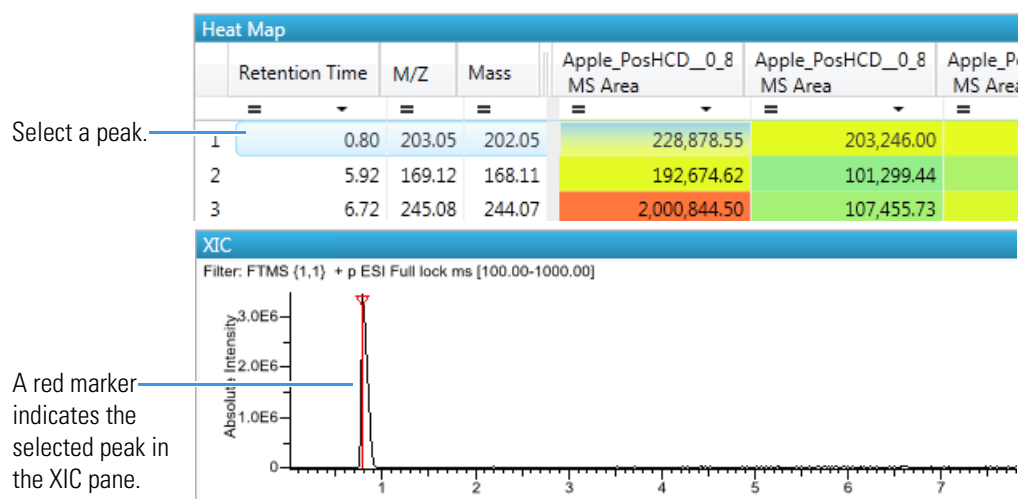
❖ To use the Heat Map pane with the XIC chromatogram pane

1. Click the **XIC** tab to display the pane.

The extracted ion chromatogram (XIC) pane displays the absolute intensity of the selected peak.

2. In the Heat Map pane, select a peak.

The application identifies the selected peak in the XIC, scales the chromatogram's *y* axis to fit the peak, and indicates it with a red marker.



Or, you can select a peak in the XIC pane, and the application scales the chromatogram to fit the peak, indicates it with a red marker, and scrolls the heat map to the selected peak.

Figure 215. Heat Map pane

Heat Map						
	Retention Time	M/Z	Mass	Apple_PosHCD_0_81_01 MS Area	Apple_PosHCD_0_8 MS Area	Apple_PosHCD_4_0 MS Area
1	5.92	169.12	168.11	192,674.62	101,299.44	112,746.64
2	6.72	245.08	244.07	2,000,844.50	107,455.73	170,410.11
3	6.72	163.04	162.03	1,156,472.00	205,919.31	107,573.62


Table 148. Heat Map pane columns

Column	Description
Retention Time	The time after injection when the compound elutes. The total time that the compound is retained on the column.
M/Z	Mass-to-charge ratio found in the spectra for the peak. Assumes that the charge is 1.
Mass	The uncharged mass found in the spectra for the peak.
Sample <i>n</i> MS Area	The MS peak area for each sample.

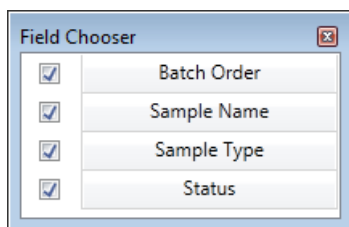
Sample List Pane

Use the Sample List pane to select a sample of interest. The application displays the associated results for the selected sample in all panes of the Unknown Screening view. See [Sample List pane](#).

❖ To hide or display columns in the Sample List pane

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Sample List pane.



2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

The application immediately displays or hides the column in the Sample List pane.


3. When you are finished modifying the column display, click  to close the Field Chooser.

Figure 216. Sample List pane

	Batch Order	Status	Sample Name	Sample Type
1	1		Unknown1	Unknown
2	2		Unknown2	Unknown
3	3		Unknown3	Unknown
4	4		Unknown4	Unknown

Table 149. Sample List pane columns

Column	Description
Batch Order	The order in which the samples were acquired.
Status	<ul style="list-style-type: none"> Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring. <p>Note When you include unknown screening features in a quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed ().</p> <p>Note When you include unknown screening features in a target screening method and you choose to process with only the unknown screening criteria, both the Samples view and the Unknown Screening View show the Status for the samples as acquired and processed ().</p>
Sample Name	A user-defined name that identifies a sample.
Sample Type	<p>Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC Std, or Unknown</p> <p>Default: Unknown</p>

Peak List Pane

Use the Peak List pane to select a specific peak found in the selected sample. The Peak List displays each peak that the application identified in the sample. See [Peak List pane](#).

❖ To display information for a peak

In the Peak List, click anywhere in the peak row.

The application displays information for the selected peak in the other Data Review panes.

Note Do not confuse a check mark in the Selected column with the currently selected peak. The row for the current, selected peak is highlighted in blue. A selected check box in the Selected column does not indicate the current, selected peak (see [Selected](#)).

Figure 217. Peak List pane

The figure shows three overlapping windows from the software interface:

- Peak List Table:** A table with columns: Selected, Peak ID, M/Z, Retention Time, Area, Height, Potential ID, and Mass. It lists four peaks, with the first peak selected (highlighted in blue).
- Library Search Table:** A table with columns: Mono Isotopic Mass, Charge State, Filter String, NIST, and Library Manager. It shows search results for the selected peak.
- Elemental Composition Table:** A table with columns: Elemental Composition, Database, and Chemspider. It shows the elemental formula and search results for the selected peak.

Selected	Peak ID	M/Z	Retention Time	Area	Height	Potential ID	Mass
<input checked="" type="checkbox"/>	peak @ 0.80 203.05	203.05	0.80	203,246.00	3,412,897.50	7	202.04
<input type="checkbox"/>	peak @ 11.48 312.3	312.36	11.48	455,449.00	7,354,474.69	7	311.54
<input type="checkbox"/>	peak @ 13.04 338.3	338.34	13.04	262,451.75	3,939,006.44	7	337.53
<input type="checkbox"/>	peak @ 14.20 278.9	278.97	14.20	166,002.72	513,232.62	9	277.96

Mono Isotopic Mass	Charge State	Filter String	NIST	Library Manager
284.27	1	FTMS + p ESI Full ms [100.00-1000.00]	N/A	N/A
100.00	1	FTMS + p ESI Full ms [100.00-1000.00]	N/A	N/A
293.15	1	FTMS + p ESI Full ms [100.00-1000.00]	N/A	N/A
260.07	1	FTMS + p ESI Full ms [100.00-1000.00]	N/A	N/A

Elemental Composition	Database	Chemspider
C18H37O2	N/A	N/A
N/A	N/A	N/A
C13H23O4N2Na	N/A	N/A
C7H21O2N2S3	N/A	N/A

Table 150. Peak List pane columns (Sheet 1 of 2)

Column	Description
Selected	Identifies peaks to display when you select the Selected option in the XIC Overlay pane, or identifies which peaks to process when you click the Submit ... for Processing icon, . Do not confuse a check mark in the Selected column with the currently selected peak. The row for the current, selected peak is highlighted in blue.

Table 150. Peak List pane columns (Sheet 2 of 2)

Column	Description
Peak ID	Identifies the peak as “peak @ <i>retention time m/z</i> .” Example: peak @ 0.80 203.05
<i>m/z</i>	Mass-to-charge ratio found in the spectra for the peak. Assumes the charge is 1.
Retention Time	The time after injection when the compound elutes. The total time (in minutes) that the compound is retained on the column.
Area	The area obtained by integrating peak intensities from the start to the end of the peak.
Height	The distance from the peak maximum to the peak base, measured perpendicular to the ordinate.
Potential ID	The number of returned peak IDs.
Mass	The uncharged mass found in the spectra for the peak.
Monoisotopic Mass	The sum of the masses of the most abundant isotope.
Charge State	The charge state of the ion (the <i>z</i> value in <i>m/z</i>). For example, a charge state of 2 with a negative polarity means that the compound has 2 more electrons than protons. Valid range: 1 through 10 Default: 1
Filter String	Filter used to identify the peak. Specified in the raw data file or the master method.
NIST	The NIST match result name for the identified peak. If there is no match or if the Library search was not specified in the method, this shows as “N/A.”
Library Manager	The library match result name for the identified peak. If there is no match or if the Library Search was not specified in the method, this shows as “N/A.”
Elemental Composition	The chemical formula for the identified peak. If there is no match or the Elemental Composition search was not specified in the method, this shows as “N/A.”
Database	The compound database match result name for the identified peak. If there is no match or the Database Search was not specified in the method, this shows as “N/A.”
ChemSpider	The ChemSpider database match result name for the identified peak. If there is no match or the ChemSpider Search was not specified in the method, this shows as “N/A.”

Peak Identifications Pane

Use the Peak Identifications pane to display the name and formula for identified peaks and the source of the identification.

Figure 218. Peak Identifications pane

Selected	ID Source	ID Source Detail	Match Result Name	Formula
<input checked="" type="checkbox"/>	NIST	nist_msms	5-Hydroxy-3'-methoxyflavone	C16H12O4
<input type="checkbox"/>	NIST	nist_msms	4'-Hydroxy-5-methoxyflavone	C16H12O4
<input type="checkbox"/>	NIST	nist_msms	1,3,9-Trimethylxanthine	C8H10N4O2
<input type="checkbox"/>	LibraryManager		Metamitron	C10H10N4O

Table 151. Peak Identifications pane columns (Sheet 1 of 2)

Column	Description
Selected	Identifies peaks to display when you select the Selected option in the XIC Overlay pane, or identifies which peaks to process when you click the Submit ... for Processing icon, . Do not confuse a check mark in the Selected column with the currently selected peak. The row for a currently selected peak is highlighted in blue.
ID Source	Specifies the search type used to identify the peak (Database Search, Library Search (NIST or LibraryManager), Elemental Composition, or ChemSpider Search). To specify search types in the method, see “ To specify the search options ” on page 313 .
ID Source Detail	Specifies the name of the library, the compound database, or the ChemSpider hyperlink where the peak was identified.
Match Result Name	Specifies the compound name that was found in the library, in the compound database, or in the ChemSpider hyperlink.
Formula	Specifies the chemical formula that was found in the library, in the compound database, in the elemental composition, or in the ChemSpider hyperlink.
Isotope Pattern Score %	The percentage of matched isotopes in the total number of isotopes.
Number of Isotopes Matched	The number of isotopes matched in the calculated isotope spectra relative to the total number of isotopes used in the score calculation, in the format “x of y”, where <ul style="list-style-type: none"> x = the number of isotopes matching the elemental composition used for the Isotope Pattern Score calculation. y = the total number of isotopes considered in the Isotope Pattern Score calculation. This is the number of isotope peaks expected to be above the spectral noise.

Table 151. Peak Identifications pane columns (Sheet 2 of 2)

Column	Description
Score	The score from the library fit. When the application finds a match in the library, in the compound database, or through the ChemSpider hyperlink, this column displays the highest score associated with the Match Result Name parameter. Valid range: 1 through 100%
SI/Dot Product	Search index method used to search the NIST library.
RSI/Rev Product	(Reverse search index) A method used to search the NIST library. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
Library Probability Percent	The probability ranking from the NIST library. When you use a reverse search, this value is "N/A."
Fragments	The number of fragments matched in the calculated spectra relative to the total number of expected fragments.

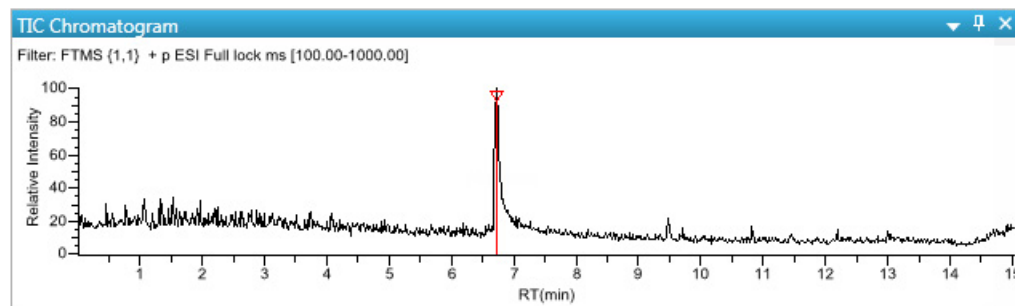
TIC Chromatogram Pane

Use the TIC Chromatogram pane to display the relative intensity of a trace along the length of the sample data retention window.

❖ To focus on a specific peak

In the TIC Chromatogram pane, click any displayed peak.

The application indicates the selected peak with a red, vertical marker and updates the focus in the other Data Review panes with data for that peak.

Figure 219. TIC Chromatogram pane

XIC Pane

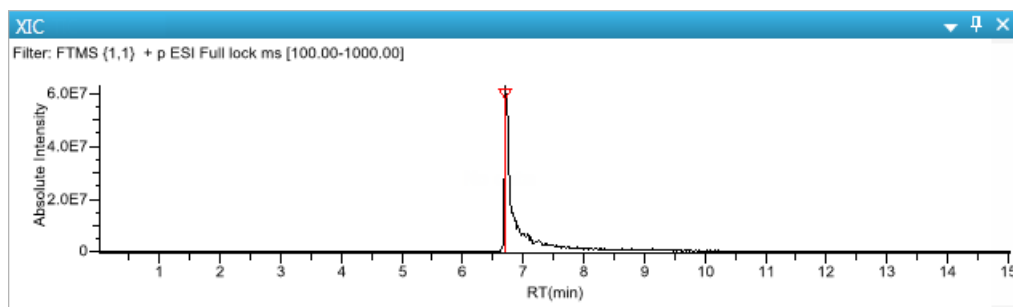
Use the XIC pane to display the absolute intensity of an extracted trace along the length of the sample data retention window.

❖ To focus on a specific peak

In the XIC pane, click any displayed peak.

The application indicates the selected peak with a red, vertical marker and updates the focus in the other Data Review panes with data for that peak.

Figure 220. XIC pane



XIC Overlay Pane

Use the XIC Overlay pane to view specific groups of peaks. You can choose to view all peaks, selected peaks only, or the top twenty most intense peaks (by area). The XIC Overlay plot is a collection of overlaid, extracted m/z ion plots that use a different color for each peak.

Follow these procedures:

- To display all peaks in a sample
- To display only selected peaks in a sample
- To display the top twenty peaks in a sample
- To focus on a specific peak

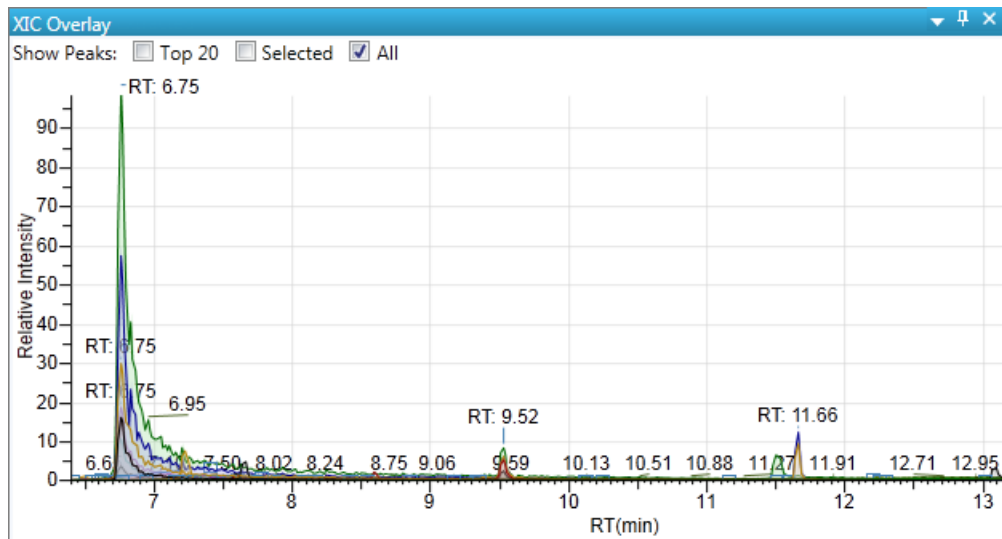
❖ To display all peaks in a sample

1. In the Sample List pane, select the sample whose peaks you want to view.
2. In the XIC Overlay pane, select the **All** check box.

The application displays all the peaks in the selected sample. See [XIC Overlay plot showing all peaks](#).

Note If there are more than 1000 peaks in the sample, performance might be slow.

Figure 221. XIC Overlay plot showing all peaks



❖ **To display only selected peaks in a sample**

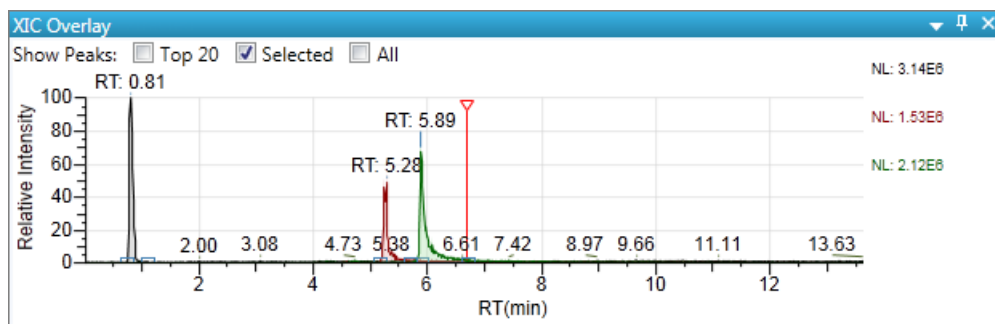
1. In the Sample List pane, select the sample whose peaks you want to view.
2. In the Peak List pane, select the **Selected** check box for each peak that you want to view.

Peak List			
<input type="checkbox"/>	<input checked="" type="checkbox"/> Selected	Peak ID	M/Z
1	<input checked="" type="checkbox"/>	peak @ 0.81 203.05	203.05
2	<input checked="" type="checkbox"/>	peak @ 5.27 158.19	158.19
3	<input checked="" type="checkbox"/>	peak @ 5.90 169.12	169.12

3. In the XIC Overlay pane, select the **Selected** check box.

The application displays all selected peaks.

Figure 222. XIC Overlay plot showing selected peaks

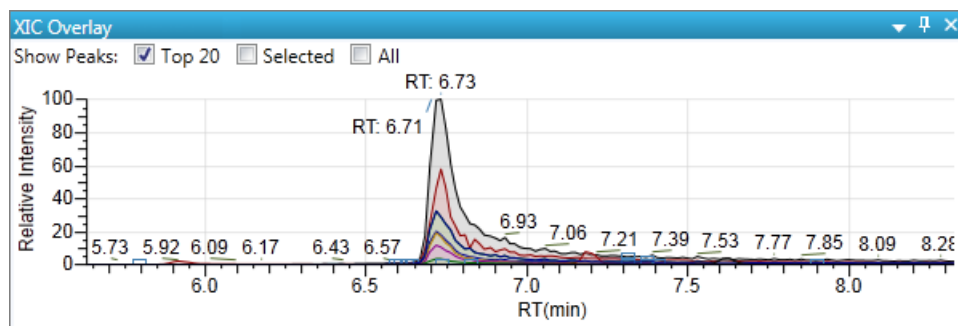


❖ **To display the top twenty peaks in a sample**

1. In the Sample List pane, select the sample whose peaks you want to view.
2. In the XIC Overlay pane, select the **Top 20** check box.

The application displays the top twenty peaks in the selected sample.

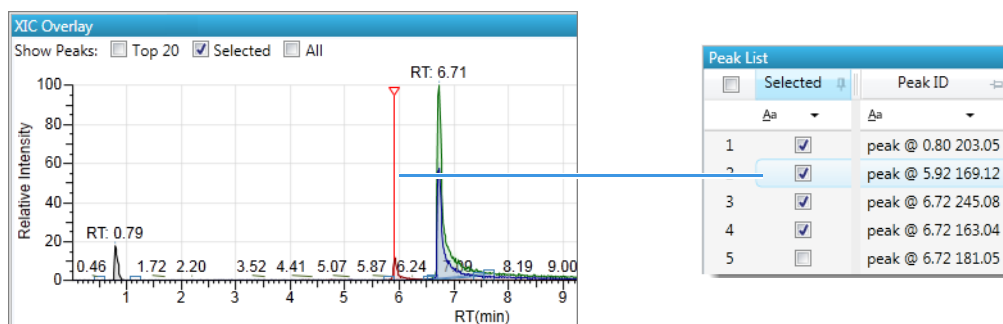
Figure 223. XIC Overlay plot showing the top 20 peaks



❖ **To focus on a specific peak**

In the XIC Overlay pane, click any displayed peak.

The application indicates the selected peak with a red, vertical marker and updates the focus in the other Data Review panes with data for that peak.



Group Averages Pane

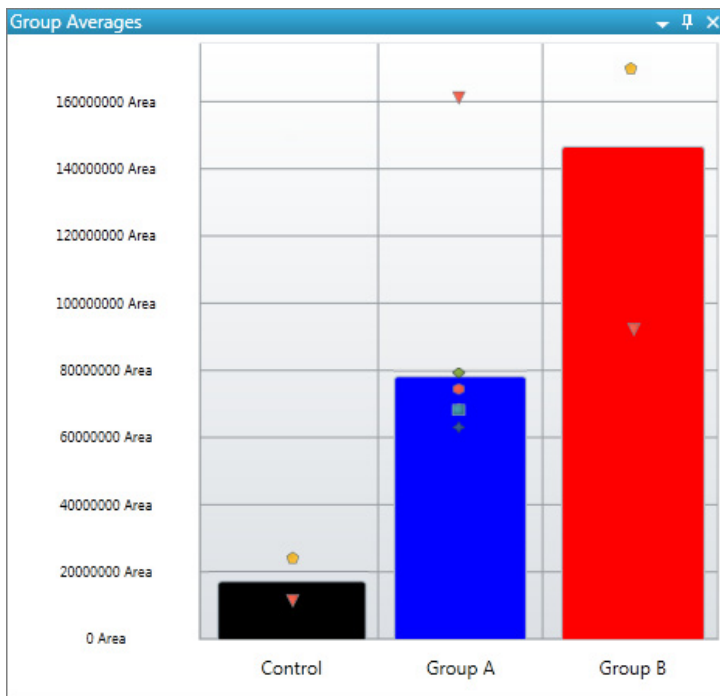
Use the Group Averages pane to compare the peak areas of different samples to a control group of samples.

The Group Averages pane is available only when you select the Alignment and Gap Filling option in the method (see “Editing the Peak Settings” on page 311) or select the RT Alignment option when you submit the batch (see “Submitting a Batch” on page 633).

The control group is displayed to the left, and other samples and groups are listed in the order in which they appear in the Batch View. To specify a group as the control group, see “Groups” on page 610.

Each group displays a colored bar that indicates the average response of the group, as displayed in the Average Area column in the Cross Sample Peak List pane (“Cross Sample Peak List Pane” on page 643). The color of the bar matches the colors assigned to the samples and peaks in the Cross Sample Peak Overlay pane (“Cross Sample Peak Overlay Pane” on page 662).

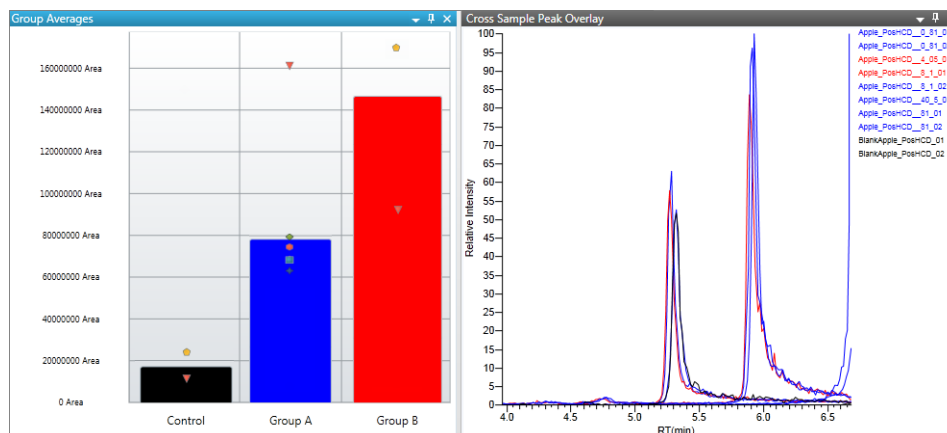
Figure 224. Group Averages pane



❖ **To use the Group Averages pane with the Cross Sample Peak Overlay pane**

Display both the Group Averages pane and the Cross Sample Peak Overlay pane.

The color of the bars in the Group Averages pane matches the colors assigned to the group samples and peaks in the Cross Sample Peak Overlay pane.



Peak Chromatogram Pane

Use the Peak Chromatogram pane to display the selected chromatogram peak. The Peak Chromatogram pane initially displays the apex scan for the detected peak. You can manually integrate the peak and use the updated peak to generate reports. See “[Peak Chromatogram Pane](#)” on page 660.

Follow these procedures:

- [To zoom in on a peak](#)
- [To remove a peak](#)
- [To customize the labels in the display](#)
- [To display surrounding apex times](#)
- [To manually integrate a peak](#)
- [To switch between method and manual integration modes](#)

❖ **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 remove a peak**

Right-click the Peak Chromatogram pane, and choose **Delete Peak** from the shortcut menu.

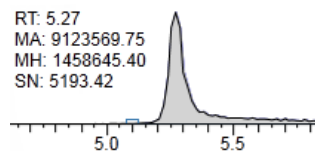
The application removes the peak displayed in the Peak Chromatogram pane. All data for this peak are removed from the Unknown Screening View panes.

❖ **To customize the labels in the display**

1. Right-click the Peak Chromatogram pane, and choose **Peak Display Settings** from the shortcut menu.

The Peak Settings dialog box opens. For detailed descriptions of commands, see “[Peak Settings Dialog Box](#)” on page 661.

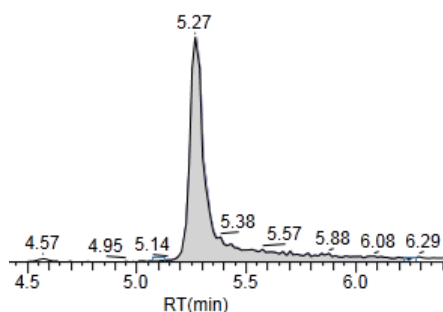
2. To display labels for the peak retention time (RT), mass height (MH), mass area (MA), or signal-to-noise (SN), select the appropriate check box.
3. Click **OK** in the Peak Settings dialog box.


Figure 225. Example of displayed labels❖ **To display surrounding apex times**

1. Right-click the Peak Chromatogram pane, and choose **Peak Display Settings** from the shortcut menu.

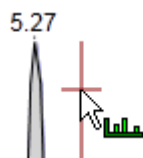
The Peak Settings dialog box opens. For detailed descriptions of commands, see “[Peak Settings Dialog Box](#)” on page 661.

2. Select the **Show All Apex Times** check box.
3. Click **OK** in the Peak Settings dialog box.

Figure 226. Example of displayed apex times❖ **To manually integrate a peak**

1. Right-click the Peak Chromatogram pane, and choose **Swipe Manual Integration** from the shortcut menu, or click the **Swipe Manual Integration** icon, .

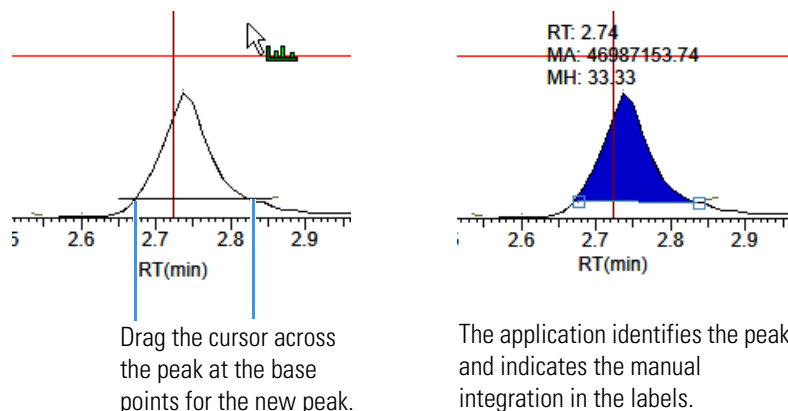
The cursor changes to indicate the manual integration mode.



2. Drag the cursor to define the beginning and ending base points for the new peak. See [Manually integrated peak](#).

Note You must drag the cursor inside the x axis and y axis.

Figure 227. Manually integrated peak



The application updates the area of the peak to the baseline that you just added. When you regenerate the reports, they display the manually modified data.

- To return to the original peak as defined by the method, right-click and choose **Toggle Integration Settings (Method)** from the shortcut menu.

❖ To switch between method and manual integration modes

Right-click the Peak Chromatogram pane and choose **Toggle Integration Settings (Manual or Method)** from the shortcut menu.

Initially, the method integration and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the Peak Chromatogram plots update and the result set updates 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.

Peak Chromatogram Pane

Use the Peak Chromatogram pane to display the selected chromatogram peak.

Figure 228. Peak Chromatogram pane

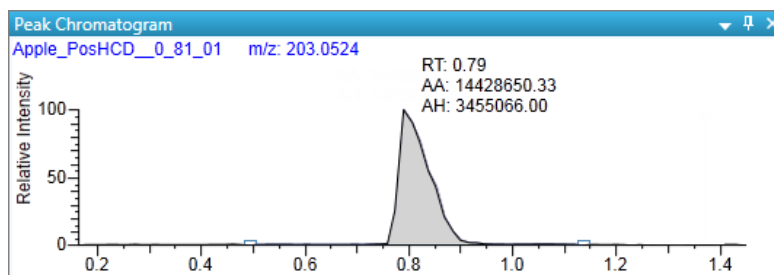






Table 152. Peak Chromatogram pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Swipe Manual Integration	Switches to manual integration mode, where you can manually define the peak.  Also available from the icon in the upper right corner,  .
Toggle Integration Settings (Manual or Method)	Switches the display between manual and method integration modes.
Delete Peak	Removes the peak and all data for this peak from the Unknown Screening View panes.  Also available from the icon in the upper right corner,  .
Peak Display Settings	Opens the Peak Settings dialog box. See Peak Settings Dialog Box .

Peak Settings Dialog Box

Use the Peak Settings dialog box to custom the display settings.

Figure 229. Peak Settings dialog box

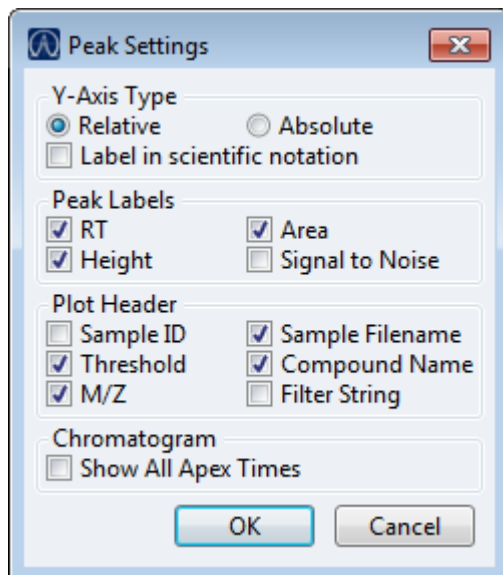


Table 153. Peak Settings dialog box parameters (Sheet 1 of 2)

Command	Description
Y-Axis Type	
Relative	Displays the <i>y</i> -axis scale from 0 through 100.

Table 153. Peak Settings dialog box parameters (Sheet 2 of 2)

Command	Description
Absolute	Displays the <i>y</i> -axis scale from 0 to the actual value of the most intense peak in the group.
Label in Scientific Notation	Displays the <i>y</i> -axis scale in scientific notation.
Peak Labels	
RT	Displays the retention time (RT) label in the peak chromatogram pane.
Height	Displays the peak height (AH) label in the peak chromatogram pane.
Area	Displays the peak area (AA) label in the peak chromatogram pane.
Signal to Noise	Displays the signal-to-noise (SN) label in the peak chromatogram pane.
Plot Header	
Sample ID	Displays a user-defined, alphanumeric string that identifies a sample.
Threshold	
<i>m/z</i>	Displays the mass-to-charge ratio found in the spectra for the peak. Assumes the charge is 1.
Sample Filename	Displays the name of the current, selected sample where the peak was found.
Compound Name	Displays the compound name match in the library or compound database.
Filter String	Displays the filter used to identify the peak. Specified in the raw data file or the master method.
Chromatogram	
Show All Apex Times	Displays all surrounding apex times in the plot.

Cross Sample Peak Overlay Pane

Use the Cross Sample Peak Overlay pane to compare instances of a selected peak across all samples in the batch. The application overlays all occurrences of the peak in the batch. See “[Cross Sample Peak Overlay Pane](#)” on [page 664](#).

The application displays the names of all samples in the batch where the selected peak is found. Samples that are assigned to groups are color coded, and the peaks found in those samples are color coded in the plot. To assign samples to groups, see “[Groups](#)” on [page 610](#).

The retention time window displayed in the Cross Sample Peak Overlay pane is the RT window that you specified in the method.

Follow these procedures:

- To select the peak to display in the Cross Sample Peak Overlay pane
- To zoom in on a peak
- To use the Cross Sample Peak Overlay pane with the Group Averages pane

❖ **To select the peak to display in the Cross Sample Peak Overlay pane**

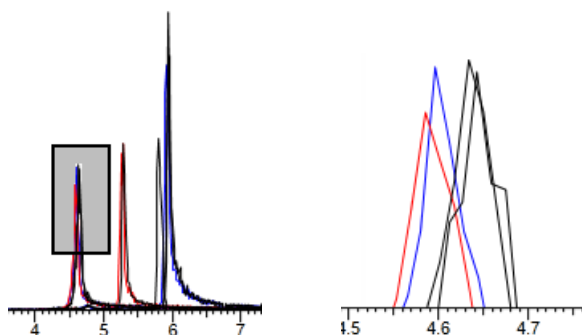
Select a peak in either the Peak List pane or the Cross Sample Peak List pane.

See “Peak List Pane” on page 650 or “Cross Sample Peak List Pane” on page 643.

❖ **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.

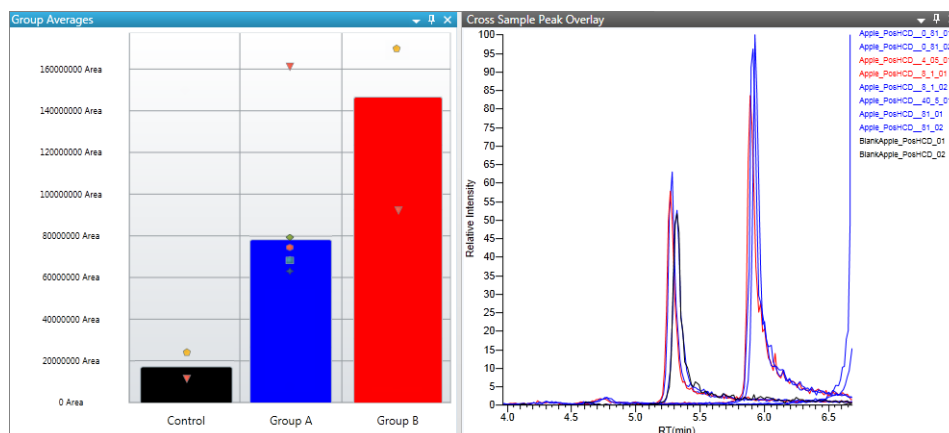


2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

❖ **To use the Cross Sample Peak Overlay pane with the Group Averages pane**

Display both the Cross Sample Peak Overlay pane and the Group Averages pane.

The color of the bars in the Group Averages pane matches the colors assigned to the group samples and peaks in the Cross Sample Peak Overlay pane.



Cross Sample Peak Overlay Pane

Use the Cross Sample Peak Overlay pane to compare instances of a selected peak across all samples in the batch

Figure 230. Cross Sample Peak Overlay pane

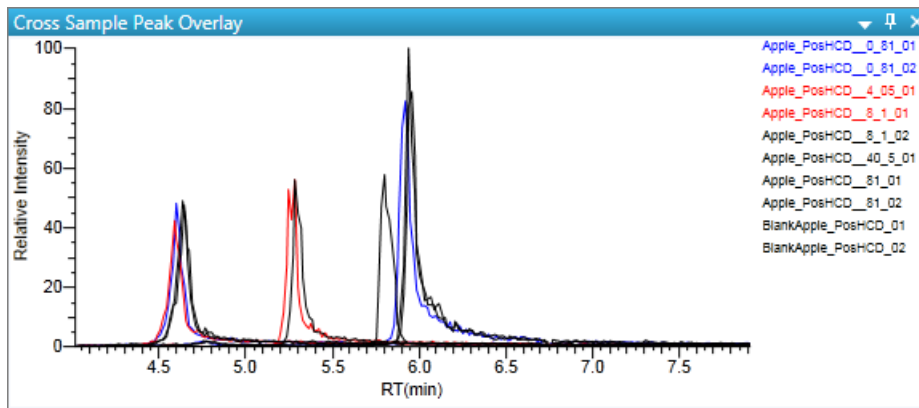


Table 154. Cross Sample Peak Overlay pane shortcut menu commands

Column	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Library Search Pane

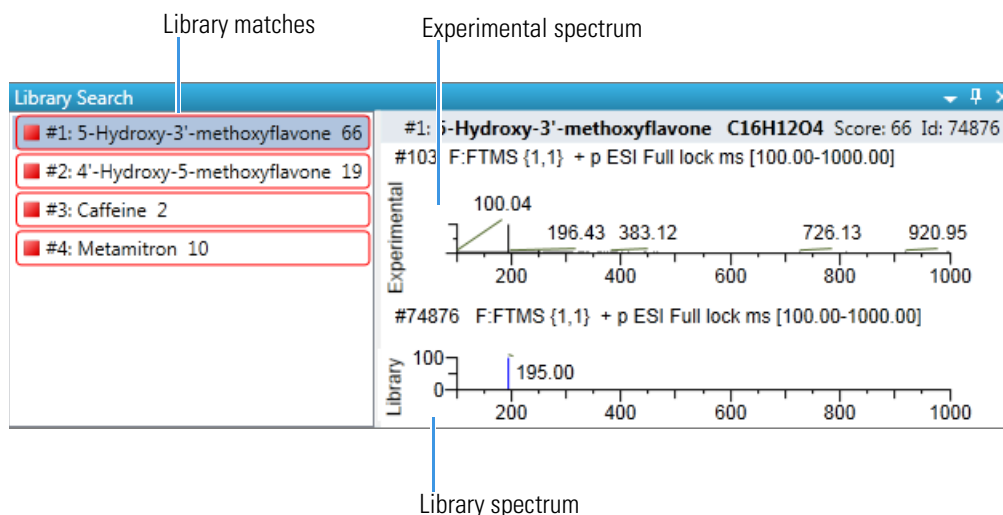
The Library Search pane displays the best library matches for the selected peak, with the highest score listed first. For detailed descriptions of the Library Search pane parameters, see “Library Search Pane” on page 667.

Follow these procedures:

- To view the spectrum for a library match
- To display the difference between experimental and library spectra

❖ To view the spectrum for a library match

In the Library Search pane, select a library entry.

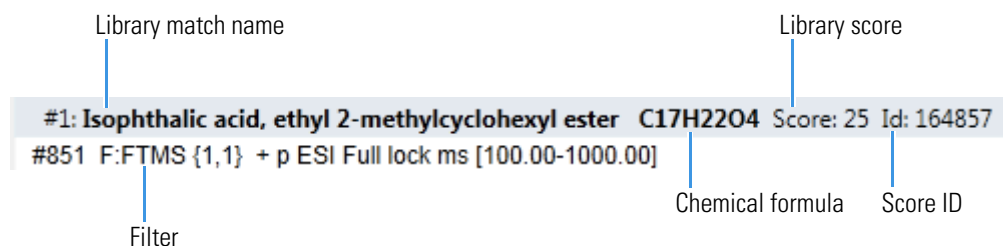


The Experimental plot displays the measured spectra for the selected compound. Library matches are colored red.

The Library plot displays the expected spectra in the library. Library matches are colored blue.

The spectra header displays the following:

- The library match name
- The chemical formula for the peak
- The score from the library fit when the library type is Library Manager or NIST
- SI and RSI when the library type is NIST
- Dot Prod or Rev Dot Prod when the library is HRAM
- Molecular weight when the library type is NIST
- The ID record from the library when the library type is Library Manager or NIST
- The scan number and scan filter when either is present in the library

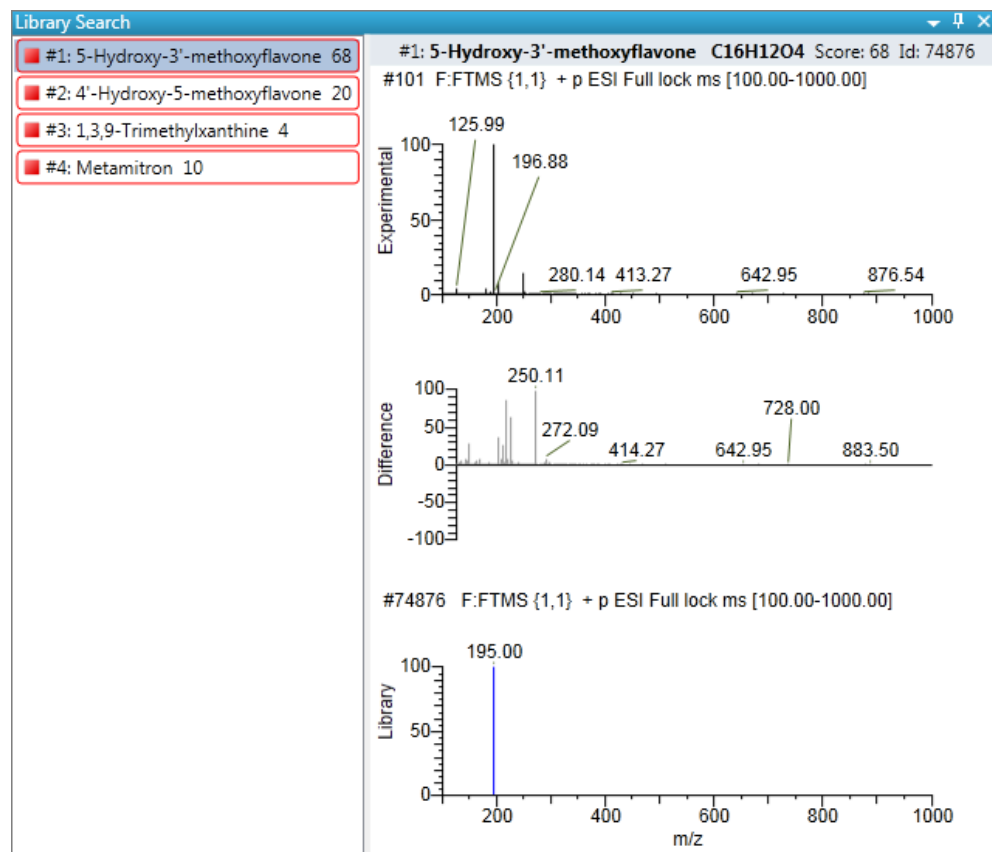


❖ **To display the difference between experimental and library spectra**

1. Right-click the spectrum plot and choose **Show Difference Plot** from the shortcut menu.

The application displays the Experimental and Library plots and a Difference plot that shows the difference between the experimental and library spectra. When you read a difference plot, the match between the experimental and library spectra is better when fewer peaks appear.

Figure 231. Library Search pane showing a Difference plot



2. To specify how the difference plot displays the mass tolerance, do the following:
 - a. Right-click the spectrum plot and choose **Set Difference Plot Mass Tolerance** from the shortcut menu.
 - b. In the dialog box that opens, select either **MMU** or **PPM** as the unit of measure.
The default value is the tolerance set in the NIST library or Library Manager library.
 - c. Type a mass tolerance value.
 - d. Click **OK**.

Note This command is available only when you display the difference plot.

Library Search Pane

Use the Library Search pane to display the best library matches for the selected peak.

Figure 232. Library Search pane

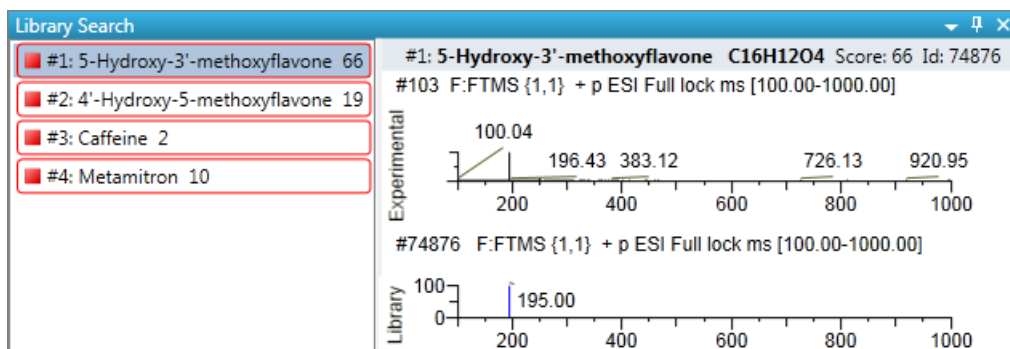


Table 155. Library Search pane shortcut menu commands

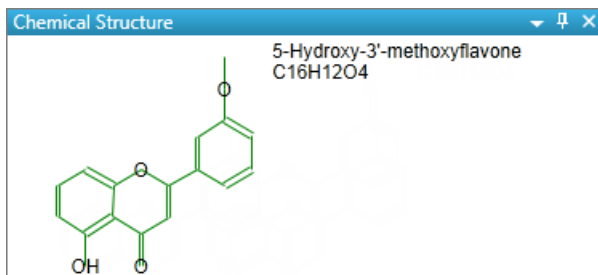
Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra Display Stack Spectra	Overlays the two spectrum displays, or stacks the Experimental and Library spectra. When you display the Difference plot, this spectrum also displays the Difference spectrum.
Show/Hide Difference Plot	Displays or hides the Difference spectrum plot.
Set Difference Plot Mass Tolerance	Opens a dialog box where you specify the mass tolerance in either MMU or PPM units. Available only when you display the Difference Plot.

Chemical Structure Pane

Use the Chemical Structure pane to view the chemical formula and structure for the peak that is currently selected in the Peak List pane.

The application displays the chemical formula (and CAS number when available) that was found in the search database that you specified in the method. See [“Editing the Processing Pages”](#) on page 311.

Figure 233. Chemical Structure pane



Fragments Pane

The Fragments pane displays the maximum number of fragments as specified in the unknown screening method. See [“Editing the Processing Pages”](#) on page 311.

When a compound database search returns a match for a peak that has fragments, the Fragments pane displays the theoretical fragments.

When the data has an MS/MS element that is identified as belonging to the chromatographic peak, the Fragments pane displays the fragments found in the MS/MS scan.

The Fragments pane displays the fragments in one of two ways:

- [All Fragments](#)
- [Individual Fragments](#)

All Fragments

The All Fragments view displays a composite of all fragments found in the peak. The application displays the measured peak as a solid red line; the application displays the expected peak as a dashed blue line.

The application displays these headers for the All Fragments view:

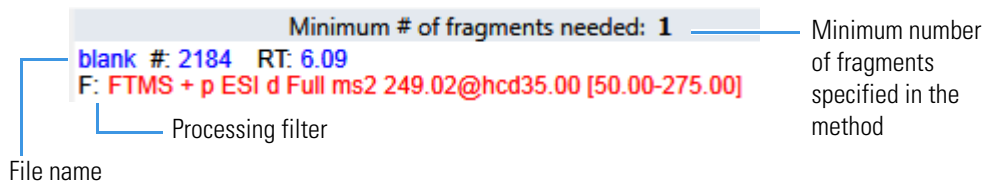
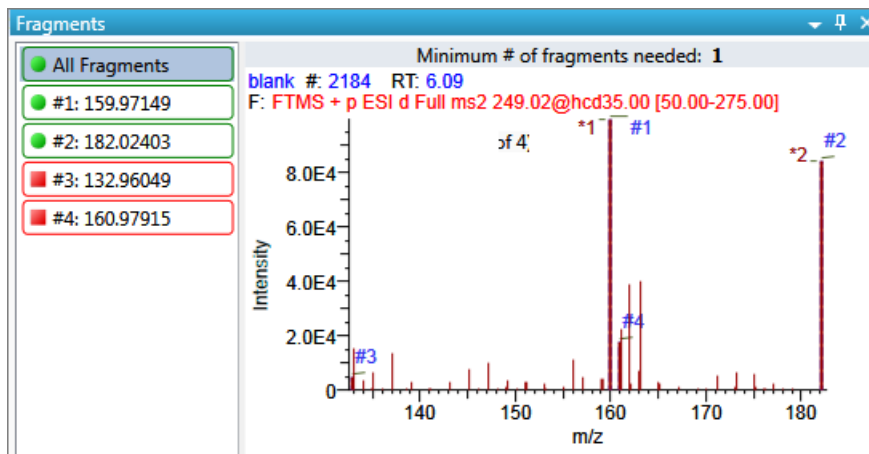


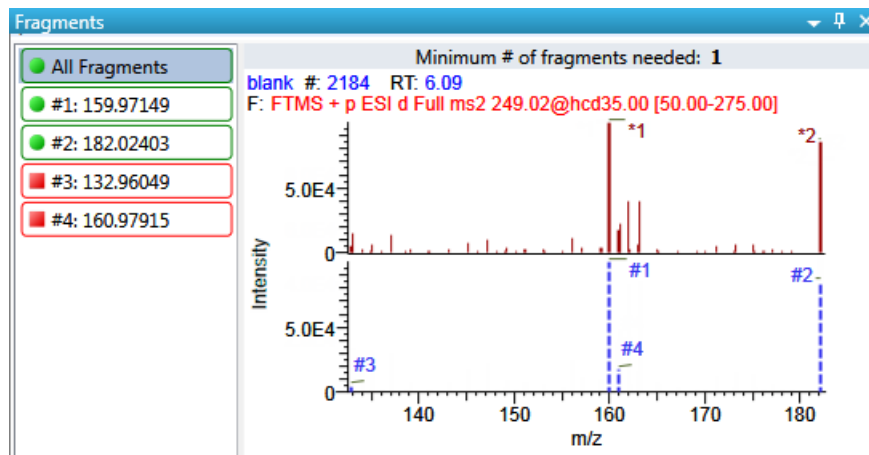
Figure 234. Fragments pane with overlaid spectra for all fragments



Expected spectrum in blue

Measured spectrum in red

Figure 235. Fragments pane with stacked spectra for all fragments



Expected spectrum in blue

Measured spectrum in red

Individual Fragments

The individual fragments view displays the expected and measured peaks for a single fragment.

The application displays these headers for the individual fragments view:

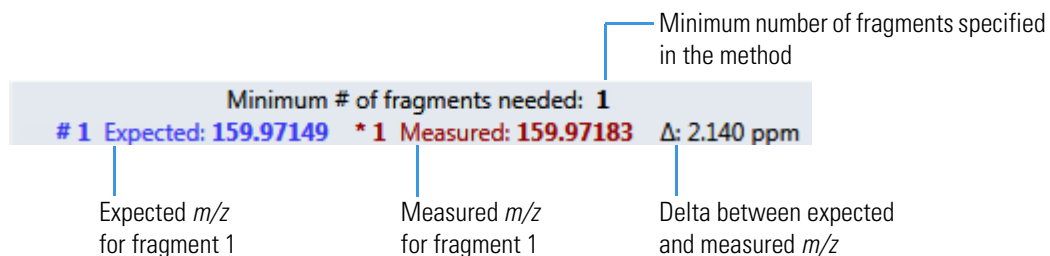


Figure 236. Fragments pane with overlaid spectra for a single fragment

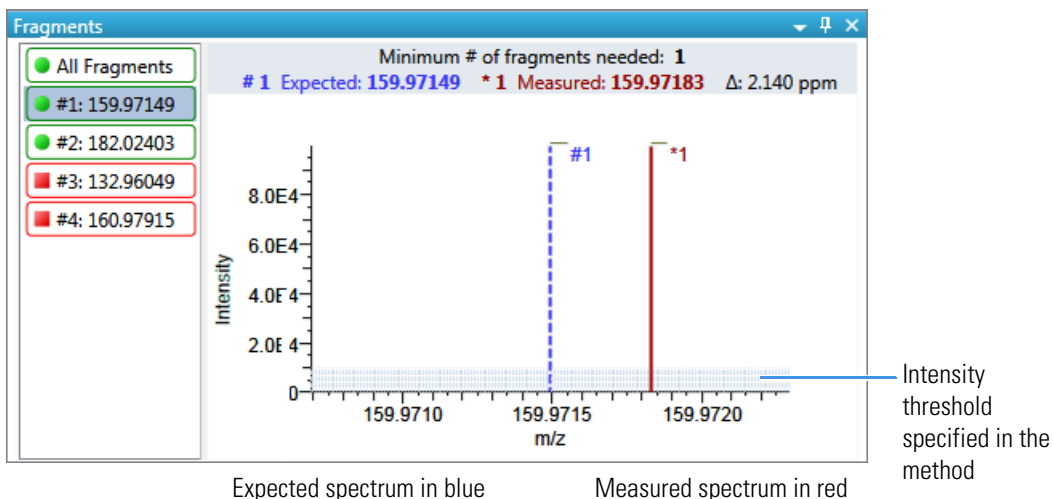
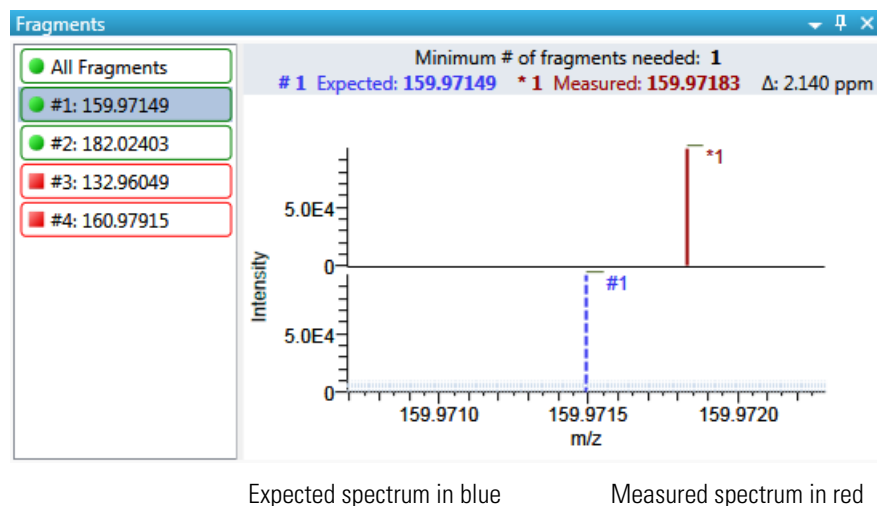


Figure 237. Fragments pane with stacked spectra for a single fragment



Isotopes Pane

The isotopes pane displays isotopic pattern results for all adducts of a compound according to the threshold and deviation parameters defined in the unknown method.

To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

- An isotope peak is not found if its intensity, relative to the monoisotopic ion's intensity, is more than the specified intensity deviation percentage away from the theoretical relative intensity of the isotope ion.
- An isotope peak is found if its measured m/z is less than the specified mass deviation amount away from its expected m/z .

To specify the peak threshold and deviation parameters, see [“Editing the Element Settings”](#) on page 327.

The Isotopes pane displays the isotopes in one of three ways:

- [All Isotopes](#)
- [Multi-Isotopes](#)
- [Individual Isotopes](#)

All isotopes panes use a shortcut menu so that you can specify how to display the data. See [“Isotopes pane shortcut menu commands”](#) on page 675.

All Isotopes

The All Isotopes view displays a composite of all isotopes found in the compound. The application scales the window with respect to the most intense isotope. The most intense isotope is usually the first isotope unless you are using halogenated compounds. The application displays the measured peak as a solid red line; the application displays the expected peak as a dashed blue line.

The application displays these headers for the All Isotopes view:

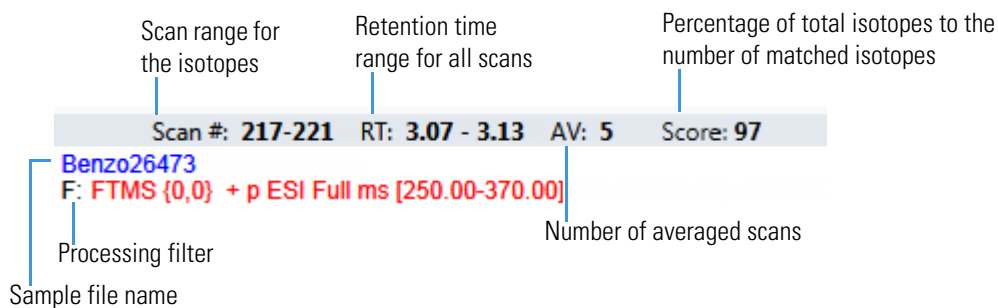


Figure 238. Isotopes pane with stacked spectra for all isotopes

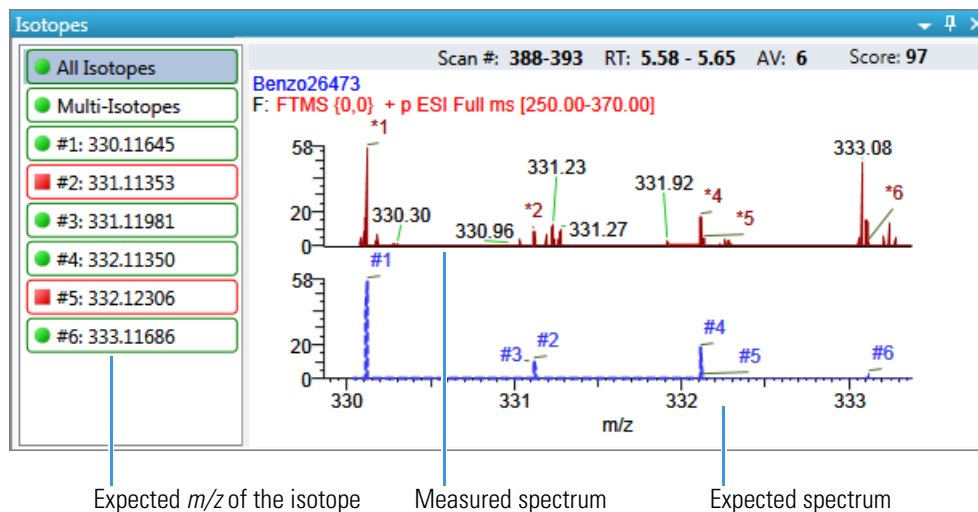
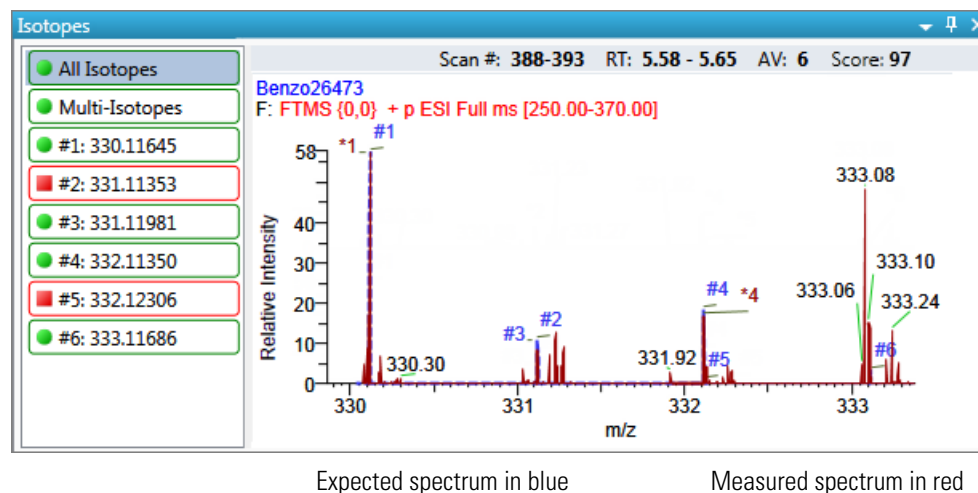


Figure 239. Isotopes pane with overlaid spectra for all isotopes



Multi-Isotopes

The Multi-Isotopes view displays individual plots for each isotope. You can individually stack or overlay the plots for each isotope.

The application displays these headers for the Multi-Isotopes view:

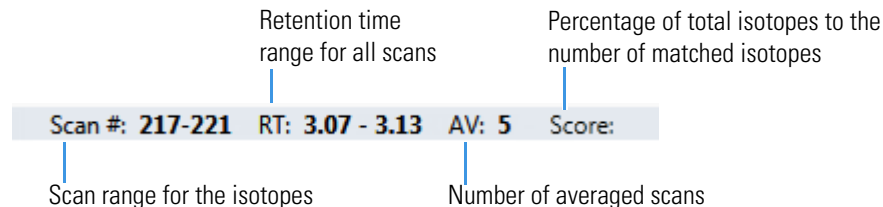
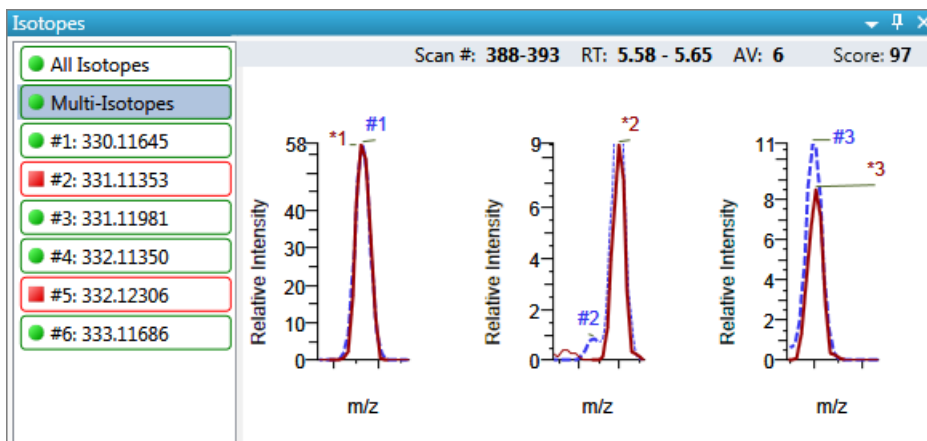


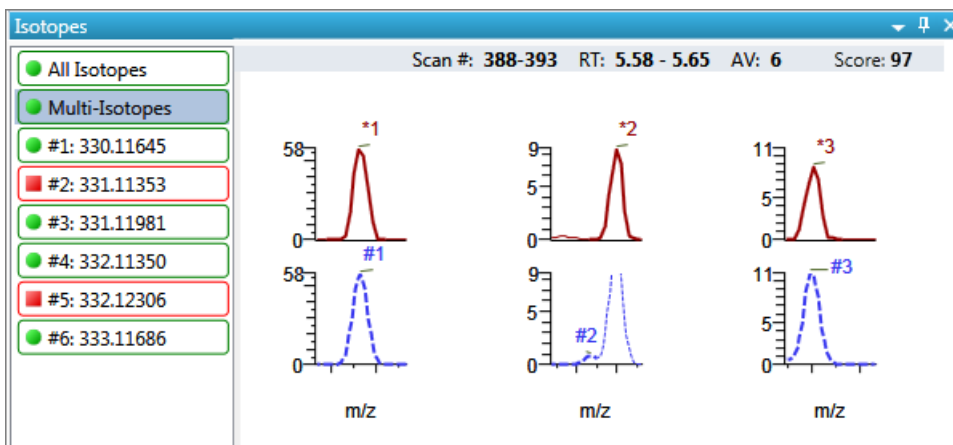
Figure 240. Isotopes pane with overlaid spectra for multi-isotopes



Expected spectrum in blue

Measured spectrum in red

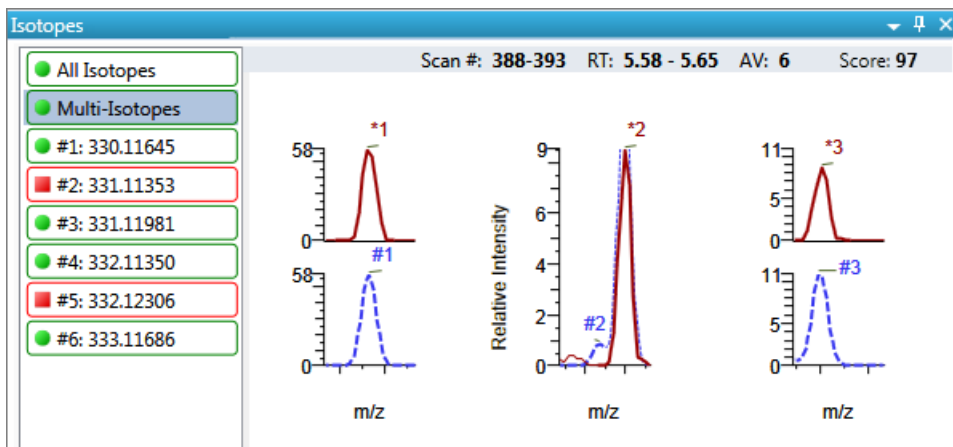
Figure 241. Isotopes pane with stacked spectra for multi-isotopes



Expected spectrum in blue

Measured spectrum in red

Figure 242. Isotopes pane with stacked and overlaid spectra for multi-isotopes



Expected spectrum in blue

Measured spectrum in red

Individual Isotopes

The individual isotopes view displays the expected and measured peaks for a single isotope.

The application displays these headers for the individual isotopes view:

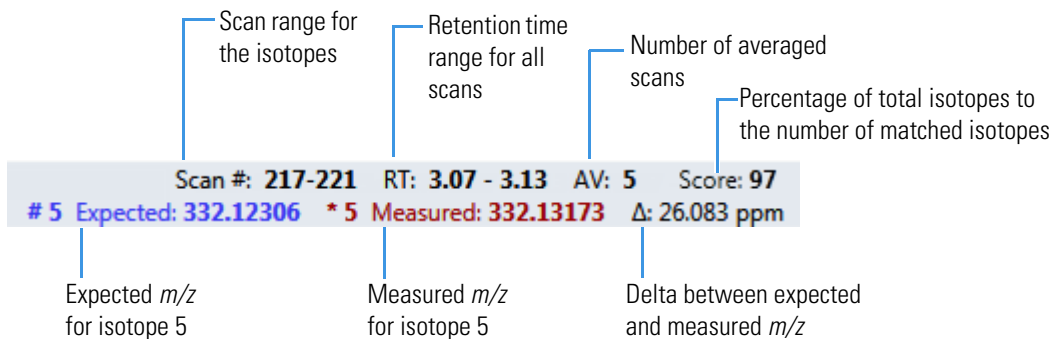


Figure 243. Isotopes pane with overlaid spectra for a single isotope

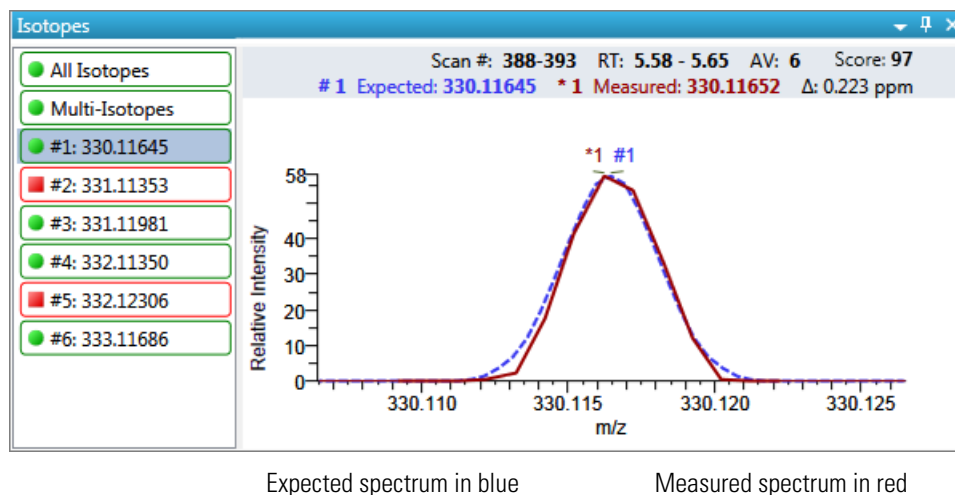


Figure 244. Isotopes pane with stacked spectra for a single isotope

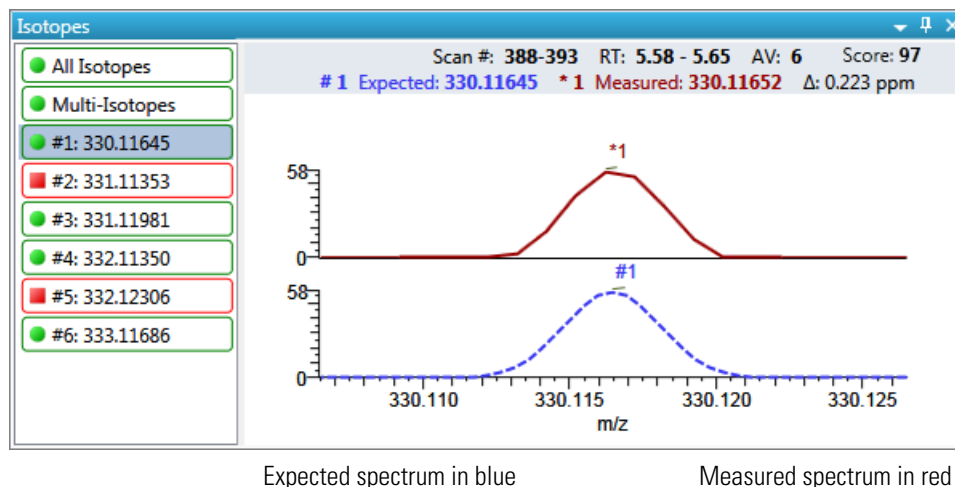
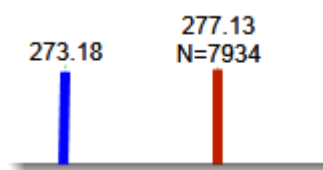


Table 156. Isotopes pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Show/Hide Noise Label	Adds a noise label to each peak. Expected isotope peaks (displayed in blue) do not display a noise label.

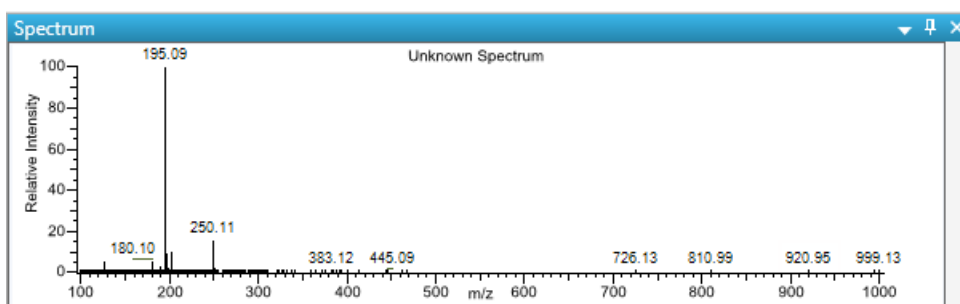


Show/Hide Resolution Label	Adds a resolution label to each peak. Expected isotope peaks (displayed in blue) do not display a resolution label.
----------------------------	---



Spectrum Pane

When data is available, the plot width is the full mass range in the raw data file. Otherwise, the application scales the width to the scan range.

Figure 245. Spectrum pane**Table 157.** Spectrum pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Working in the Report View

The Report View displays example reports for the current batch. You must have an open batch to use the features in the Report View.

Follow these procedures:

- [To open the Report View](#)
- [To preview a report](#)
- [To generate a report as a PDF, an Excel, or a CSV file](#)
- [To print a report](#)
- [To display a generated report](#)
- [To edit a report template](#)
- [To create a new report template](#)

❖ To open the Report View

Click **Report View** in the navigation pane.



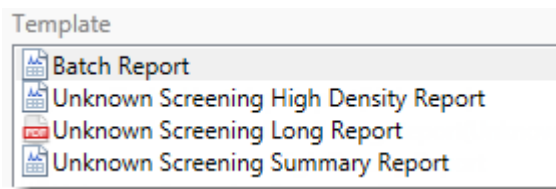
The application opens the Report View. For detailed descriptions of all parameters, see [“Report View”](#) on [page 680](#).

❖ To preview a report

1. In the Template pane, select a report template.

The template list shows all the report templates that you configured in the Configuration console. See [“Specifying the Reports”](#) on [page 71](#).

Figure 246. Example template list for unknown screening batches




2. Click **Preview**, .

The application opens the Report Designer, showing the report information for the current batch in the selected report template format.

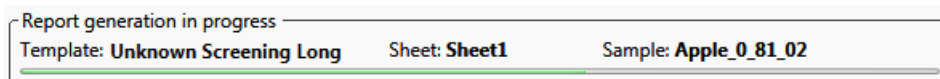
For details about using the Report Designer, see [Chapter 12, “Using the Report Designer.”](#)

❖ To generate a report as a PDF, an Excel, or a CSV file

1. In the Template pane, select a report template.
2. Select the check box for each of the file types that you want to create: **PDF**, **Excel**, or **CSV**.
3. Click **Generate**,  **Generate**.


The application does the following:

- Displays a green progress bar as it generates the reports.



- Creates a report for the current batch as a PDF, an Excel, or a CSV file, using the selected report template format.
- Adds information about the generated report to the Generated Reports pane.
For details about the Generated Reports pane, see [“Report View” on page 680](#).
- Saves the report files to the ...\\TraceFinderData\\3.3\\Projects*batch*\\ReportOutput folder.

❖ To print a report

1. In the Template pane, select a report template.
2. Select the check box for the **Print** file format.
3. Click **Generate**,  **Generate**.

The application does the following:

- Creates a report for the current batch using the selected report template format.
- Prints the report to your default printer.
- Adds information about the generated report to the Generated Reports pane.
For details about the Generated Reports pane, see [“Report View” on page 680](#).
- Saves the report files to the ...\\TraceFinderData\\3.3\\Projects*batch*\\ReportOutput folder.

❖ To display a generated report

In the Generated Reports pane, click **View** for the report that you want to see.

Figure 247. Generated Reports pane showing a PDF report

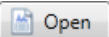
Generated Reports				
Template	Rule	Sample	Output	Generated Report File
Batch Report	Batch		pdf	View... Batch Report_20140113092939.pdf (3 pages)

↓
Opens the generated file.

The application opens the output file.

❖ To edit a report template

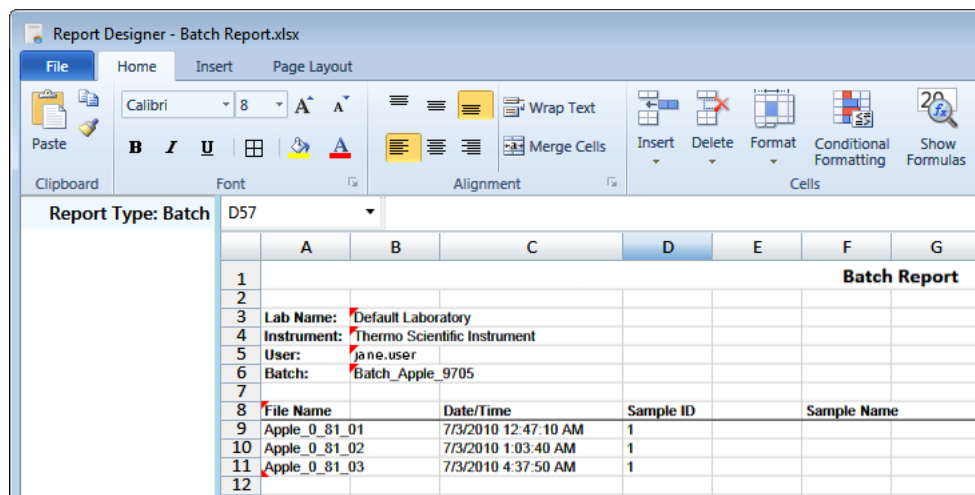
Note You cannot edit report templates that were provided with the TraceFinder application; however, you can open a TraceFinder template, make changes, and save it to a new template name.

1. In the Template pane, select a report template.
2. Click **Open**, .

The application opens the Report Designer showing the template in an Excel spreadsheet. See [Report Designer showing the template for the selected report](#).

Note When user security is activated, you must have Template Editing permission to edit report templates created by your laboratory. If the Open button is not active, user security is activated and you do not have Template Editing permission.

Figure 248. Report Designer showing the template for the selected report



Report Designer - Batch Report.xlsx

File Home Insert Page Layout

Clipboard Font Alignment Cells

Report Type: Batch D57

	A	B	C	D	E	F	G
1	Batch Report						
2							
3	Lab Name:	Default Laboratory					
4	Instrument:	Thermo Scientific Instrument					
5	User:	jane.user					
6	Batch:	Batch_Apple_9705					
7							
8	File Name	Date/Time	Sample ID	Sample Name			
9	Apple_0_81_01	7/3/2010 12:47:10 AM	1				
10	Apple_0_81_02	7/3/2010 1:03:40 AM	1				
11	Apple_0_81_03	7/3/2010 4:37:50 AM	1				
12							

3. Use the features in the Report Designer to edit the template.
See [Chapter 12, “Using the Report Designer.”](#)
4. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

❖ To create a new report template

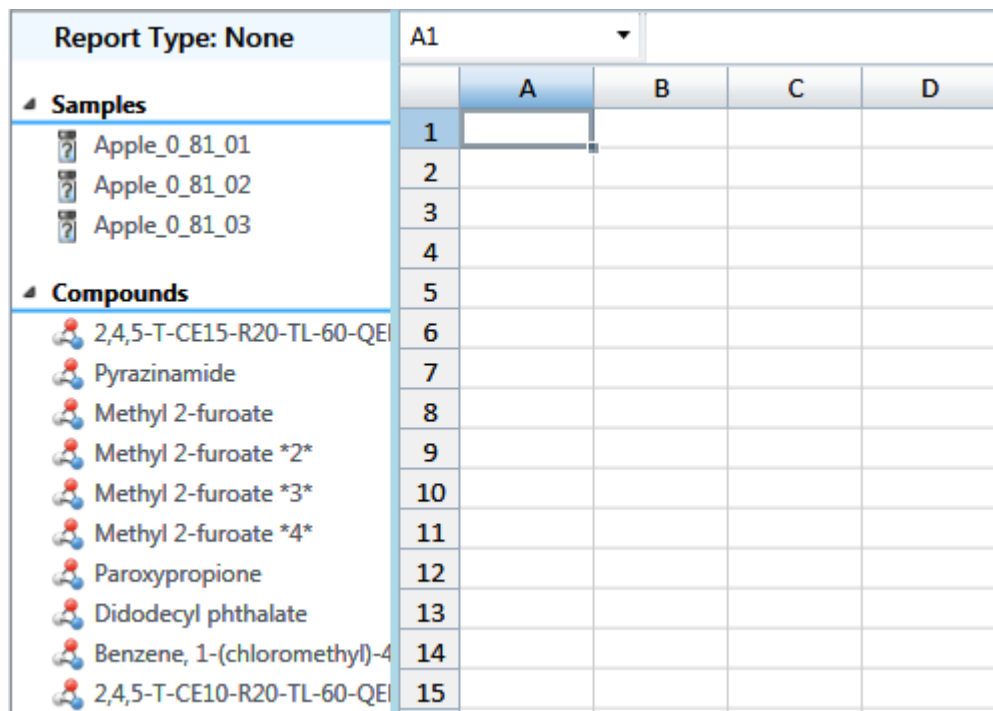
1. Click **New**, .

The application opens the Report Designer showing an empty template in an Excel spreadsheet. See [Report Designer showing a new, empty template](#).

The Report Type is None.

In the left pane, the spreadsheet lists all samples in the current batch and all compounds in the method used for the batch.

Figure 249. Report Designer showing a new, empty template



Report Type: None		A1			
		A	B	C	D
▲ Samples					
Apple_0_81_01					
Apple_0_81_02					
Apple_0_81_03					
▲ Compounds					
2,4,5-T-CE15-R20-TL-60-QEI					
Pyrazinamide					
Methyl 2-furoate					
Methyl 2-furoate *2*					
Methyl 2-furoate *3*					
Methyl 2-furoate *4*					
Paroxypropione					
Didodecyl phthalate					
Benzene, 1-(chloromethyl)-4					
2,4,5-T-CE10-R20-TL-60-QEI					

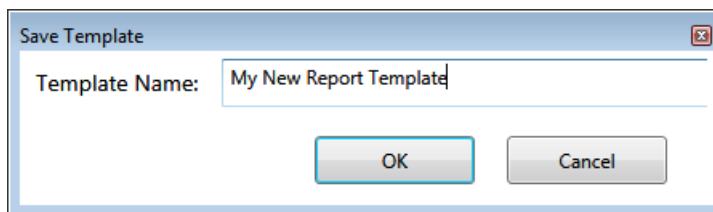
2. Use the features in the Report Designer to create the report template.

See [Chapter 12, “Using the Report Designer.”](#)

3. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

The Save Template dialog box opens.

Figure 250. Save Template dialog box



Save Template

Template Name: My New Report Template

OK Cancel

4. Type a name for the new report template and click **OK**.

11 Using the Analysis Mode for Unknown Screening Batches

Working in the Report View

Report View

Use the features in the Report View to display example reports for the current batch.

Figure 251. Report View

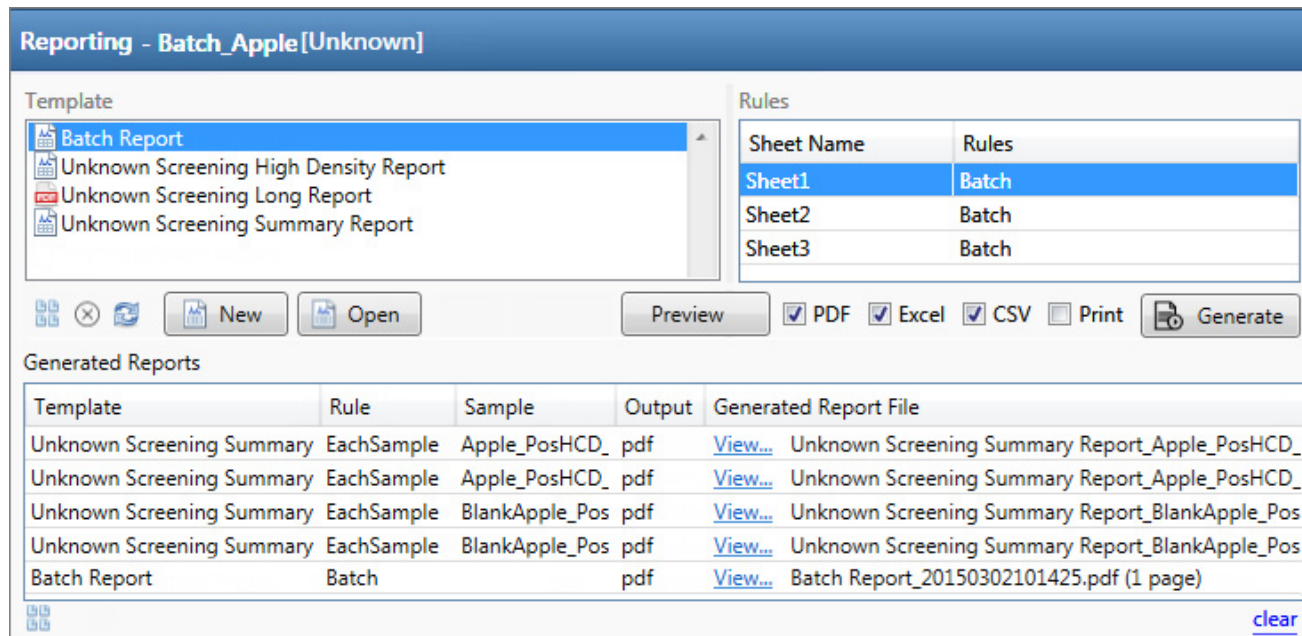





Table 158. Report View parameters (Sheet 1 of 2)

Parameter	Description
Template	
	Displays all available unknown screening report templates.
Rules	
Sheet Name	Specifies each sheet in the report.
Rules	Specifies the type of data used in each sheet in the selected report. <ul style="list-style-type: none"> • Batch • EachSample • SampleType: <i>SampleType</i> • CompoundType: <i>CompoundType</i> • SampleCustomFormula:
Buttons	
View Report Templates	Displays the C:\TraceFinderData\3.3\Templates\ReportTemplates folder that contains all report templates.
Open	Opens the selected report template in the Report Designer.
New	Opens a blank report template in the Report Designer.

Table 158. Report View parameters (Sheet 2 of 2)

Parameter	Description
 Preview	Opens the Report Designer showing the report information for the current batch in the selected report template format.
PDF	Writes the generated report to a PDF file in the ...\\TraceFinderData\\3.3\\Projects\\ <i>batch</i> \\ReportOutput folder.
Excel	Writes the generated report to a PDF file in the ...\\TraceFinderData\\3.3\\Projects\\ <i>batch</i> \\ReportOutput folder.
CSV	Saves the generated report as a PDF file in the ...\\TraceFinderData\\3.3\\Projects\\ <i>batch</i> \\ReportOutput folder. When the report contains multiple sheets, the application writes each sheet as a separate CSV file.
Print	Prints the generated report to your default printer.
 Generate	Generates the selected type of reports for the current batch using the selected report template.
Generated Reports	
Template	Report template used for the report. See “Example template list for unknown screening batches” on page 676.
Rule	Type of data used in each sheet of the report. See Rules .
Sample	For sample-level reports, the name of each sample in the report.
Output	Type of output specified for the report: PDF, Excel, CSV, or Print.
Generated Report File	Lists the output file name for each report in the ...\\TraceFinderData\\3.3\\Projects folder.
View	Displays the generated output file.
 View Generated Reports	Displays the C:\\TraceFinderData\\3.3\\Projects folder that contains all report outputs.
Clear	Removes all reports from the Generated Reports display. This does not delete the reports from the C:\\TraceFinderData\\3.3\\Projects folder.

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 *Batch_MasterMethod*.

❖ To open the Local Method View

1. Click **Analysis** in the navigation pane.
2. Click **Local Method**.



The Local Method view for the currently selected batch opens. See [Local Method View](#).

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 “[Editing a Master Method](#)” on [page 307](#).

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 252. Local Method View

Analysis ▾

▶ Batch View

▶ Data Review

Report View

▾ Local Method ▶

Acquisition

Unknown Screening

Processing

Peak Detection Settings

Reports

Local Method View - Apple_batch1

Master method: [Method Unknown Screening](#)

Lab Name:

Assay type:

Injection Volume:

Mass Precision:

Instrument Method:

Notes

Using the Report Designer

This chapter includes instructions about using the features of the Report Designer.

Contents

- [Editing a Template](#)
- [Toolbar Reference](#)
- [Quick Tips](#)

Use the features in the Report Designer to create new report templates or edit your laboratory's report templates. You cannot edit report templates that were provided with the TraceFinder application; however, you can open a TraceFinder template, make changes, and save it to a new template name.

When user security is activated, you must have Template Editing permission to edit report templates created by your laboratory. To use the administration tools to set Reports permissions, refer to the instructions in the *TraceFinder Administrator Console User Guide*.

With the Report Designer, you can do any of the following to create or edit a report template:

- Make changes to the template as you would in an Excel application.
- Add or remove graphics.
- Add repeated areas of many types.
- Format fonts and colors.
- Add or edit formulas.
- Edit template text and headers.

In addition to the procedures in this chapter, you can view video instructions at <http://mytracefinder.com/plugins/reporting/>.

Note To edit or create a template, you must have an open batch.

Editing a Template

Use the Report Designer to add or remove graphics, add tables, add repeated areas, and format headings, data, or cells.

Follow these procedures:

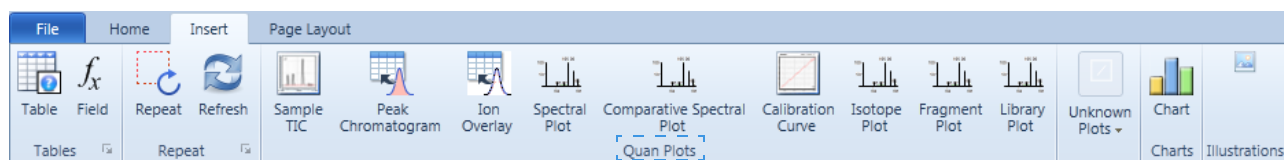
- To insert graphics into a report template
- To resize an inserted graphic
- To move an inserted graphic
- To insert a table
- To remove an inserted table
- To make changes to a table
- To format header text in the spreadsheet
- To format data in the report grid
- To format cells in the report grid
- To add repeated areas
- To insert a new sheet in a report

❖ To insert graphics into a report template

1. Click the **Insert** tab.

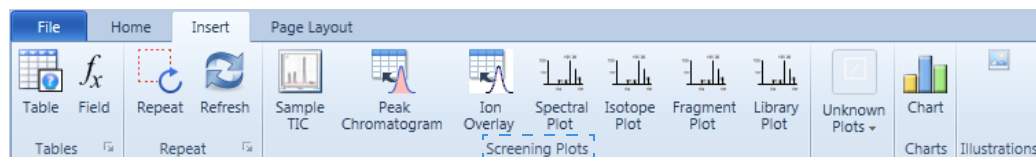
The Insert page displays the available objects that you can insert in a quantitation, a target screening, or an unknown screening report template.

Figure 253. Quan Plots features for quantitation batch report templates



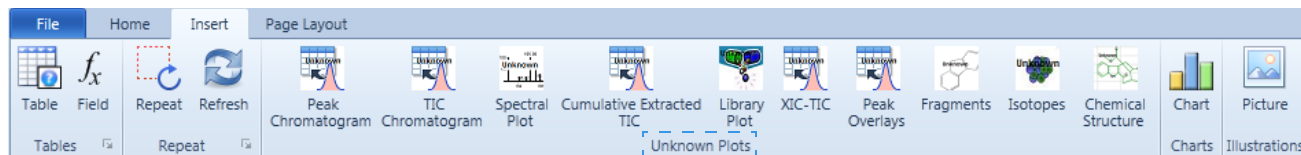
For a description of each graphic element, see “[Insert Toolbar – Quantitation Reports](#)” on page 700.

Figure 254. Screening Plots features for target screening batch report templates



For a description of each graphic element, see “[Insert Toolbar – Target Screening Reports](#)” on page 702.

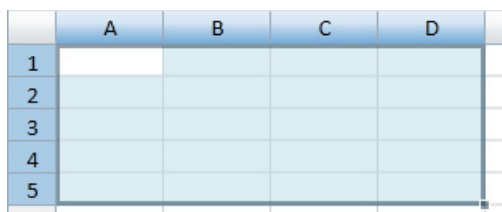
Figure 255. Unknown Plots features for unknown screening batch report templates



For a description of each graphic element, see “[Insert Toolbar – Unknown Screening Reports](#)” on page 703.

Note The Insert features for quantitation and target screening report templates also include Unknown Plots. You can insert unknown plots when your quantitation or target screening batch also uses unknown features.

- In the template grid, drag to select cells where you want to place the item.



Note You can also select a single row, and the application inserts the upper left corner of the graphic at the first cell, using a minimum default size.

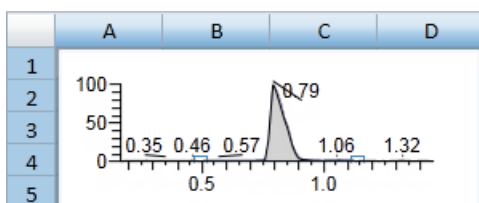
- Select a sample from the list of samples in the left pane.

The application uses graphical data from the selected sample when you insert a graphical plot.

- Click a graphical plot in the toolbar to insert into the selected cells.

The application inserts the selected plot in the template grid.

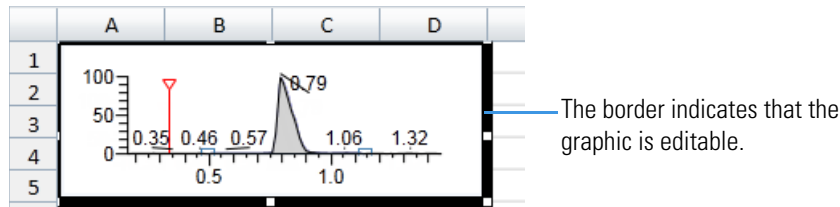
Figure 256. Inserted peak chromatogram



❖ **To resize an inserted graphic**

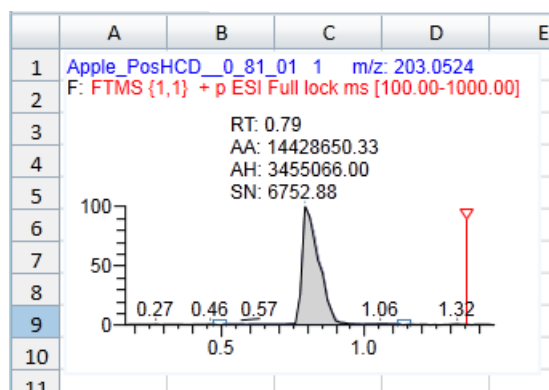
1. Right-click the graphic to make it editable.

Figure 257. Editable graphic



2. Grab a corner of the graphic and stretch it to the new size.

Figure 258. Resized graphic

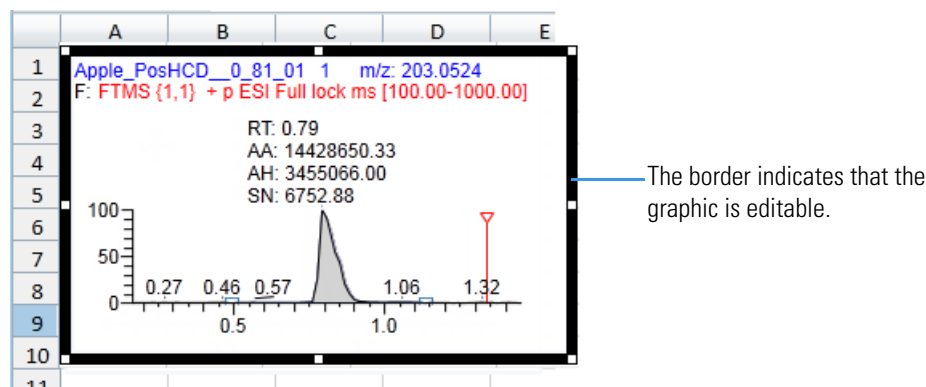


Note In this example, the original graphic was too small to display all the chromatogram data. Stretching the graphic reveals the sample name, mass, filter, and labeling.

❖ **To move an inserted graphic**

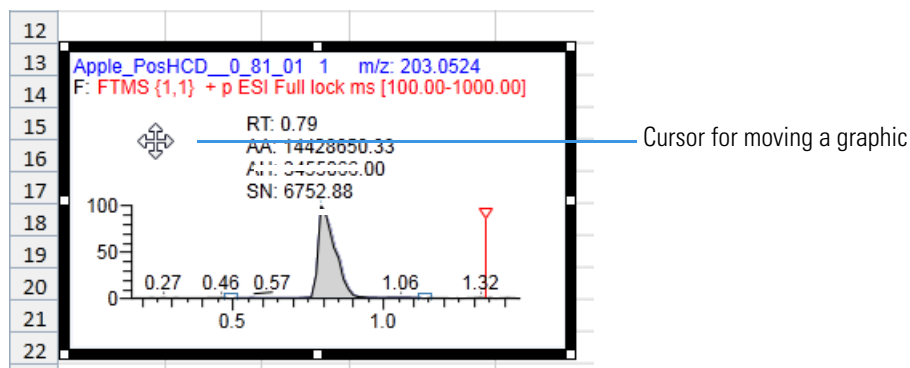
1. Right-click the graphic to make it editable.

Figure 259. Editable graphic




2. Click the graphic (notice the cursor change), and drag it to a new location.

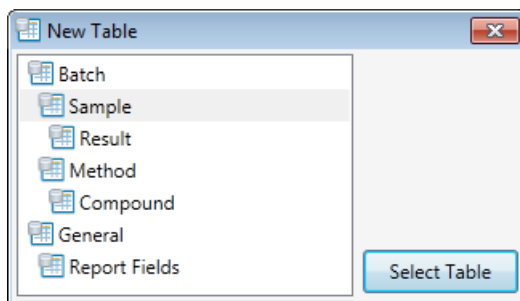
Figure 260. Moved graphic



❖ **To insert a table**

1. Select a row in the report grid where you want to insert the table.
2. Click the **Insert** tab, and then click the **Table** icon, .

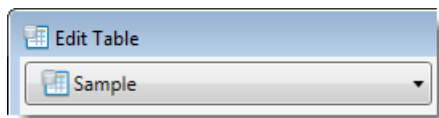
The New Table dialog box opens.



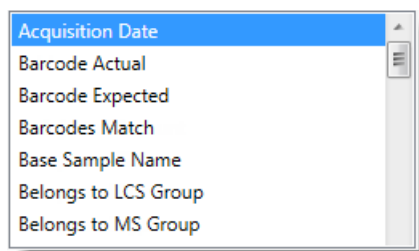
3. Select the type of table that you want to insert and click **Select Table**.

The Edit Table dialog box opens. For descriptions of all parameters, see [“Edit Table Dialog Box”](#) on page 697.

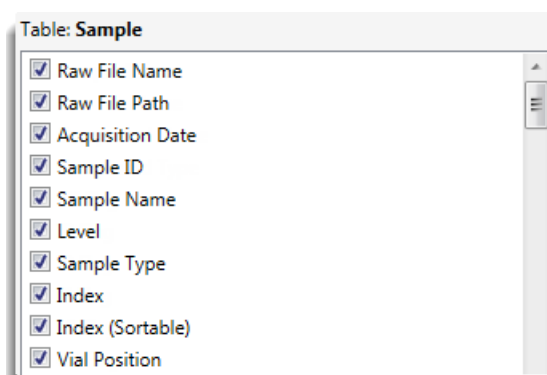
The dropdown list in the upper left corner displays the data type for the table you selected.



The left pane displays an alphabetical list of all available fields for the selected data type that you can include in the table. To display fields for a different data type, see [step 4](#).

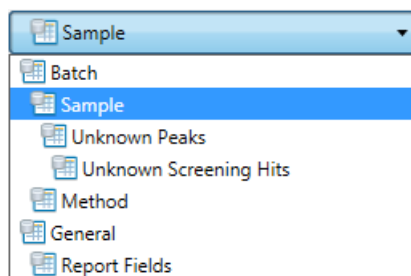


The right pane lists the fields that are included in the new table.




You can select as many additional fields as you want. The table you create displays each selected field as a table column. By default, all available fields for the original data type are included in the table. The first field in the list is the leftmost column in the table. The last field in the list is the rightmost column in the table. To change the order of the columns, see [step 6](#).

4. To add fields to the table from a different data type, do the following:
 - a. Click the dropdown list and select a different data type.





The left pane displays an alphabetical list of all available fields for the new data type.

- b. Select a field in the left pane and then click .

The application moves the selected field to the rightmost pane to indicate that it is included in the inserted table.

5. To select a field that you do not want in the table, in the rightmost pane, clear the check box next to the field name.

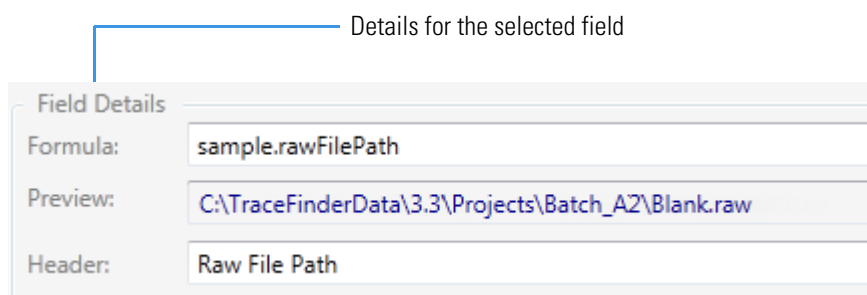
6. To move a column up or down in the table, select the field name in the rightmost pane and click the **Up** arrow, , or **Down** arrow, .
7. To edit the header for a table column, select the field in the list on the right, and then type new header text in the Header box in the Field Details area.

The default header name is the same as the field name.

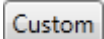
8. To find the formula for a field, select the field.

The application displays the formula in the Formula box.

- Raw File Name — Field not selected
- Raw File Path — Field selected (blue background)



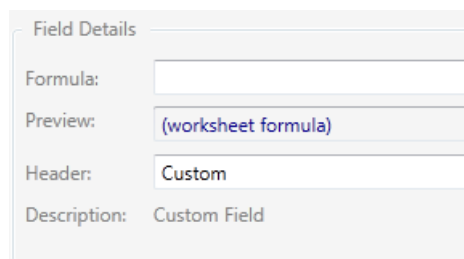
This video demonstrates how to use the Report Designer to create your own formula: www.Working with Formulas.

9. To create a custom column, do the following:
 - a. Click **Custom**, .

The application adds a Custom field to the fields list.

- b. Select the Custom field in the list.

The application display the details for the new, custom column.

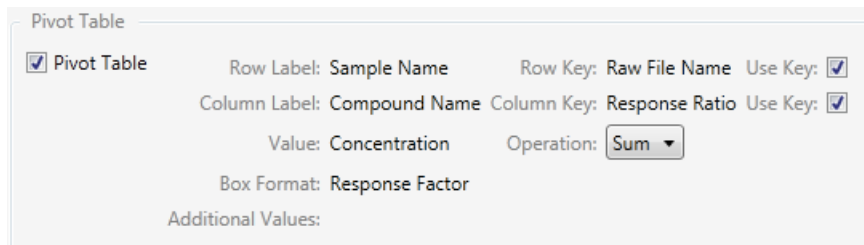


- c. Enter values for the Formula and Header.

10. To create a pivot table, do the following:

- a. Select the **Pivot Table** check box.

The Pivot Table area expands to display the pivot table options.



Pivot Table

Pivot Table

Row Label: Sample Name Row Key: Raw File Name Use Key:

Column Label: Compound Name Column Key: Response Ratio Use Key:

Value: Concentration Operation: Sum

Box Format: Response Factor

Additional Values:

- b. Select the **Use Key** check box for the row label.
- c. Select the **Use Key** check box for the column label.
- d. Select the operation that you want to use to calculate the aggregate value: **Sum**, **Count**, **Average**, **First**, or **Last**.

11. When you have made all your table selections, click **OK**.

The application inserts the table into the report template.

❖ To remove an inserted table

1. Select all rows and cells in the table.
2. Right-click and choose **Delete – Delete Cells and Shift Cells Left** from the shortcut menu.

The application removes the entire table from the report template.

❖ To make changes to a table

1. In the table that you want to edit, right-click and choose **Data Table** from the shortcut menu.

The Edit Table dialog box opens, displaying all of the available fields for the selected template. The Edit Table dialog box is virtually identical to the Edit Table dialog box that you used to create a table.

For descriptions of all parameters, see [“Edit Table Dialog Box”](#) on page 697.

2. Edit the fields for the table and click **OK**.

❖ **To format header text in the spreadsheet**

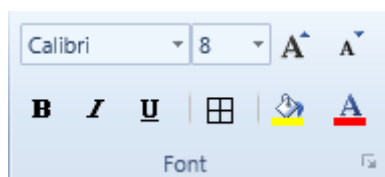
1. In the Report Designer window, select the header in the spreadsheet table.

To change all headers, select the entire header row.

To change a single header, select the specific header cell.

Tip You can also use the SHIFT key to select sequential cells or the CTRL key to select nonsequential cells anywhere in the grid.

2. Click the **Home** tab.
3. Use the Font icons to change the font format.



❖ **To format data in the report grid**

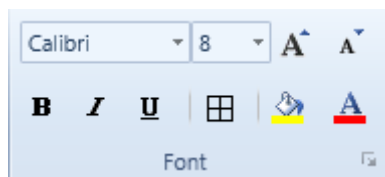
1. Select the data that you want to format.

To format all rows in a column, select the header row.

To format a single cell of data, select only that cell.

Tip You can also use the SHIFT key to select sequential cells or the CTRL key to select nonsequential cells anywhere in the grid.

2. Click the **Home** tab and use the toolbar icons to edit the font or cells as appropriate:



- Change the font or font size.
- Make the selected text bold.
- Make the selected text italics.
- Underline the selected text.
- Apply borders to the currently selected cells.
- Increase or decrease font size.
- Apply color to the background for selected cells.
- Change the font color.

❖ **To format cells in the report grid**

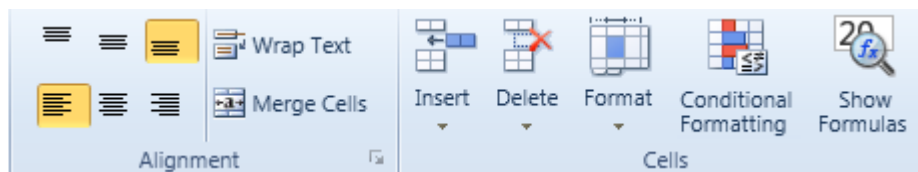
1. Select the cells that you want to modify:

To change all cells in a row, select the entire row.

To change a single cell, select only that cell.

Tip You can also use the SHIFT key to select sequential cells or the CTRL key to select nonsequential cells.

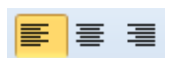
2. Click the **Home** tab and use the Alignment or Cells toolbar icons to edit the cells.



3. To align the cell text to the top, center, or bottom of the cell, click one of these icons:



4. To align the cell text to the left, center, or right of the cell, click one of these icons:



5. To make all contents visible within a cell, click **Wrap Text**.
6. To join selected cells into one cell, click **Merge Cells**.
7. To insert cells, rows, or columns into the template, click **Insert**.
8. To delete rows or columns from the template, click **Delete**.
9. To change the row height or column width, organize sheets, or protect or hide cells, click **Format**.
10. To highlight or emphasize useful cells based on specific criteria, click **Conditional Formatting** to use data bars, color scales, or icon sets.
11. To show formulas for selected cells instead of the resulting value, click **Show Formulas**.

❖ **To add repeated areas**

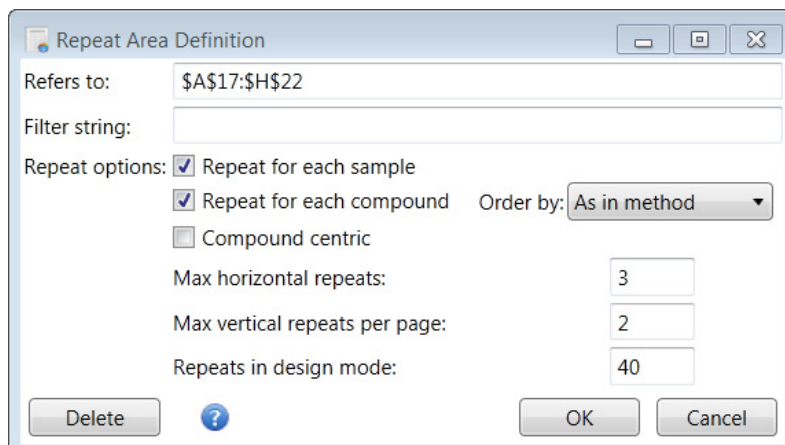
1. To define a repeat area, select the cells that you want to repeat.

You can repeat only one area per worksheet, but you can repeat it many times. You cannot insert data tables beneath a repeated area. See [“Example of repeated areas”](#) on page 696.

2. Click the **Insert** tab and then click **Repeat**.



The Repeat Area Definition dialog box opens.

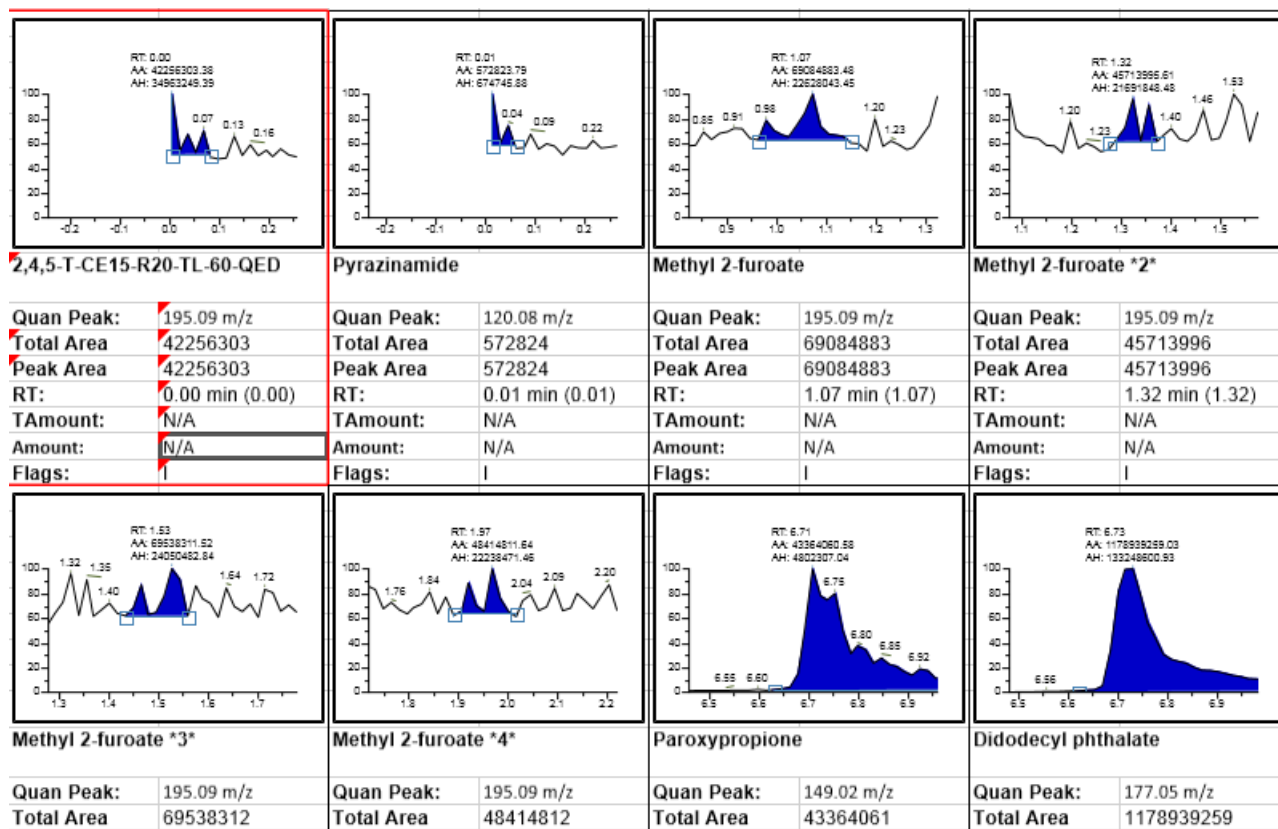


3. To filter the repeat area according to the filter criteria, type the string syntax in the Filter String box.
4. Select to repeat for each sample, for each compound, or for both.
5. Define whether the repeat area repeats first for samples or first for compounds:
 - To have the repeat area repeat first for samples and then for compounds, clear the **Compound Centric** check box.
 - To have the repeat area repeat first for compounds and then for samples, select the **Compound Centric** check box.
6. To define the number of times to repeat horizontally before wrapping to the next row, type a number in the Max Horizontal Repeats box.
7. To define the number of times to repeat vertically before inserting an auto-page break, type a number in the Max Vertical Repeats Per Page box.
8. To define the maximum suggested number of repeats, type a number in the Repeats in Design Mode box.

This maximum number of repeats is intended to limit the size of the report while you are editing the report in the Report Designer. When generating an actual report, the application does not enforce this limit.

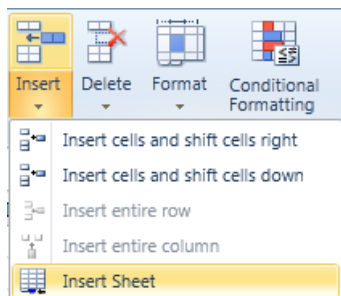
In this example, the repeated area (outlined in red) displays the peak chromatogram, target peak, total area, peak area, retention time, theoretical amount, actual amount, and reported flags, if any, for each compound.

Figure 261. Example of repeated areas



❖ To insert a new sheet in a report

1. Click the **Home** tab.
2. In the Cells area, choose **Insert Sheet** from the Insert menu.



The application adds a new sheet to the report.

Edit Table Dialog Box

Use the options in the Edit Table dialog box to edit the fields in a table.

Figure 262. Edit Table dialog box

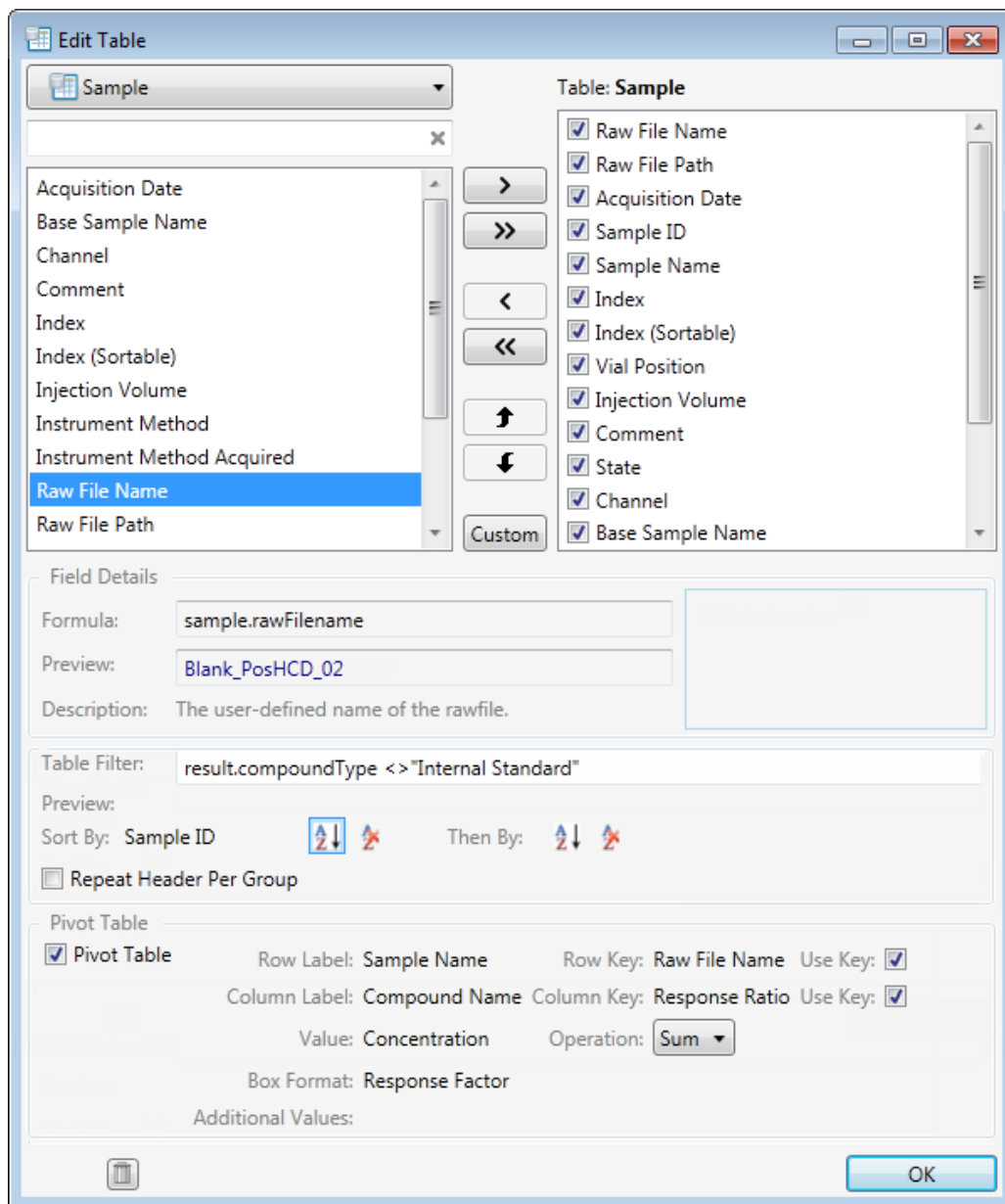



Table 159. Edit Table dialog box parameters (Sheet 1 of 2)

Parameter	Description
Dropdown List	Specifies the type of table you are editing.
Field List	Lists all available table fields.
Table	Displays the selected table type and the fields included in the table.

Table 159. Edit Table dialog box parameters (Sheet 2 of 2)

Parameter	Description
Field Details	
Formula	Specifies the functions and arguments used to define the field.
Preview	Specifies the name of the raw data file used for the report.
Header	Specifies the header name for the column in the spreadsheet.
Description	Specifies the type of field.
Table Filter	
Table Filter	Specifies the filter used for the sample compounds.
Preview	–
Sort By	Sorts the data by ascending or descending values.
Pivot Table	
Pivot Table	Enables the Pivot Table features.
Row Label	–
Row Key	–
Column Label	–
Column Key	–
Value	–
Operation	Specifies the operation used to calculate the aggregate value. Valid values: Sum, Count, Average, First, Last
Box Format	–
Additional Values	–
 Delete	Deletes the selected table from the template.

Toolbar Reference

The Report Designer includes the following toolbars.

- [Home Toolbar](#)
- [Insert Toolbar – Quantitation Reports](#)
- [Insert Toolbar – Target Screening Reports](#)
- [Insert Toolbar – Unknown Screening Reports](#)
- [Page Layout Toolbar](#)

Home Toolbar

Use the options in the Home toolbar to modify fonts, align cell data, and format cells.

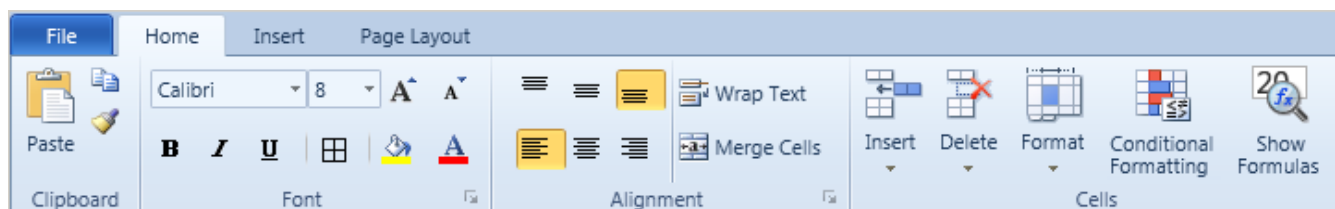


Table 160. Home toolbar options (Sheet 1 of 2)

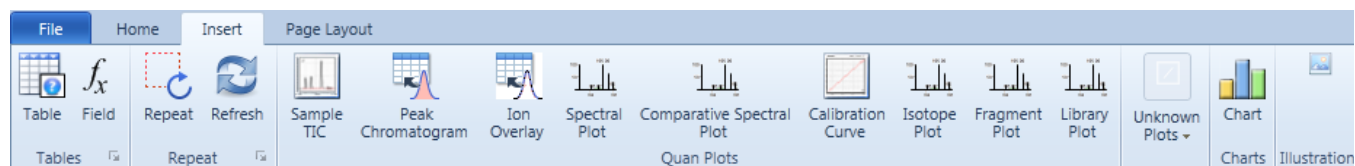
Parameter	Description
Clipboard	
Paste	Paste the contents of the Clipboard. You can also paste only formatting or only a formula.
Copy	Copy text or graphics to use in another place.
Font	
Font and size lists	Use the dropdown lists to change the font or font size.
Bold	Make the selected text bold.
Italic	Make the selected text italics.
Underline	Underline the selected text.
Border	Apply borders to the currently selected cells.
Font size	Increase or decrease the font size.
Fill color	Apply color to the background for selected cells.
Font color	Change the font color.
Alignment	
Vertical alignment	Align the cell text to the top, center, or bottom of the cell.
Horizontal alignment	Align the cell text to the left, center, or right of the cell.

Table 160. Home toolbar options (Sheet 2 of 2)

Parameter	Description
Wrap text	Make all contents visible within a cell.
Merge cells	Join selected cells into one cell.
Cells	
Insert	Insert cells, rows, columns, or sheets into a template.
Delete	Delete rows or columns from a template.
Format	Change the row height or column width, organize sheets, or protect or hide cells.
Conditional Formatting	Based on specific criteria, highlight or emphasize useful cells using data bars, color scales, and icon sets.
Show Formulas	Show formulas for selected cells instead of the resulting value.

Insert Toolbar – Quantitation Reports

Use the options in the Insert toolbar to add graphics, plots, and other objects to a template or report. You can also set up repeating objects and define functions.

**Table 161.** Insert toolbar options (Sheet 1 of 2)

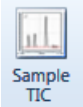
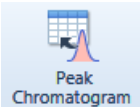
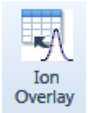
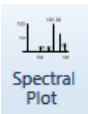
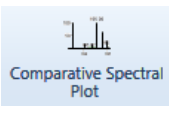
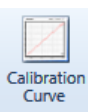
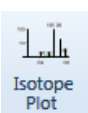
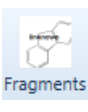

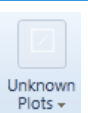
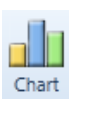

Parameter	Description
Table	
Table	Create a table to manage and analyze data.
Field	Edit the formula for a field by choosing functions and editing arguments.
Repeat	
Repeat	Repeat text, cell, or graphic elements.
Refresh	Update the view to reflect recent changes.
Plots	
	Add a sample TIC. For information about sample TIC data in the Data Review results, see “Peaks Pane” on page 478 .
	Add a peak chromatogram. For information about peak chromatogram data in the Data Review results, see “Quan Peak” on page 499 .

Table 161. Insert toolbar options (Sheet 2 of 2)

Parameter	Description
	<p>Add an ion overlay.</p> <p>For information about ion overlay data in the Data Review results, see “Ion Overlay” on page 512.</p>
	<p>Add a spectral plot.</p> <p>For information about spectral plot data in the Data Review results, see “Spectra” on page 515.</p>
	<p>Add a comparative spectral plot.</p> <p>For information about comparative spectral data in the Data Review results, see “Spectra” on page 515.</p>
	<p>Add a calibration curve plot.</p> <p>For information about calibration curve data in the Data Review results, see “Calibration Curve” on page 510.</p>
	<p>Add an isotope plot to display the number of isotopes found, the score, a pass/fail flag, and a plot of the isotopes.</p> <p>For information about isotope plot data in the Data Review results, see “Isotope” on page 516.</p>
	<p>Add a fragment plot.</p> <p>For information about fragment plot data in the Data Review results, see “Fragments” on page 517.</p>
	<p>Add a library plot.</p> <p>For information about library plot data in the Data Review results, see “Library Match” on page 515.</p>
	<p>Add plots for unknown screening when your quantitation batch includes unknown screening features. See Insert Toolbar – Unknown Screening Reports.</p>
Charts	
	<p>Add a custom chart. To define the chart, double-click the inserted blank chart.</p>
Illustrations	
	<p>Insert a picture from a file.</p>

Insert Toolbar – Target Screening Reports

Use the options in the Insert toolbar to add graphics, plots, and other objects to a template or report. You can also set up repeating objects and define functions.

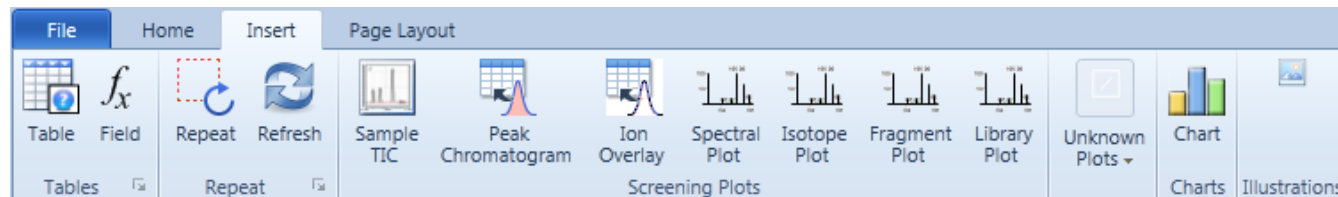


Table 162. Insert toolbar options (Sheet 1 of 2)

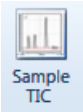
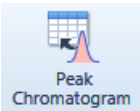
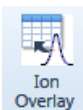
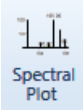



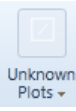


Parameter	Description
Table	
Table	Create a table to manage and analyze data.
Field	Edit the formula for a field by choosing functions and editing arguments.
Repeat	
Repeat	Repeat text, cell, or graphic elements.
Refresh	Update the view to reflect recent changes.
Plots	
	Add a sample TIC.
	Add a peak chromatogram. For information about peak chromatogram data in the Data Review results, see “Chromatogram Pane” on page 583 .
	Add an ion overlay.
	Add a spectral plot. For information about spectral plot data in the Data Review results, see “Spectrum” on page 584 .
	Add an isotope plot to display the number of isotopes found, the score, a pass/fail flag, and a plot of the isotopes. For information about isotope plot data in the Data Review results, see “Isotopes” on page 585 .
	Add a fragment plot. For information about fragment plot data in the Data Review results, see “Fragments” on page 591 .

Table 162. Insert toolbar options (Sheet 2 of 2)

Parameter	Description
	Add a library plot. For information about library plot data in the Data Review results, see “ Library ” on page 594 .
	Add plots for unknown screening when your target screening batch includes unknown screening features. See Insert Toolbar – Unknown Screening Reports .
Charts	
	Add a custom chart. To define the chart, double-click the inserted blank chart.
Illustrations	
	Insert a picture from a file.

Insert Toolbar – Unknown Screening Reports

Use the options in the Insert toolbar to add graphics, plots, and other objects to a template or report. You can also set up repeating objects and define functions.

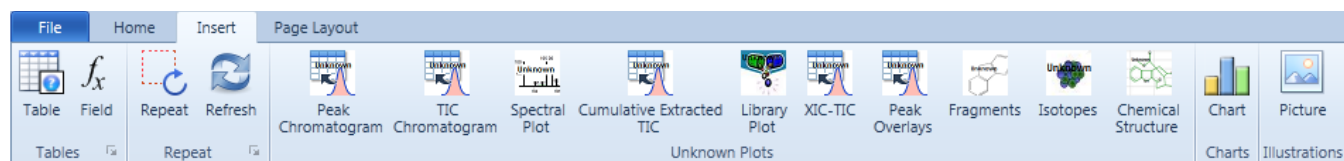


Table 163. Insert toolbar options (Sheet 1 of 2)

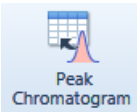
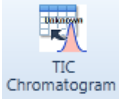
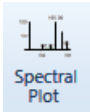
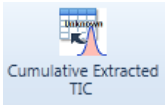
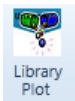




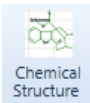


Parameter	Description
Table	
Table	Create a table to manage and analyze data.
Field	Edit the formula for a field by choosing functions and editing arguments.
Repeat	
Repeat	Repeat text, cell, or graphic elements.
Refresh	Update the view to reflect recent changes.
Plots	
	Add a peak chromatogram. For information about peak chromatogram data in the Data Review results, see “ Peak Chromatogram Pane ” on page 658 .

Table 163. Insert toolbar options (Sheet 2 of 2)

Parameter	Description
	<p>Add a TIC chromatogram.</p> <p>For information about TIC chromatogram data in the Data Review results, see “TIC Chromatogram Pane” on page 653.</p>
	<p>Add a spectral plot.</p> <p>For information about spectral plot data in the Data Review results, see “Spectrum Pane” on page 675.</p>
	<p>Add an XIC overlay plot.</p> <p>For information about XIC overlay data in the Data Review results, see “XIC Overlay Pane” on page 654.</p>
	<p>Add a library plot.</p> <p>For information about library plot data in the Data Review results, see “Library Search Pane” on page 664.</p>
	<p>Add an XIC plot.</p> <p>For information about XIC plot data in the Data Review results, see “XIC Pane” on page 654.</p>
	<p>Add a cross-sample peak overlay plot.</p> <p>For information about cross-sample peak overlay data in the Data Review results, see “Cross Sample Peak Overlay Pane” on page 662.</p>
	<p>Add a fragments plot.</p> <p>For information about fragments plot data in the Data Review results, see “Fragments Pane” on page 668.</p>
	<p>Add an isotopes plot.</p> <p>For information about isotopes plot data in the Data Review results, see “Isotopes Pane” on page 671.</p>
	<p>Add a chemical structure plot.</p> <p>For information about chemical structure plot data in the Data Review results, see “Chemical Structure Pane” on page 668.</p>
Charts	
	<p>Add a custom chart. To define the chart, double-click the inserted blank chart.</p>
Illustrations	
	<p>Insert a picture from a file.</p>

Page Layout Toolbar

Use the options in the Page Layout toolbar to adjust margins, orientation, paper size, and page breaks. To see your changes, click **Print Preview**.

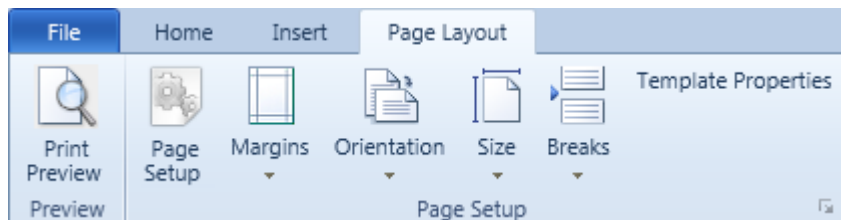
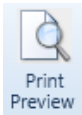
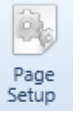
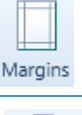
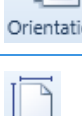




Table 164. Page Layout toolbar options

Command	Description
	View the report before printing it.
	Define page details.
	Select page margins for the current view or the entire document.
	Switch the pages from portrait to landscape view.
	Choose a page size for the current view or the entire document.
	Specify where a new page begins in the printed copy.
Template Properties	<p>Open the Template Properties dialog box where you can specify the expected batch type for the report template.</p> <p>The Template Properties dialog box also displays the Used Range so that you can identify when there is empty white space in the report template. Extra white space to the right or left of the report content can cause unwanted page breaks.</p>

Quick Tips

Follow these tips to make the most of the Report Designer features.

❖ To move a report to the Archive folder

1. With a report open for editing, choose **File > Archive** from the Report Designer main menu.
2. At the confirmation prompt, click **Yes**.

The application deletes the report from the ...*batch*\ReportOutput folder.

❖ To insert items in the Report Designer

- Insert a data table when the selected cell is above or below any other table, but not in the same row as a field. You cannot insert tables in repeat areas.
- Insert a data field when the selected cell is not in the same row as a table.
- Use these shortcut keys:

CTRL+T	Insert a table.
CTRL+T	Edit a table when the selected cell is inside a table.
CTRL+SHIFT+T	Insert or edit a field.
CTRL+R	Insert or edit a repeating area.

❖ To format cells and group headers

Because the first row of a data table retains formatting information, edit the formatting of the first row.

The application copies the formatting to all other rows.

For group header items, the application copies the formatting of the first group header to the remaining group headers.

❖ To sort fields

Select a field, and then click **A-Z** to sort the data in ascending or descending order.

Using the Audit Viewer

This chapter includes instructions about using the features of the Audit Viewer. For detailed descriptions of parameters in the Audit Viewer, see “[Audit Viewer](#)” on [page 716](#).

The TraceFinder application records all user access, including logging in, logging out, data creation and editing (batches, methods, and templates), and manual integration. You can use the Audit Viewer to view the resulting log files to track modifications to the data. When an event requires confirmation (as specified in the Administrator Console), the Audit Viewer records who confirmed each change to a batch, method, or template. When no confirmation is required, then the Audit Viewer records the user who was logged in when the change occurred.

In the Administration Console, a user with Auditing permissions can configure the auditing service by specifying which events are logged, which events require confirmation, a list of default reasons for a specific event, and whether a user can submit a custom reason. To use the auditing administration tools, refer to the instructions in the *TraceFinder Administrator Console User Guide*.

Contents

- [Audit Trail Log Files](#)
- [Audit Log File Functions](#)
- [Audit Viewer](#)

Audit Trail Log Files

The application creates the following audit trail log files:

- **Application:** Records all user access, such as starting and stopping the application, logging in, logging out, or accessing or saving data in batches and methods. The application saves the data in the following log file: C:\Thermo\TraceFinder\3.3\Logs\AuditLog.adb.
- **Master Method:** Records all user interactions with master methods, such as creating, opening, or editing a master method. The application saves the data in the following log file: C:\TraceFinderData\3.3\Methods*MasterMethodName*\AuditLog.adb.

- **Batch Template:** Records all user interactions with batch templates, such as creating, opening, or editing a batch template. The application saves the data in the following log file: C:\TraceFinderData\3.3\Templates\Batches*BatchTemplateName*\AuditLog.adb.
- **Batch:** Records all user interactions with batches, such as creating, opening, editing, acquiring, processing, or generating reports for a batch. The application saves the data in the following log file:
C:\TraceFinderData\3.3\Projects*SubFolder**BatchName*\AuditLog.adb.


Audit Log File Functions

The Audit Viewer displays all saved audit log files, and you can filter and sort the audit data.

Follow these procedures:

- [To access the Audit Viewer](#)
- [To select an audit log](#)
- [To view only application, method, batch, or batch template events](#)
- [To create a filter for audit log events](#)
- [To view audit event details](#)
- [To create a filter for an audit log history](#)
- [To display the history for an event](#)

❖ To access the Audit Viewer

Choose **Tools > Audit Trail** from the TraceFinder main menu or click the **Audit Viewer** icon,  .

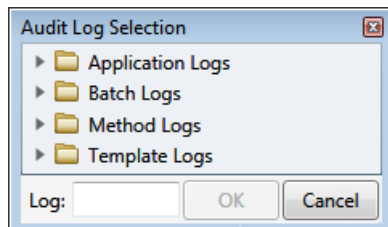
The Audit Viewer opens. For detailed descriptions of parameters in the Audit Viewer, see “[Audit Viewer](#)” on [page 716](#).

Note The Tools > Audit Trail menu command always opens to application log files, whereas the Audit Viewer icon is context sensitive and opens to the appropriate type of log files (application, method, batch, or batch template).

❖ **To select an audit log**

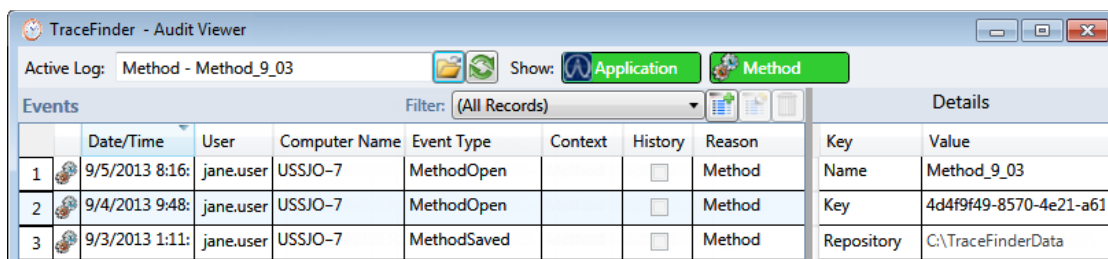
1. Click the **Open Audit Log** icon, .

The application opens the Audit Log Selection dialog box.



2. Expand a log folder to select an application, batch, method, or batch template audit log file, and click **OK**.

The Audit Viewer displays the contents of the selected audit log file, as in this example for a method.



❖ **To view only application, method, batch, or batch template events**

1. In the Active Log list, select an Active Log file.
 - Application logs include application and security events.
 - Method logs include application and method events.
 - Batch logs include application, method, and batch events.
 - Batch template logs include application and batch template events.

The Audit Viewer displays icons for each of the event types included in the log file.



2. Click an icon to turn the display on or off.

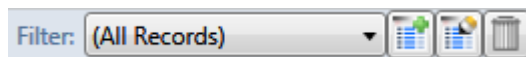
In this example, the Events pane displays Batch and Method events and hides Application events.



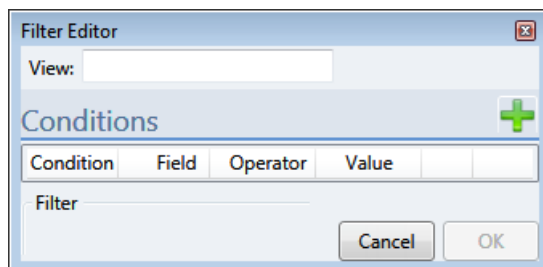
Note There is no icon for security events in an application log file. You cannot hide the display of security events.

❖ **To create a filter for audit log events**

1. In the Events pane, click the **Create New Filter** icon, .



The Filter Editor dialog box opens.

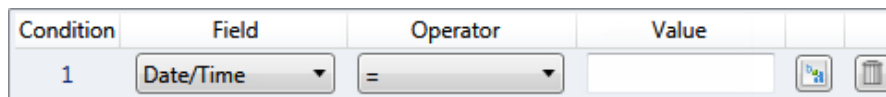


2. In the View box, type a name for the new filter.

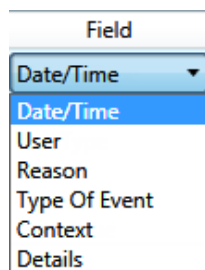
You can also leave the View box empty when you enter your filter criteria. When you finish adding conditions and click OK (step 8), the application filters the current events list based on the filter criteria you specify, but the filter is not saved. The Filter list in the viewer identifies this filter as (Custom).

3. Click the **Add** icon, .

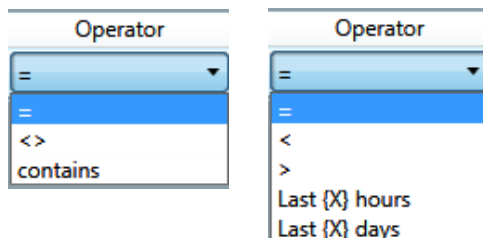
The application adds a new, undefined condition to the Condition list.



4. In the Field list, select one of the following field types.

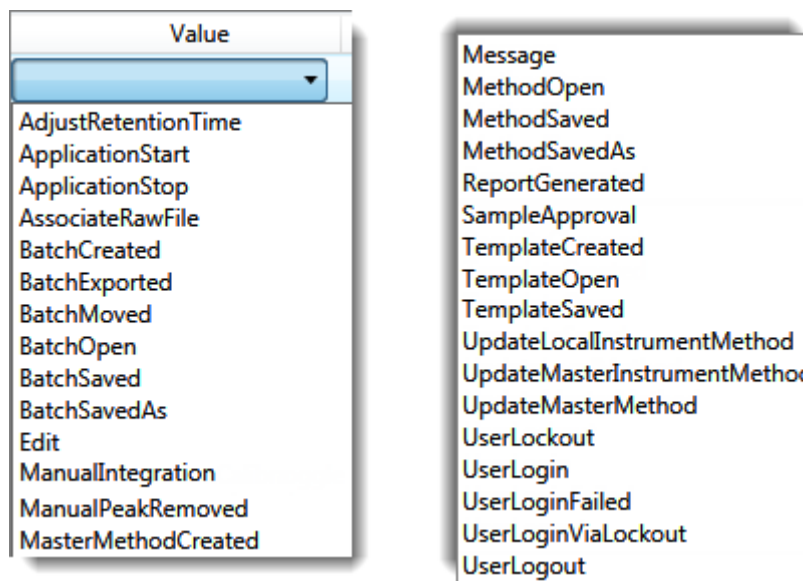



5. In the Operator list, select one of the available operators.

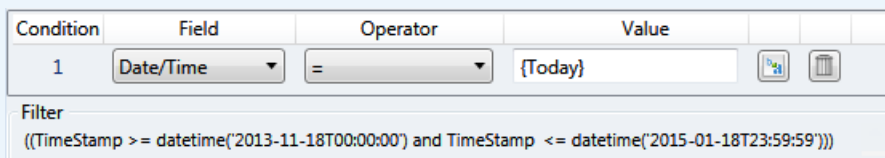


The available operators depend on the field type that you selected.

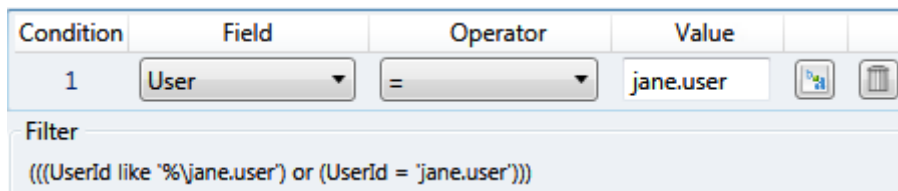
6. In the Value box, type a value or select a value from the list.
 - For the Date/Time field, type a numerical value in the Value box.
 - For the User, Reason, Context, or Details field, type the appropriate text in the Value box. This value is case sensitive.
 - For the Type of Event field, select one of the following values.



Note You can also click the Tokens icon, , and select a token for the Value. Tokens are predefined values, such as dates and sample or compound identifiers.



The Filter at the bottom of the dialog box displays the complete definition for the filter.



7. Repeat [step 3](#) (on [page 710](#)) through [step 6](#) (on this page) for each condition that you want to include in your filter.
8. When you have added all your conditions, click **OK**.

The application creates the new filter with the specified conditions.

❖ **To view audit event details**

In the Events pane, select an event.

The Details pane displays key values based on the type of log you select.



Details for batch log files include the name of the batch.



Details for method log files include the name of the method and the method type.



Details for batch template log files include the name of the batch template, the location of the data repository, and the subproject folder where the template was created.




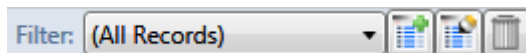
Details for Application log files include whether the events are for a batch or method, the location of the data repository, and, for a batch, the subproject folder where the batch was created.



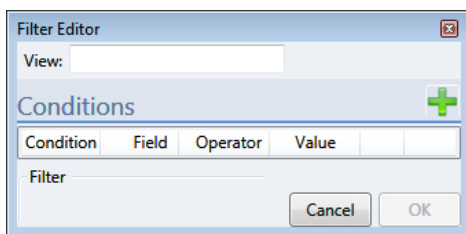
Details for Security log files include the authentication method used (Windows Active Directory or local machine) and the location of the administrator repository.

❖ **To create a filter for an audit log history**

1. In the History pane, click the **Create New Filter** icon, .



The Filter Editor dialog box opens.

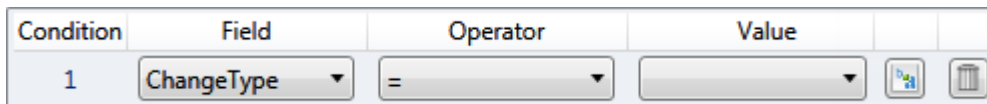


2. In the View box, type a name for the new filter.

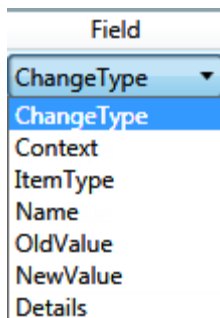
You can also leave the View box empty when you enter your filter criteria. When you finish adding conditions and click OK (step 8), the application filters the current history list based on the criteria you specify, but the filter is not saved. The Filter list in the viewer identifies this filter as (Custom).

3. Click the **Add** icon, .

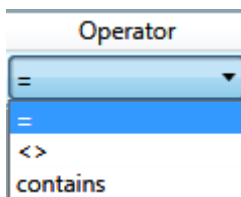
The application adds a new, undefined condition to the Conditions list.



4. In the Field list, select one of the following field types.



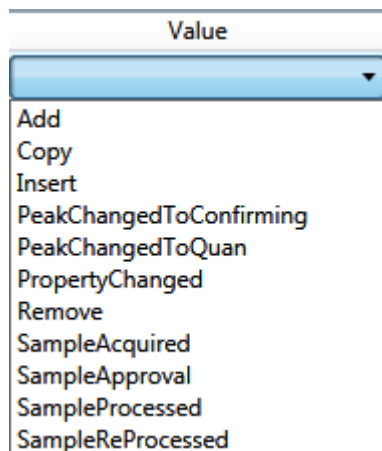
5. In the Operator list, select from *equals*, *less than/greater than*, or **contains**.



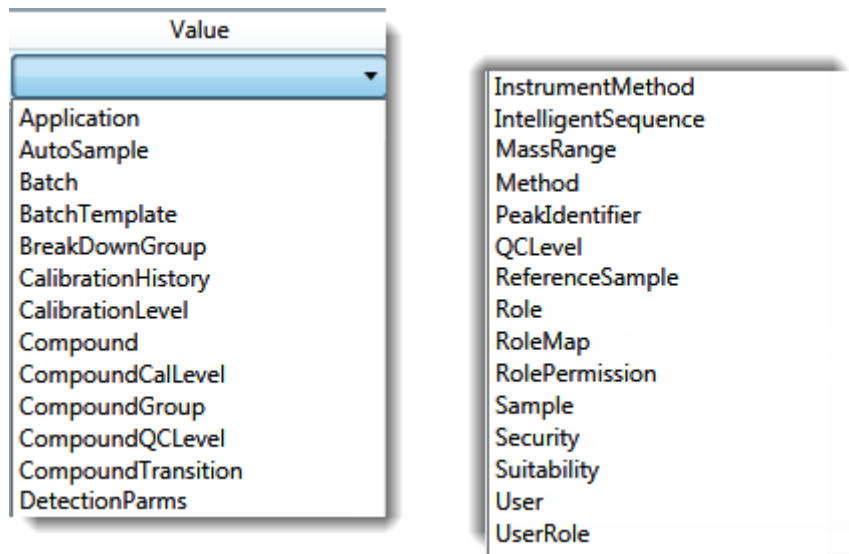
The available operators depend on the field type that you selected.


6. In the Value list, type or select a value from the list.

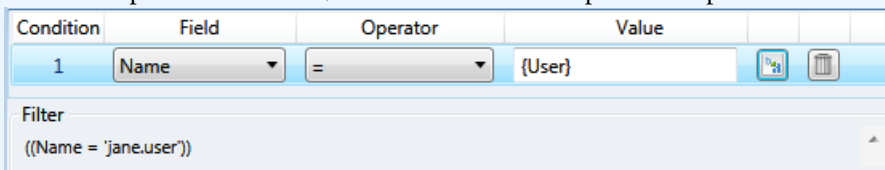
- For the Name, Context, or Details field, type the appropriate text in the Value box. This value is case sensitive.
- For the OldValue or NewValue field, type a numerical value in the Value box.
- For the ChangeType field, select one of the following values.



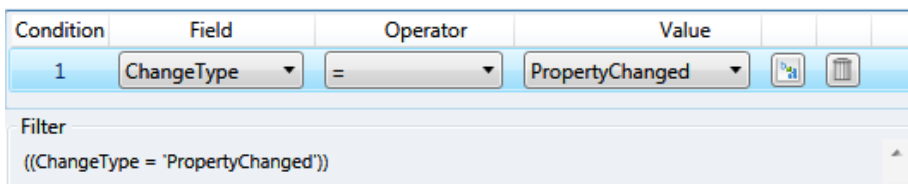
- When the selected Field is **ItemType**, select one of the following values.



Note You can also click the Tokens icon, , and select a token for the Value. Tokens are predefined values, such as dates and sample or compound identifiers.



The Filter at the bottom of the dialog box displays the complete definition for the filter.



- Repeat steps 3 through 6 for each condition that you want to include in your filter.
- When you have added all your conditions, click **OK**.

The applications created the new filter with the specified conditions.

❖ **To display the history for an event**

- In the Events pane, select an event that has a selected check box in the History column.

Event Type	Context	History	Reason
BatchOpen		<input type="checkbox"/>	Batch
BatchCreated		<input type="checkbox"/>	Batch
BatchSaved		<input checked="" type="checkbox"/>	Batch

Select an event that has the History check box selected.

The History pane displays all unsaved (queued) actions for the selected event.

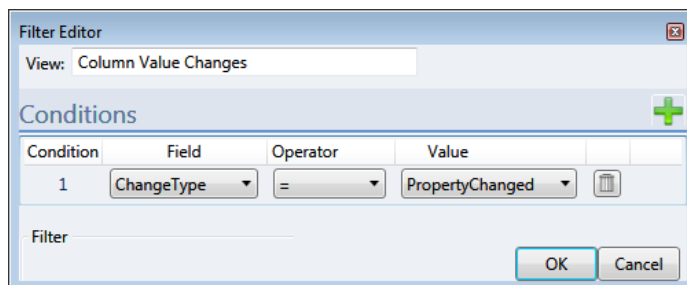
History							
							Filter: (All Records)
Order	Change Type	Context	Item Type	Item Name	Old Value	New Value	
1	1	Add	Unknown2	Sample	n/a	n/a	1
2	2	Add	Unknown3	Sample	n/a	n/a	2
3	3	Add	Unknown4	Sample	n/a	n/a	3
4	4	PropertyChanged	Apple_0_81	Sample	RawFileName	Unknown1	Apple_0_81_01
5	5	PropertyChanged	Apple_0_81	Sample	SampleID		1
6	6	PropertyChanged	Apple_0_81	Sample	VialPosition		CStk1-01:14
7	7	PropertyChanged	Apple_0_81	Sample	BarcodeExpected		2134

- To limit the actions in the history list, select a filter from the Filter list.

See [“To create a filter for an audit log history”](#) on page 712.

Figure 263. Example History filter

When you select this filter,



the History pane displays only these actions for the selected event:

History							
							Filter: Column Value Changes
Order	Change Type	Context	Item Type	Item Name	Old Value	New Value	
1	1	PropertyChanged	Apple_0_81	Sample	RawFileName	Unknown1	Apple_0_81_01
2	2	PropertyChanged	Apple_0_81	Sample	SampleID		1
3	3	PropertyChanged	Apple_0_81	Sample	VialPosition		CStk1-01:14
4	4	PropertyChanged	Apple_0_81	Sample	BarcodeExpected		2134

Audit Viewer

Use the Audit Viewer to view the audit log files to track user access and modifications to the data. See [Audit Viewer parameters](#).

Figure 264. Application log in the Audit Viewer

TraceFinder - Audit Viewer

Active Log: Application - Logs Show: Application

Events Filter: (All Records)

Log	Date/Time	User	Computer Name	Event Type	Context	History	Reason
1	10/24/2013 1:2	jane.user	USSJO-7	UserLogin		<input type="checkbox"/>	Security
2	10/24/2013 1:2		USSJO-7	ApplicationStart	1.0	<input type="checkbox"/>	Application
3	10/24/2013 11	jane.user	USSJO-7	ApplicationStop		<input type="checkbox"/>	Security
4	10/24/2013 11		USSJO-7	ApplicationStart		<input type="checkbox"/>	Security
5	10/24/2013 10	jane.user	USSJO-7	ApplicationStop		<input type="checkbox"/>	Application
6	10/24/2013 10	jane.user	USSJO-7	UserLogin		<input type="checkbox"/>	Security
7	10/24/2013 10		USSJO-7	ApplicationStart	1.0	<input type="checkbox"/>	Application

Details

Key	Value
UserId	jane.user
UsersValid	True
UsersEnabled	True
SecurityEnabled	Yes
SecurityMode	ActiveDirectory
SecurityDomain	AMER
FromLockout	False

History Filter: (All Records)

Order	Change Type	Context	Item Type	Item Name	Old Value	New Value

Details

Key	Value
UniqueId	4d5a1806-4f23-4f03

Logged in user: AMER\jane.user

Figure 265. Batch log in the Audit Viewer

TraceFinder - Audit Viewer

Active Log: Batch - Project1\Apple_10_17 Show: Application Batch Method

Events Filter: (All Records)

Log	Date/Time	User	Computer Name	Event Type	Context	History	Reason
1	10/24/2013 8:53	jane.user	USSJO-7	BatchOpen	Apple_10_17	<input type="checkbox"/>	Batch
2	10/24/2013 7:31	jane.user	USSJO-7	BatchSaved	Apple_10_17	<input checked="" type="checkbox"/>	Batch
3	10/24/2013 6:51	jane.user	USSJO-7	BatchSaved	Apple_10_17	<input checked="" type="checkbox"/>	Batch

Details

Key	Value
Repository	C:\TraceFinderData
SubFolder	Project1

History Filter: (All Records)

Order	Change Type	Context	Item Type	Item Name	Old Value	New Value
1	1	Unknown2	Sample	n/a	n/a	1
2	2	Unknown3	Sample	n/a	n/a	2
3	3	Unknown4	Sample	n/a	n/a	3
4	4	Apple_0_81_01	Sample	RawFileName	Unknown1	Apple_0_81_01
5	5	Apple_0_81_01	Sample	SampleID		1
6	6	Apple_0_81_01	Sample	VialPosition		CStk1-01:14

Details

Key	Value
UniqueId	4d5a1806-4f23-4f03

Logged in user: AMER\jane.user

Table 165. Audit Viewer parameters (Sheet 1 of 2)



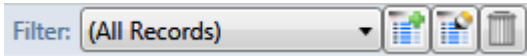








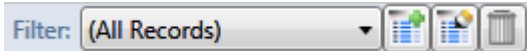



Parameter	Description
Active Log	Name of the current audit log file.
	Opens the Audit Log Selection dialog box where you can open a different audit log file. You can select from these audit log files: application, batch, method, or batch template.
	Refreshes the current audit log file in the viewer.
Show	Select to display only specific types of events in the Events list. The selected log file can contain batch, method, and application events.
Events	
Filter	Select a filter view to use for displaying the event log entries.  <ul style="list-style-type: none">  Opens the Filter Editor dialog box where you can create a filter view.  Opens the Filter Editor dialog box where you can edit the current filter view.  Deletes the current event filter view.
Log	<ul style="list-style-type: none">  Indicates an event that occurred at the main application level, such as logging in or opening a batch.  Indicates an event that occurred in the Administration Console.  Indicates an event that occurred in a method template.  Indicates an event that occurred in a method.  Indicates an event that occurred in a batch.
Date/Time	Time stamp of the event.
User	When an event requires confirmation (as specified in the Administrator Console), <i>User</i> is the user who confirmed each change to a batch, method, or template. When no confirmation is required, <i>User</i> is the user who was logged in when the change occurred.
Computer Name	Name of the computer on which the application recorded the event.
Event Type	Specific event that triggered the log file entry. For a complete list of event types, refer to the <i>TraceFinder Administration Console User Guide</i> .
Context	Name of the sample, batch, method, or application version where the event occurred.

Table 165. Audit Viewer parameters (Sheet 2 of 2)


Parameter	Description
History	Indicates that there is a history log of queued actions for the event.
Reason	Default or custom reason that the user entered for the event.
Details Key/Value	Identifying parameters and their values for the selected auditing event. These key parameters are different for each type of auditing event.
History	
Filter	<p>Select a filter view to use for displaying the change history.</p>  <p>  Opens the Filter Editor dialog box where you can create a filter view. </p> <p>  Opens the Filter Editor dialog box where you can edit the current filter view. </p> <p>  Deletes the current history filter view. </p>
Order	The sequence of actions that occurred.
Change Type	One of the predefined ChangeType values. See ChangeType .
Context	Name of the specific value on which the action occurred.
Item Type	One of the predefined ItemType values. See ItemType .
Item Name	A user-defined name for the filter.
Old Value/New Value	Original parameter value and the changed value.
Details Key/Value	Identifying parameters and values for the selected history event.

Using Quick Acquisition

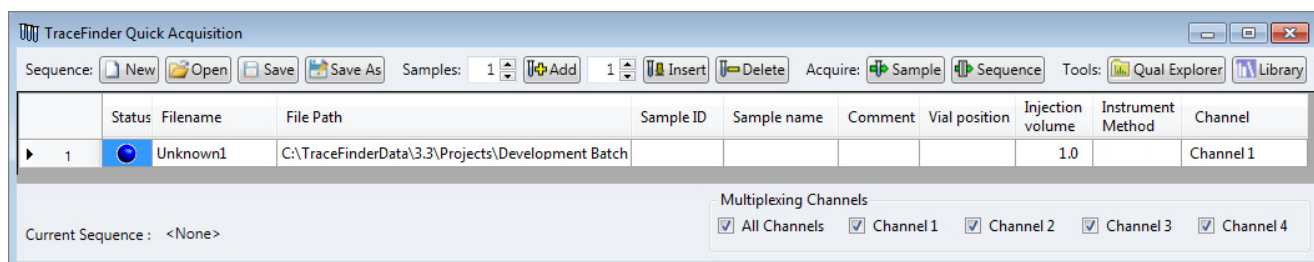
Use the quick acquisition feature to quickly submit samples from any mode in the application.

Note The Quick Acquisition feature is available only when you activate it in the Configuration console. See “[Quick Acquisition](#)” on [page 57](#).

❖ To run a quick acquisition





1. Choose **Tools > Quick Acquire Sample** from the main menu or click the **Quick Acquire Sample** icon, .





The TraceFinder Quick Acquisition window opens.



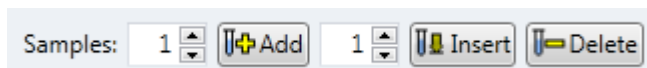
2. To create the sequence of samples that you want to acquire, do any of the following:

- Use the Sequence buttons in the toolbar to open and save Xcalibur sequence files.

Sequence:    

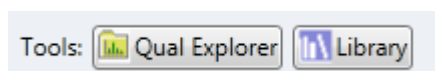
Button	Description
	Replaces the current sequence with a new sequence that contains one Unknown sample.
	Opens the Open dialog box where you can open a saved SLD file.
	Saves the current sequence as an SLD file in the C:\TraceFinderData\Sequences folder.
	Opens the Save As dialog box where you can save the current sequence to a new file name or location.

- Use the Samples buttons in the toolbar to create a sequence of samples.



Button	Description
	Adds the specified number of new, empty samples to the end of the sample list.
	Inserts a new, empty sample or samples above the selected sample.
	Removes the selected samples from the sample list.

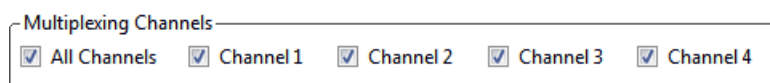
- (Optional) Use the Tools buttons in the toolbar to open a qualitative browser or the NIST library browser.



Button	Description
	Opens the qualitative explorer that you configured as your default qualitative explorer in the Configuration console. See “Launching a Qualitative Explorer” on page 18.
	Opens the NIST library browser. See “Launching the NIST Library Browser” on page 17.

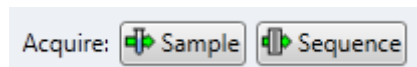
3. (Optional) When using multiplexing, select a channel for each imported sample.

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 console. See [“Multiplexing”](#) on page 61.

4. When you have completed your sequence of samples, click either of the Acquire buttons.



Button	Description
	Submits only the selected samples for acquisition, processing, or report generation.
	Submits the sequence for acquisition, processing, or report generation.

The application submits the samples for acquisition, processing, and report generation. See [“Acquisition Page”](#) on page 389.

Isotopic Pattern Details

The TraceFinder application calculates an isotopic pattern score based on the settings in the method. The application displays this score in the Data Review view. This appendix describes the isotopic distribution concepts and provides calculation details with examples for the isotopic pattern score.

Contents

- [Isotopic Distribution in Exact Mass Spectra](#)
- [Isotopic Pattern Score Calculations](#)

Isotopic Distribution in Exact Mass Spectra

To determine the elemental compositions, the TraceFinder application uses an isotopic pattern matching algorithm that considers the isotope accurate mass and intensity ratios. Using a single exact mass, usually the monoisotopic mass of a measured isotope pattern, the application calculates all possible elemental compositions that lie within a mass tolerance window. You can filter this list of possible elemental compositions and narrow the results by using the natural isotopic distribution of elements.

Natural Isotopic Distribution

The following table lists the natural isotopic distribution of the most common elements.

Table 166. Natural isotopic distribution (Sheet 1 of 2)

Element	Isotope	Isotope order	Exact mass	Mass difference	Abundance (%)
Hydrogen	¹ H	A0	1.0078		99.9985
	² H	A1	2.014102	+1.006302	0.015
Carbon	¹² C	A0	12.0		98.890
	¹³ C	A1	13.003355	+1.003355	1.110
Nitrogen	¹⁴ N	A0	14.003074		99.634
	¹⁵ N	A1	15.00109	+0.998016	0.366

Table 166. Natural isotopic distribution (Sheet 2 of 2)

Element	Isotope	Isotope order	Exact mass	Mass difference	Abundance (%)
Oxygen	¹⁶ O	A0	15.994915		99.762
	¹⁷ O	A1	16.999132	+1.004217	0.038
	¹⁸ O	A2	17.999161	+2.004246	0.200
Fluorine	¹⁹ F	A0	18.99840		100
Phosphorus	³¹ P	A0	30.971459		100
Sulfur	³² S	A0	31.972071		95.020
	³³ S	A1	32.971459	+0.999388	0.750
	³⁴ S	A2	33.967867	+1.995796	4.210
	³⁶ S	A4	35.967081	+3.995010	0.020

where:

- A0 represents the monoisotopic peak, which is the most abundant and usually the isotope with the lowest mass.

For example: ¹H, ¹²C, ¹⁴N, ¹⁶O, ¹⁹F, ³¹P, and ³²S

- A1 represents the isotope where one atom in the molecule is statistically replaced by another atom approximately 1 amu heavier.

For example: ²H, ¹³C, ¹⁵N, ¹⁷O, and ³³S

- A2 represents the isotope where:

Two atoms in the molecule are statistically replaced by two other atoms, each approximately 1 amu heavier.

–or–

One atom is replaced by another atom approximately 2 amu heavier.

For example: ¹⁸O and ³⁴S

- A3 represents the isotope where:

Three atoms in the molecule are statistically replaced by three other atoms, each approximately 1 amu heavier.

–or–

One atom is replaced by another atom approximately 1 amu heavier and one atom is replaced by another atom approximately 2 amu heavier.

–or–

One atom is replaced by another atom approximately 3 amu heavier.

- A4 represents the isotope where:

Four atoms in the molecule are statistically replaced by four other atoms, each approximately 1 amu heavier.

–or–

Two atoms are replaced by two other atoms, each approximately 1 amu heavier, and one atom is replaced by another atom approximately 2 amu heavier.

–or–

Each atom of the two atoms is replaced by another atom approximately 2 amu heavier.

–or–

One atom is replaced by another atom approximately 1 amu heavier, and one atom is replaced by another atom approximately 3 amu heavier.

–or–

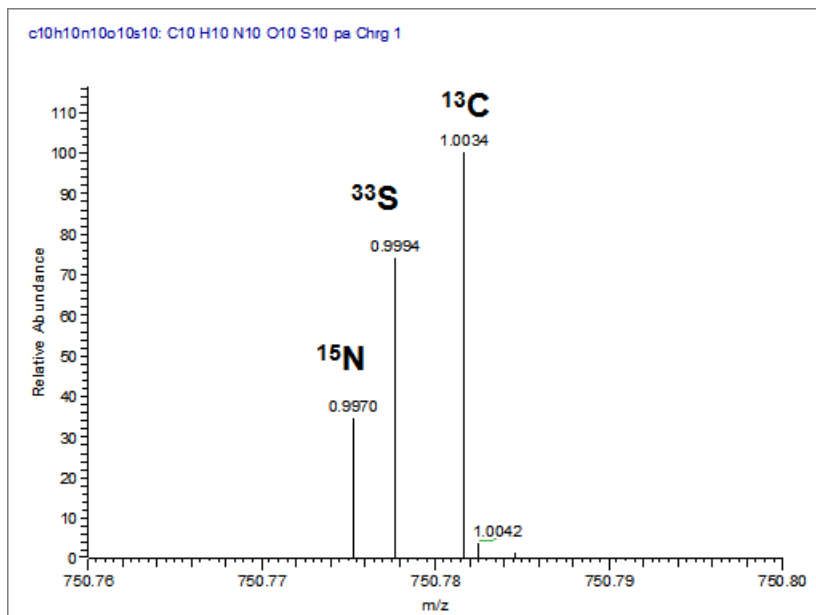
One atom is replaced by another atom approximately 4 amu heavier.

For example: ^{36}S

- Mass difference is the difference in mass between the A0 isotope and another isotope (A1, A2, A3, A4, and so on) of the same element.
- Abundance is the percentage of occurrence of each isotope normally in nature.

In the following figure, the x axis shows the mass difference of A1 relative to the monoisotopic peak (A0) of the ^{13}C , ^{15}N , and ^{33}S isotopes. The y axis shows relative abundance in intensity.

Figure 266. Mass difference and abundance of A1 relative to A0

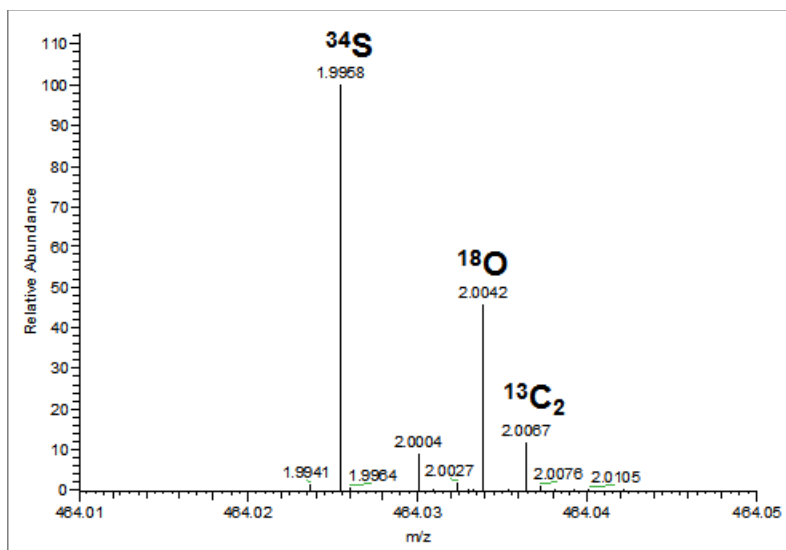


B Isotopic Pattern Details

Isotopic Distribution in Exact Mass Spectra

In the following figure, the x axis shows the mass difference of A2 relative to the monoisotopic peak (A0) of the ^{18}O , ^{34}S , and $^{13}\text{C}_2$ isotopes. The y axis shows relative abundance in intensity.

Figure 267. Mass difference and abundance of A2 relative to A0



Note For a particular isotopic spectrum, the mass difference is always the same between the A0 isotope and the other isotopes (A1, A2, and so on) of each specific element, but the intensity varies according to the composition of the molecule—that is, the number of each element in the molecule.

Isotopic Pattern Score Calculations

The TraceFinder application follows the same isotopic distribution logic as described in “Isotopic Distribution in Exact Mass Spectra” on page 721, but in a different order and with numerical limits and scores to optimize automatic processing. After the TraceFinder application determines the possible elemental compositions for a particular compound of interest, it calculates an expected isotope pattern for each elemental composition candidate and an isotopic pattern score to represent the fit between the expected and measured isotope patterns.

The following data set example describes the isotopic pattern score data and provides the score calculation details for one specific data set.

Data Set Example

This example uses the **Metribuzin** target compound in an **Apple_PosHCD_40_5_01** sample.

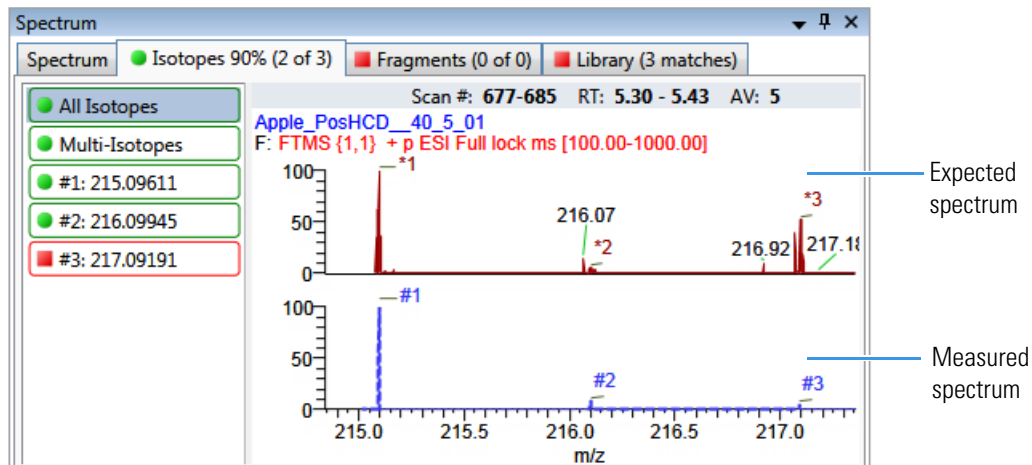
For this compound, note that the Isotopic Pattern Score column shows 90% and the Num Isotopes Matched column shows “2 of 3” in the Compounds pane in the Data Review. The compound’s formula is C₈H₁₄N₄O₅ and its adduct is H, so the modeled isotopic pattern is C₈H₁₅N₄O₅.

Figure 268. Isotopic data for Metribuzin

Compounds					
Selected	Compound Name	Formula	Isotopic Pattern Score (%)	Num Isotopes Matched	
640	Metribuzin	C ₈ H ₁₄ N ₄ O ₅	90	2 of 3	

In the Spectrum pane, click the Isotopes tab and zoom in to view the expected isotopic pattern spectrum compared to the acquired, measured spectrum. The resulting isotopic pattern score should correlate to a visual inspection of the difference between the expected isotope display and the measured display for the target compound.

Figure 269. Isotopic pattern spectra (stacked)



For this example, the processing method used to process the data contains the following isotopic pattern settings for target screening:

- Fit threshold = 90%
- Allowed Mass Deviation = 5 ppm
- Allowed Intensity Deviation = 10%
- Use Internal Mass Calibration = Cleared

The data for the **Metribuzin** compound is as follows:

Measured	Expected
A0 m/z = 215.09602	A0 m/z = 215.09611
A0 Noise = 1482	–
A0 intensity = 4.75E4	A0 intensity = 8.55E5

Because the measured and the expected spectra have different intensities, the spectral noise threshold must proportionally apply to the expected spectrum to decide which peaks are expected in the measured data.

$$\text{Noise threshold (expected)} = \text{Noise of A0 (measured)} \times \text{Intensity of A0 (expected)} \div \text{Intensity of A0 (measured)}$$

Following the previous formula, the expected noise threshold is $1482 \times 8.55E5 \div 4.75E4 = 2.6676E4$.

The expected ions in the measured spectrum are those whose intensities are above the expected noise threshold. The following table lists the ions in the expected spectrum. A “✓” in the Above Threshold column indicates the expected ions.

Table 167. Ions in expected spectrum

Isotope order	m/z (expected)	Intensity (expected)	Above threshold	Present in measured spectrum
A0	215.09611	8.55E5	✓	Yes
A1	216.09945	7.50E4	✓	Yes
A2	217.09191	3.86E4	✓	Yes
A3	218.09521	3.39E3		No

Calculating Mass and Intensity Deviations

The expected number of ions is 3, as shown by those ions with a “✓” in the Above Threshold column of the [Ions in expected spectrum](#) table. These are the ions you focus on for the scoring calculations. This number “3” shows as the value of *y* in the Num Isotopes Matched column of the Compounds pane in the Data Review. It indicates the number of expected isotopic pattern peaks based on the Fourier transform (FT) noise in the spectrum.

In this case, you expect to see the three most intense expected peaks in the measured spectrum. The masses of those peaks are (in order of intensity from high to low): 215.09611, 216.09945, and 217.09191. When the measured spectrum is more intense or the noise level is lower, you find more peaks passing the noise threshold and expected in the measured spectrum, eventually including other isotopic peaks.

The following table shows the mass deviation (delta *m/z*) data for each of the expected ions.

Table 168. Mass deviation data for the expected ions

Isotope order	<i>m/z</i> (expected)	<i>m/z</i> (measured)	Delta <i>m/z</i> (ppm)
A0	215.09611	215.09602	-0.42
A1	216.09945	216.09879	-3.05
A2	217.09191	217.09712	24

where:

$$\text{Delta } m/z \text{ (ppm)} = 1\,000\,000 \times ([m/z \text{ (measured)} - m/z \text{ (expected)}] \div m/z \text{ (expected)})$$

For example:

$$1\,000\,000 \times ([216.09879 - 216.09945] \div 216.09945) = -3.05 \text{ ppm}$$

Tip You can see the expected, measured, and delta *m/z* values on the Isotopes page of the Spectrum pane. The MS page (see [“Isotopic pattern spectra \(stacked\)”](#) on [page 725](#)) displays the profile measured *m/z* values, whereas the Isotopes page displays the centroid measured *m/z* values, which might be different.

If you want more precision, you can see extra decimal digits for the A0 *m/z* values in an exported data file.

If the absolute value of the Delta *m/z* is less than 5 ppm (the Allowed Mass Deviation value set in the processing method), the TraceFinder application determines that this ion is found—that is, the ion is present in the measured spectrum. For this data set example, the application finds only the A0 and A1 ions, so “2” shows as the value of *x* in the Num Isotopes Matched column of the Compounds pane in the Data Review. The application does not find the A2 expected ion because the absolute value of its Delta *m/z* of 24 ppm is much higher than 5 ppm.

Note You can see from zooming in on the isotopic pattern spectra (see “[Isotopic pattern spectra \(stacked\)](#)” on [page 725](#)) that there are measured peaks in the measured spectrum closely corresponding to the first two expected ions, but there is not a measured peak closely corresponding to the 217.09191 expected ion.

The following table lists the intensity deviation (delta intensity) data for each of the expected ions, relative to the A0 ion’s expected intensity of 8.55E5 and measured intensity of 4.75E4.

Table 169. Intensity deviation data for the expected ions

Isotope order	<i>m/z</i> (expected)	Intensity (expected)	Relative intensity (expected, %)	Intensity (measured)	Relative intensity (measured, %)	Delta intensity
A0	215.09611	8.55E5	100	4.75E4	100	0
A1	216.09945	7.50E4	8.77	8.75E3	18.42	9.65
A2	217.09191	3.86E4	4.51	3.47E4	73.05	68.54

where:

- Relative intensity (expected and measured) values are derived from the isotopic pattern spectra (see “[Isotopic pattern spectra \(stacked\)](#)” on [page 725](#)). Each value is a percentage of the isotope’s intensity relative to the A0 ion’s intensity.

For example: $7.50E4 \div 8.55E5 = 8.77\%$

- Delta intensity = *Relative intensity (measured)* – *Relative intensity (expected)*

For example: $18.42 - 8.77 = 9.65$

In this example, the absolute values of the Delta *m/z* for the A0 and A1 ions (see “[Mass deviation data for the expected ions](#)” on [page 727](#)) are both less than the Allowed Mass Deviation of 5 ppm; therefore, the application considers that these two ions are present in the measured spectrum. The delta intensity of the A1 isotope ion is close to the Allowed Intensity Deviation of 10% and the delta intensity of the A2 isotope ion is much higher (see “[Intensity deviation data for the expected ions](#)” on [page 728](#)).

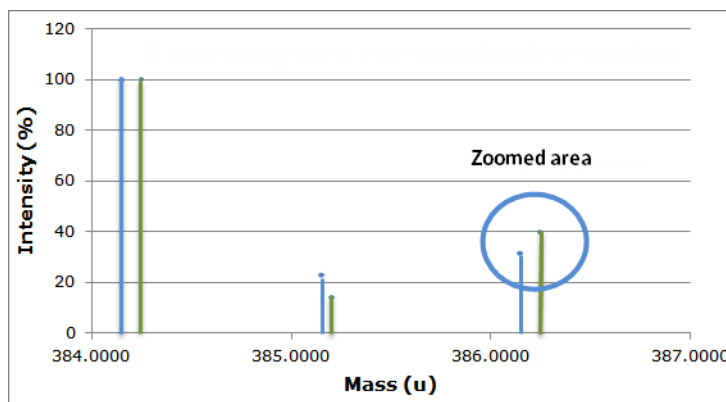
The TraceFinder application determines the isotopic pattern score value from a combination of the mass and intensity deviations between the expected and the measured spectra. In this case, the application reduces the isotopic pattern score value down to 90 from 100 to reflect the marginal quality of the intensities of the A1 and A2 isotopes and to penalize for not finding the A2 isotope.

Calculating Isotopic Pattern Score

To score the fit for an isotopic pattern, the TraceFinder application calculates each expected ion's fit and then combines the individual fit scores, weighted by their expected intensities.

For each expected ion peak, the application measures the m/z and intensity differences between the expected and the measured patterns. It then normalizes those differences (normalized deviation values) to the maximum allowed mass and intensity deviation values set in the processing method. The application then sums the normalized differences by vector addition (see [Vector sum of intensity \(I\) and mass \(M\) deviations](#)).

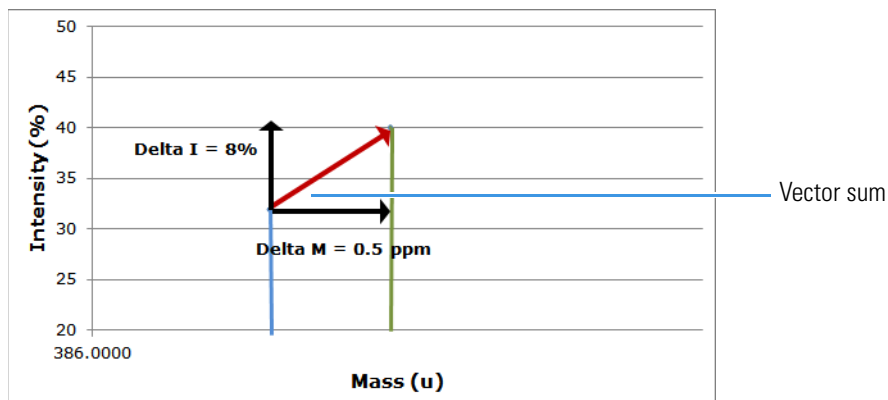
Figure 270. Measured and expected patterns



Expected spectrum in blue

Measured spectrum in green

Figure 271. Vector sum of intensity (I) and mass (M) deviations



Expected spectrum in blue

Measured spectrum in green

This example starts first with the intensity deviations. The Allowed Intensity Deviation value set in the processing method is 10, so this is the normalization value. As shown in [“Intensity deviation data for the expected ions”](#) on [page 728](#), the delta intensity value for the A1 isotope is close to 10%, resulting in a normalized intensity deviation close to 1.0.

Normalized Intensity Deviation

The following table lists the normalized intensity deviation data for each of the expected ions.

Table 170. Normalized intensity deviation data for the expected ions

Isotope order	m/z (expected)	Delta intensity	Allowed intensity deviation (%)	Normalized intensity deviation
A0	215.09611	0	10	$0 \div 10 = 0.0$
A1	216.09945	9.65	10	$9.65 \div 10 = 0.965$
A2	217.09191	68.54	10	$68.54 \div 10 = 6.854$

Next are the mass deviations. For mass deviations, you can control two settings in the processing method:

- The first setting is the Allowed Mass Deviation that functions as an outer limit in the same way as the Allowed Intensity Deviation functions as a limit for the intensity.
- The second setting is the Use Internal Mass Calibration check box. If you do not select this check box in the method, then the application considers any mass value within 2 ppm of the expected m/z as a perfect match (no deviation). If you select this check box, then the application considers only a mass value within 1 ppm of the expected m/z as a perfect match.

In this example, the Allowed Mass Deviation value set in the processing method is 5 ppm and the Use Internal Mass Calibration check box is cleared. The mass normalization is a bit more complex than the intensity normalization because mass values < 2 ppm (Use Internal Mass Calibration setting) from the expected m/z are considered to have no deviation from theory; however, for values between 2 and 5 ppm (Allowed Mass Deviation value) from the expected m/z , the normalized deviation varies from 0 through 1.

The calculated normalized mass deviation value is as follows:

- 0 if absolute value ($\Delta m/z$) < 2 ppm
where 2 ppm is the value from the Use Internal Mass Calibration setting.
- $[\text{absolute value } (\Delta m/z) - 2 \text{ ppm}] \div (5 \text{ ppm} - 2 \text{ ppm})$ if
absolute value ($\Delta m/z$) \geq 2 ppm
where 2 ppm is the value from the Use Internal Mass Calibration setting and 5 ppm is the Allowed Mass Deviation value.

In this case, the absolute value of the mass deviation for the A0 ion is less than 2 ppm; therefore, its normalized mass deviation value is 0.

Normalized Mass Deviation

The following table lists the normalized mass deviation data for each of the expected ions.

Table 171. Normalized mass deviation for each of the expected ions

Isotope order	<i>m/z</i> (expected)	<i>m/z</i> (measured)	Delta <i>m/z</i> (ppm)	Internal calibration (ppm)	Allowed mass deviation (ppm)	Normalized mass deviation
A0	215.09611	306.10356	-0.42	2	5	0
A1	216.09945	307.10691	-3.05	2	5	0.35
A2	217.09191	308.11324	24	2	5	7.33

For example: $[(24 - 2)] \div (5 - 2) = 7.33$

To calculate the combined deviations, the application uses the Pythagorean theorem to calculate the vector sum of the normalized deviations. The calculation for the vector sum is as follows:

Vector sum = Square root $[(\text{Normalized intensity deviation})^2 + (\text{Normalized mass deviation})^2]$.

However, if the vector sum > 1, then set it to 1.

Calculated Vector Sum

The following table lists the vector sum data for each of the expected ions.

Table 172. Calculated vector sum

Isotope order	<i>m/z</i> (expected)	Normalized intensity deviation	Normalized mass deviation	Vector sum
A0	215.09611	0	0	0
A1	216.09945	0.965	0.35	1
A2	217.09191	6.854	7.33	1

To calculate the final score, you must weigh the vector sum values and then express the result as a percentage value. Each ion's weighting contribution to the final isotopic pattern score is proportional to its intensity.

Weighting Factor Calculations

The following table lists the weighting factor of each of the three expected ions.

Table 173. Weighting factor calculations

Isotope order	m/z (expected)	Intensity (expected)	Weighting factor for final score
A0	215.09611	8.55E5	0.8827
A1	216.09945	7.50E4	0.0774
A2	217.09191	3.86E4	0.0399
		Sum = 9.686E5	Sum = 1.000

The weighting factor of each individual ion = *Intensity of each ion* ÷ *Sum of intensities of all expected ions*

For example: $8.55E5 \div 9.686E5 = 0.8827$

When not all of the expected ions are present in the measured spectrum, the application applies a penalty value (1, 2, or 4) to the weighted deviation of each missing ion, lowering the final isotopic pattern score even further. The penalty value depends on how strong the ion signal is expected to be in the measured spectrum. For the A2 ion that is not found, the application sets its penalty to a value of 1, causing its vector sum value of 1 (in [Table 172 on page 731](#)) to be replaced with the penalty value of 1 (in [Table 174](#)). In this case, it is the same number, but for other cases, the penalty value might be different from the vector sum value.

Calculated Isotopic Pattern Score

The following table lists the calculated isotopic pattern score using the weighting factors.

Table 174. Calculated isotopic pattern score

Isotope order	m/z (expected)	Deviation (vector sum or penalty)	Weighting factor	Weighted deviation
A0	215.09611	0 (vector sum)	0.8827	0
A1	216.09945	1 (vector sum)	0.0774	0.0774
A2	217.09191	1 (penalty)	0.0399	0.0399
				Sum = 0.12

where:

- Weighted deviation of each individual ion = *Deviation* × *Weighting factor*

For example: $1 \times 0.0774 = 0.0774$

- Isotopic pattern score = $100\% \times (1.0 - \text{Sum of all weighted deviation values})$

For this example, the calculated isotopic pattern score of $100\% \times (1.0 - 0.12)$ is 88, which is close to the 90 score displayed in the application.

Note Use these calculations to approximate the score displayed in the application. The calculated score might not match exactly the score in the application because some internal calculation details are not listed here or there is a discrepancy due to decimal digit rounding.

In certain cases, closely matching isotopes exist because heavier isotopes contribute to the isotopic pattern observed in the mass spectra. For example, the isotopes 206.0941 and 206.1006 result from the contribution of one heavier isotope of carbon and one heavier isotope of nitrogen, respectively, together making up the split A1 isotopic peak. When the application performs isotopic pattern scoring, this situation appears as a main isotopic peak with a smaller peak to the side whose m/z is included in the calculations.

Finding the Noise Value

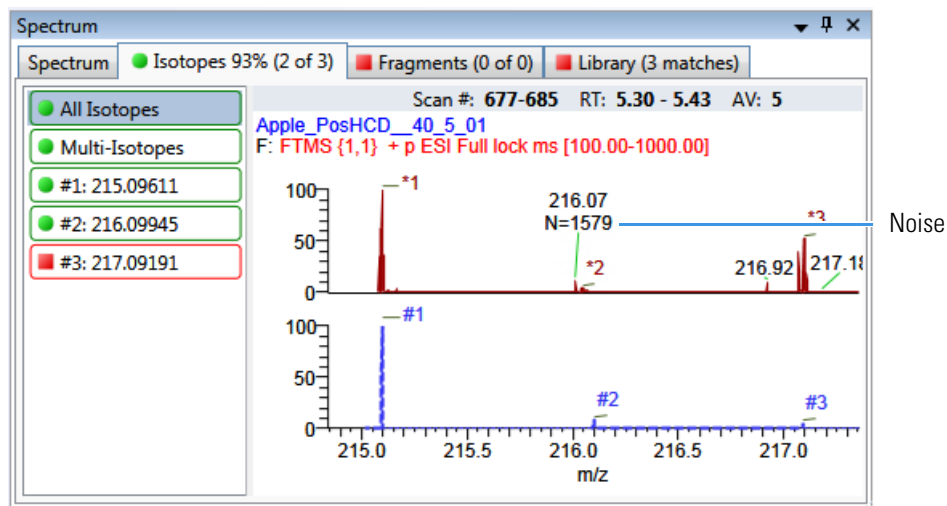
On the Isotopes page of the Spectrum pane, you can view the averaged noise value (N) for a peak in the measured spectrum.

❖ To find the noise value associated with a mass spectral peak

1. Right-click the spectrum plot area and choose **Display Stack Spectra** from the shortcut menu.
2. Zoom in to the peak of interest.

As an example, see “[Isotopic pattern spectra \(stacked\)](#)” on [page 725](#) for the compound **Metribuzin**.

3. Right-click the measured spectrum plot area and choose **Show Noise Label** from the shortcut menu.



Expected spectrum in blue

Measured spectrum in red

In this example, the averaged noise value for the peak is 1579.

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, Level, Comment, and other columns.

Follow these 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 the difference between a selected and nonselected cell.



2. Right-click and choose **Copy Down** from the shortcut menu.

The value is copied to all rows below the selected row.

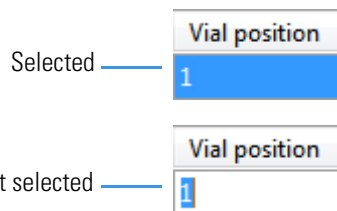
❖ To automatically enter sequential column values

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 the difference between a selected and nonselected cell.



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 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.

Filename	Sample ID	Sample name
Sample1		
Sample101		
Sample102		
Sample103		
Sample104		
Sample105		
Sample106		
Sample107		
Sample108		
Sample109		
Sample110		
Sample111		
Sample112		
Sample113		

Filename
Sample1
Sample2
Sample3
Sample4
Sample104
Sample105
Sample106
Sample107
Sample108
Sample109
Sample110
Sample111
Sample112
Sample113

Moving Data Review Panes

This appendix describes the procedures you can use to move, dock, or float panes in all Data Review views. The procedures have accompanying animations.

Follow these procedures:

- [To move a docked pane](#)
- [To make a pane floating or dockable](#)
- [To change a pane from a docked pane to a tabbed pane](#)

❖ To move a docked pane

1. Grab the title bar of the pane and begin dragging the pane.

The application displays docking arrows.

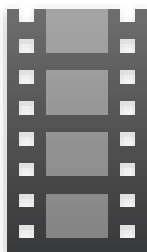


2. Drag the pane over one of the arrows.

As you hold the cursor over a docking arrow, the application displays a blue region indicating where this arrow will place the pane.

3. Drop the pane onto one of the arrows.

This animation shows the various ways that you can use the docking mechanism to move a pane. To view the animation, click the filmstrip, and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.



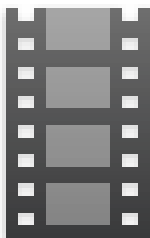
❖ To make a pane floating or dockable

Do one of the following:

- To make a dockable pane floating, right-click the title bar of the pane and choose **Floating**.

While a pane is set as floating, you cannot use the docking arrows to dock it or make it a tabbed pane.

- To make a floating pane dockable, right-click the title bar of the pane and choose **Dockable**.



This animation shows how to switch a pane from docked to floating and back to docked. To view the animation, click the filmstrip, and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.

❖ To change a pane from a docked pane to a tabbed pane

1. Grab the title bar of the pane and begin dragging the pane.

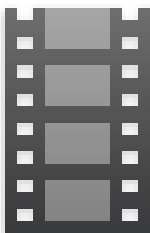
The application displays docking arrows.



Drop the pane on the center location to create a tabbed pane.

2. Hold the cursor over the center of the docking arrows to display a blue region indicating the location of the tabbed pane.
3. Drop the pane over the center of the docking arrows.

Note To change a floating pane to a tabbed pane, you must first make the pane a dockable pane, and then you can make it a tabbed pane.



This animation shows how to change a pane from a docked pane to a tabbed pane and back to a docked pane. To view the animation, click the filmstrip, and then right-click and choose **Full Screen Multimedia**. To stop the animation, press ESC.



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