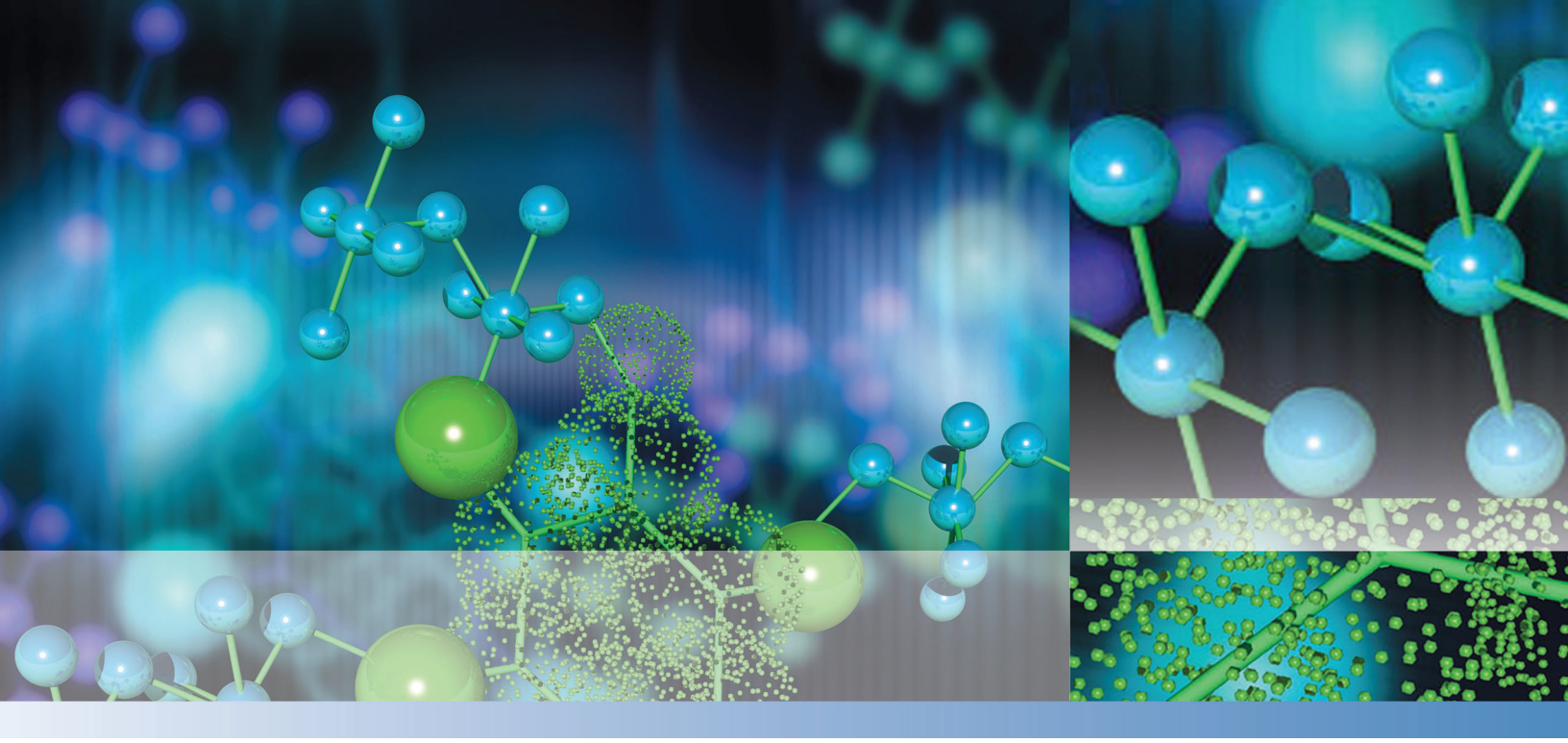

Thermo

TraceFinder

User Guide

Software Version 3.2
Optimized for Clinical Research

XCALI-97598 Revision A June 2014

DOCUMENTATION SURVEY

Thermo SCIENTIFIC

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

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Preface

This guide describes how to use the Thermo TraceFinder™ 3.2 application in the Thermo Scientific™ series of GC/MS and LC/MS analytical software.

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*

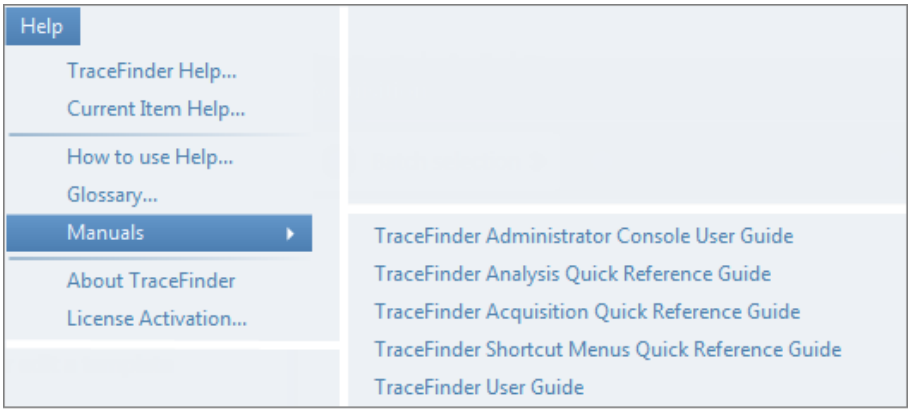
❖ **To view TraceFinder documents using the Start menu**

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***.

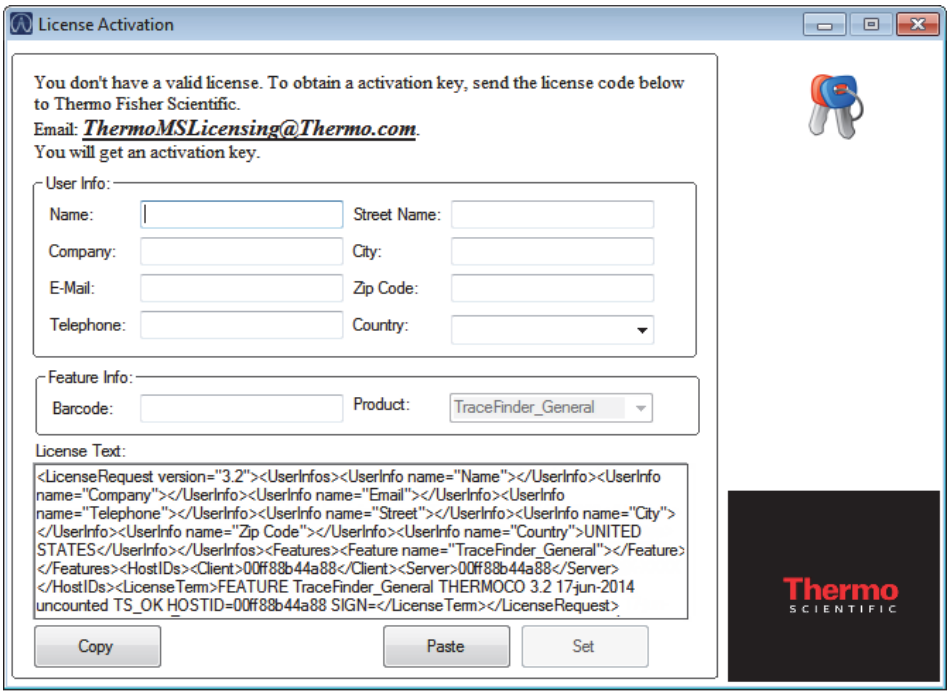
Figure 1. PDF files available from the Help menu



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 trial. If your free trial has expired, the License Activation window opens.



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

Two types of licenses are available:

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

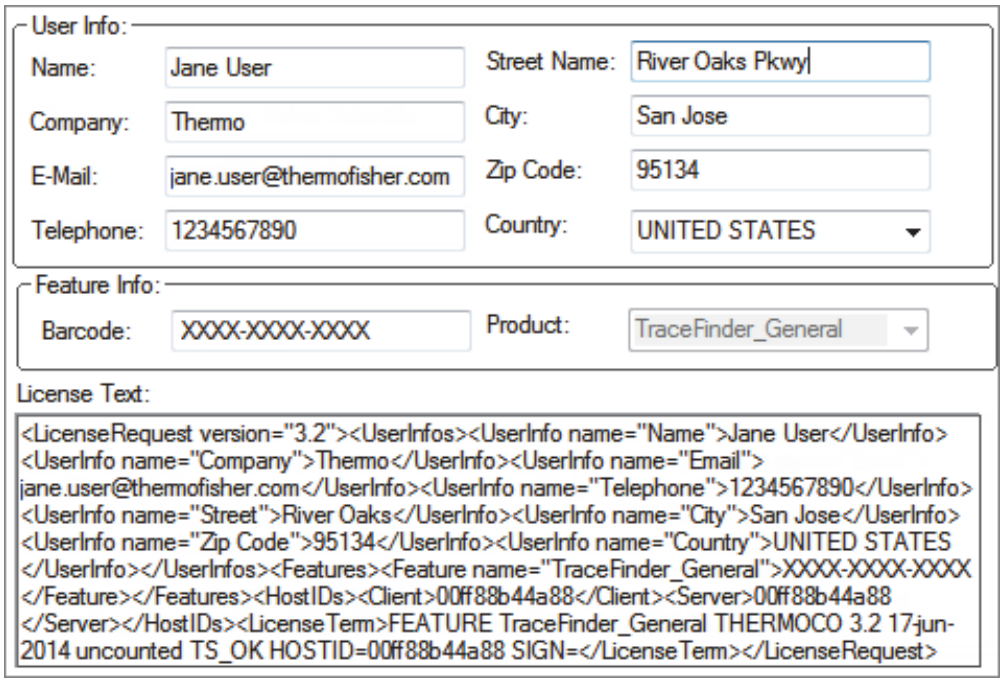
The evaluation version is full-featured and automatically expires 120 days after activation. Any attempt to set back the system date automatically terminates this version. You can purchase and then activate the full version of the TraceFinder application at any time, during or after the free evaluation, without reinstalling the software.

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

❖ To request an activation key

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

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



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

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

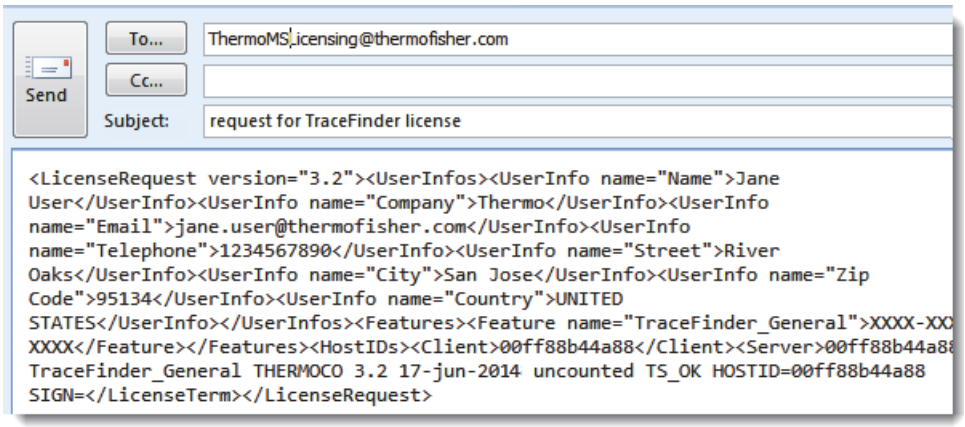
   Note The barcode might already be filled in for you.

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

   The application copies this XML text to the Clipboard.

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

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



You will receive an email response containing the activation key.

❖ To use your activation key

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

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

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

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

Special Notices

Make sure you follow the special notices presented in this guide. Special notices 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.

Contacting Us

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

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Technical Support	(U.S.) Phone: 1 (800) 532-4752 Fax: 1 (561) 688-8736 Email: us.techsupport.analyze@thermofisher.com Web—for product support, technical documentation, and knowledge bases: www.thermoscientific.com/support
Customer Service (Sales and service)	(U.S.) Phone: 1 (800) 532-4752 Fax: 1 (561) 688-8731 Email: us.customer-support.analyze@thermofisher.com Web—for product information: www.thermoscientific.com/lc-ms Web—for customizing your service request: 1. From any Products & Services web page, click **Contact Us**. 2. In the Contact Us box, complete the information requested, scroll to the bottom, and click **Send**.
User Documentation	Web—for downloading documents: mssupport.thermo.com 1. On the Terms and Conditions web page, click **I Agree**. 2. In the left pane, click **Customer Manuals**. 3. To locate the document, click **Search** and enter your search criteria. For Document Type, select **Manual**. Email—to send feedback directly to Technical Publications: techpubs-lcms@thermofisher.com Web—to complete a survey about this Thermo Scientific document: www.surveymonkey.com/s/PQM6P62

1

Introduction

This chapter describes general features of the TraceFinder software.

Contents

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

About the TraceFinder Application

The TraceFinder application targets the clinical research 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 TraceFinder application can export mass data in the Acquisition List to XML format so that other applications, including TSQ 8000, TSQ Quantum™, ISQ, and Q Exactive™, can import the files into their databases.

The TraceFinder application can import the following file types:

- Sample lists in .csv or .xml format

  See "Defining the Sample List" on page 326.

- 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 Screening Methods."

  For detailed information about creating instrument methods, see "Working with Instrument Methods" on page 113.

- Compounds from files that use the database (.xml or .cdb) format

  See "Working with the Compound Database" on page 76.

- Batches, methods, or templates from the TraceFinder 2.0, 2.1, 3.0, or 3.1 applications.

  See "Converting Legacy Data" on page 18.

The TraceFinder application checks the accuracy and precision of data against systems that have previously been certified against a standard processing program, such as the Statistical Analysis System (SAS).

Supported File Types

The TraceFinder application supports the following file types:

- Comma-separated values (.csv): A set of file formats used to store tabular data in which numbers and text are stored in plain textual form that can be read in a text editor. Lines in the text file represent rows of a table, and commas in a line separate fields in the tables row.
- Extensible Markup Language (.xml): A generic framework for storing any amount of text or any data whose structure can be represented as a tree. The only indispensable syntactical requirement is that the document has exactly one root element (also called the document element). This means that the text must be enclosed between a root start-tag and a corresponding end-tag.
- Instrument method (.meth): A proprietary file format for the Xcalibur software suite with specific instructions that enable scientific instruments to perform data acquisition.
- Processing method (.pmd): A proprietary file format for the Xcalibur software suite with specific instructions on processing data that was acquired through the instruments attached to the system.
- Raw data (.raw): The file type for acquired samples on the system.
- Compound database (.cdb): The file type for TraceFinder or ExactFinder compound database data.
- Library (.db): A library used for target screening.

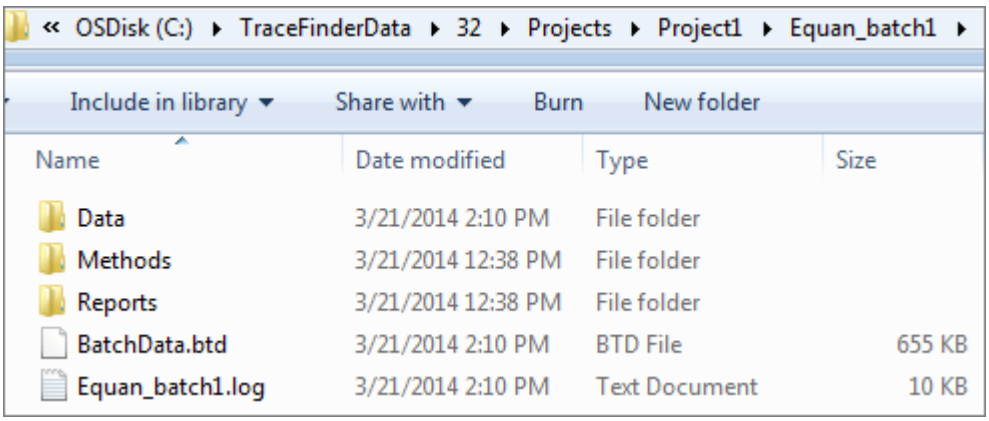
TraceFinder Directory Structure

The TraceFinder 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\32\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



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 clinical research 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 TraceFinder application uses a comprehensive processing method to provide improved handling of ion ratio calculations, reviewing, and reporting. In addition, it can compare the mass 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, supporting capabilities present in the LCquan™ and ToxLab Forms applications
- Target 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 TraceFinder 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 TraceFinder application, follow these basic steps:

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

   A master method combines the instrument method and processing method that define 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:

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 worldwide regulatory agencies, helping to track the performance of LC and GC systems and methods.

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 Report
- High Density Sample Report 1 Long
- Intelligent Sequencing Report
- Internal Standard Summary Report
- Ion Ratio Failure Report
- Manual Integration Report
- Method Report
- MSMSD Report
- Quantitation Report
- Quantitation Report - 2
- Screening Batch Report
- SGS Report
- Solvent Blank Report
- Standard Addition Report
- Surrogate Recovery Report
- Target Screening Hight Density Sample Report
- Target Screening Hight Density Sample Report 2
- Target Screening Summary Report
- TIC Report
- TIC Summary Report
- Tune Report

2

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

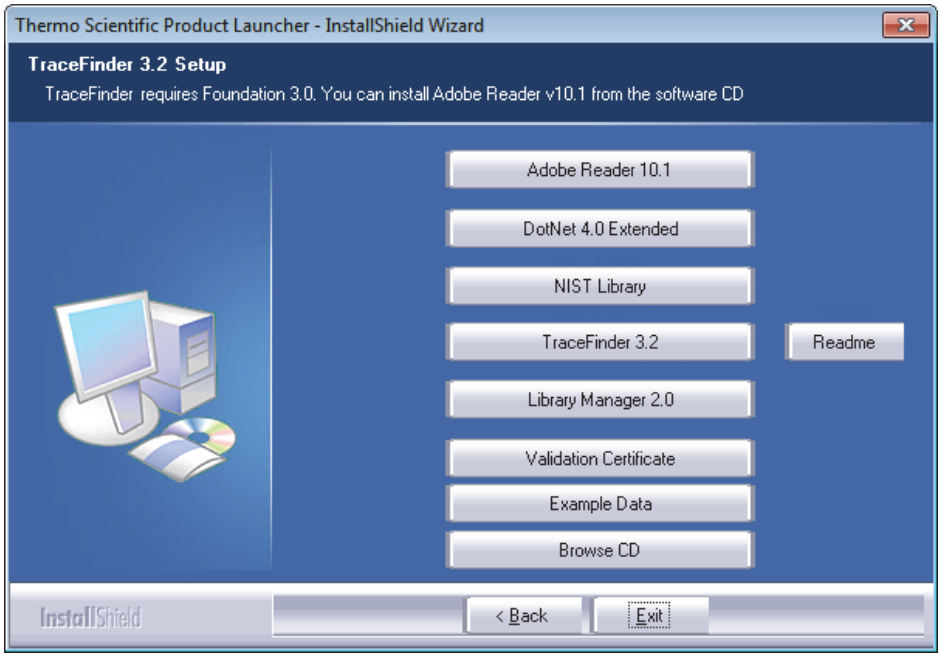
To initially install the TraceFinder 3.2 application, follow the instructions in the *TraceFinder Installation Guide*. Later, you might need to reinstall the TraceFinder application or other features on the InstallShield Wizard.

Follow these instructions to reinstall, start, and log in to the TraceFinder 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 TraceFinder application and then uninstall all Thermo instrument drivers.
3. Insert the TraceFinder CD, and install both the TraceFinder 3.2 application and the NIST library as follows:
   a. Open the TraceFinder launcher and click **Next**.

The InstallShield Wizard opens.



b. Click **TraceFinder 3.2**, and follow the instructions in the InstallShield Wizard.

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

c. At the prompt, click **Yes** to completely remove any previously installed TraceFinder applications.

d. Open the TraceFinder launcher again and click **Next**.

e. Click **TraceFinder 3.2**, and follow the instructions in the InstallShield Wizard.

> **IMPORTANT** For the TraceFinder application to properly install, you might be prompted to uninstall Thermo Foundation™. 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. If you have not previously installed the NIST library, click **NIST Library** and follow the instructions to install the library.

i. (Optional) Click **Example Data**.

The application installs example compound databases, instrument methods, and batch data.

4. Install the appropriate device drivers, and configure the instruments in the Thermo Foundation Instrument Configuration window.

❖ 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 > TraceFinder Clinical Research**.

   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*.

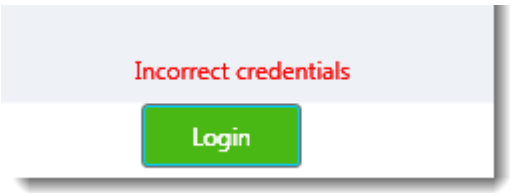
❖ To log in to the TraceFinder application (when user security is activated)

> **Note** Before you can log in to the TraceFinder 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 11.

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.

Figure 3. TraceFinder main window, showing the Analysis mode

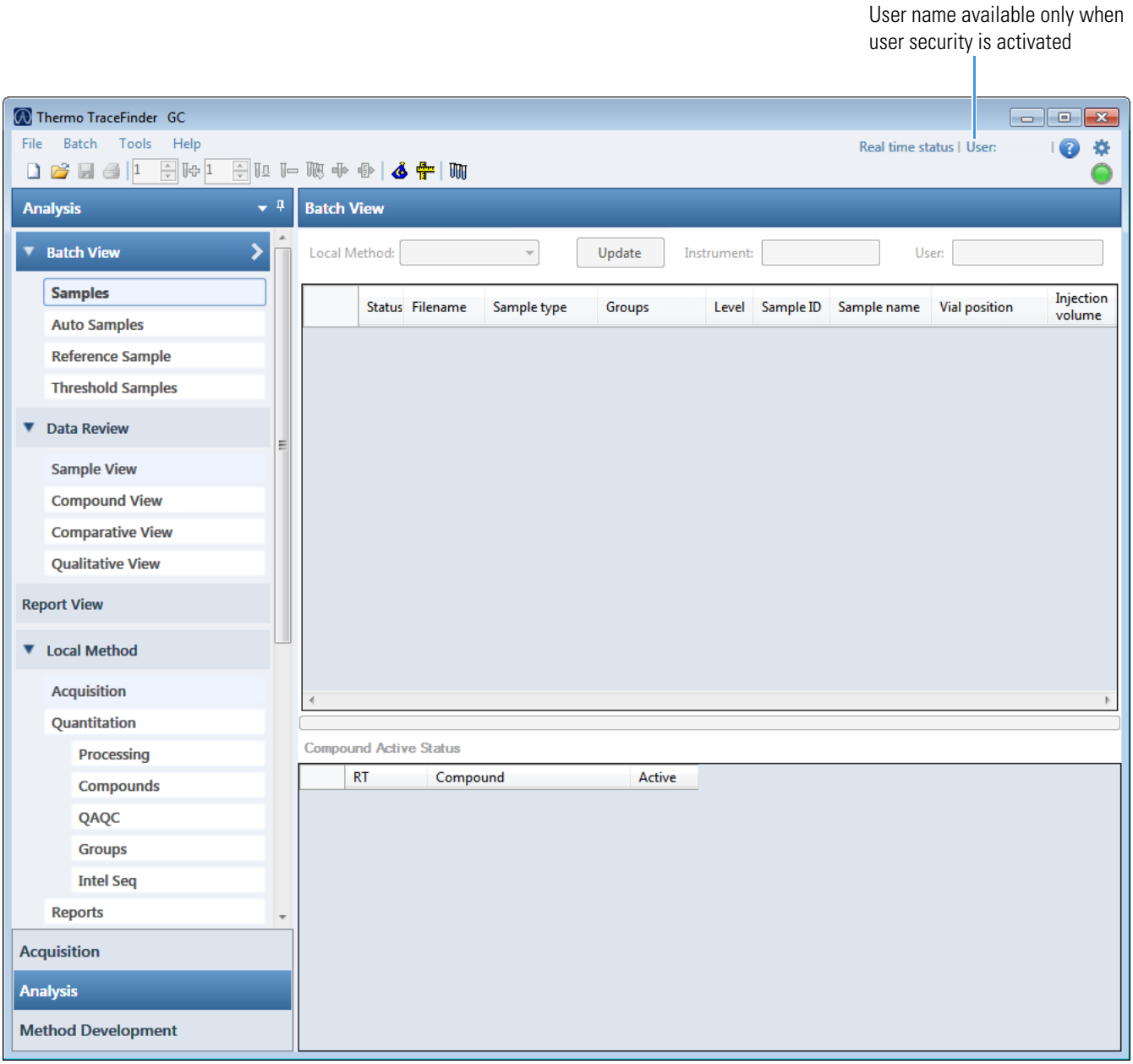


Table 1. TraceFinder main window features (Sheet 1 of 2)

Parameter	Description
Toolbar	See "Toolbar Reference" on page 536.
Application Configuration	See Chapter 3, "Using the Configuration Console."
Acquisition	See Chapter 7, "Using the Acquisition Mode."

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

Parameter	Description
Analysis	See Chapter 8, "Using the Analysis Mode."
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 Screening Methods."

Figure 4. TraceFinder login window

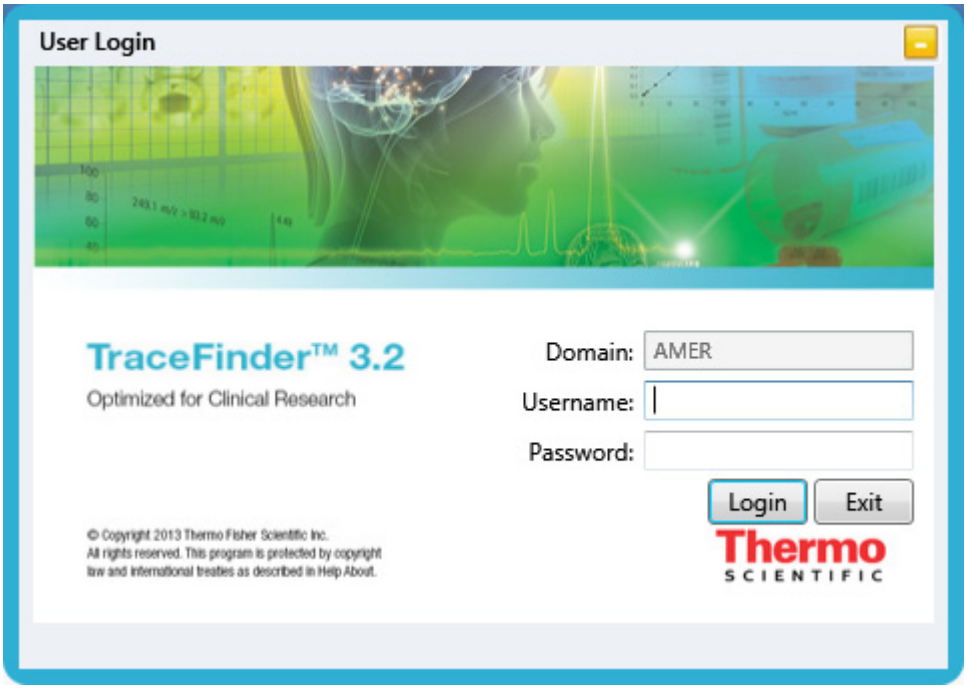


Table 2. Login window parameters

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 TraceFinder 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

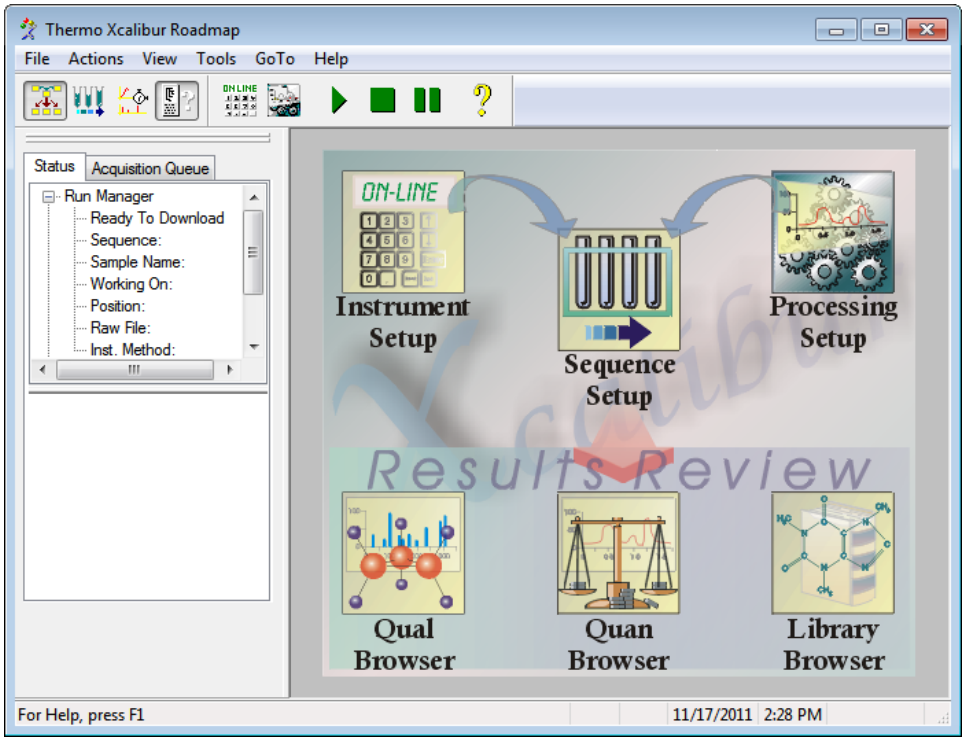
1. Open the TraceFinder launcher, and click **Next**.
2. Click **NIST Library**.

   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.

❖ To install the QED library

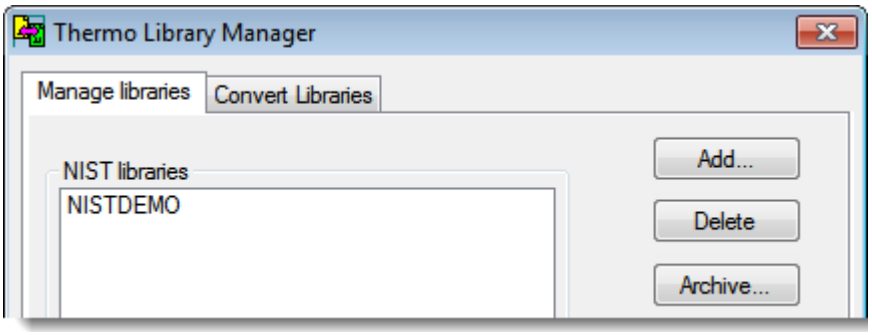
1. On your desktop, double-click the **Xcalibur** icon, .

   The Thermo Xcalibur Roadmap opens.



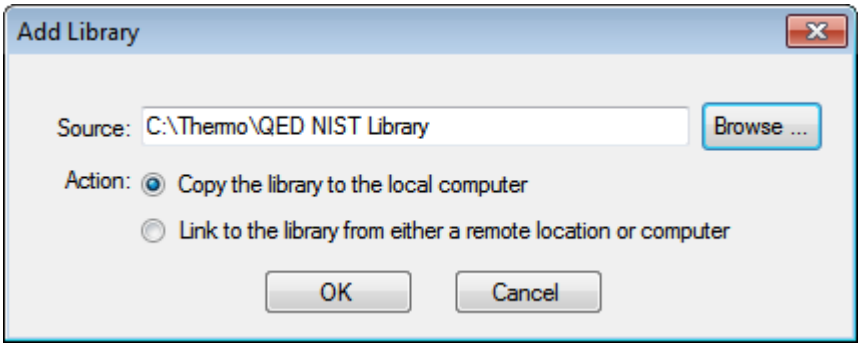
2. Choose **Tools > Library Manager** from the main menu.

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



3. Click **Add**.

   The Add Library dialog box opens.

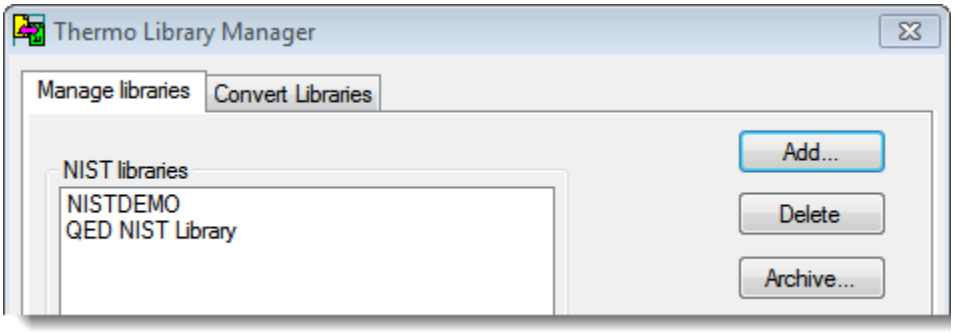


4. Click **Browse**, and locate your QED library in the C:\Thermo folder.
5. Click **OK**.

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

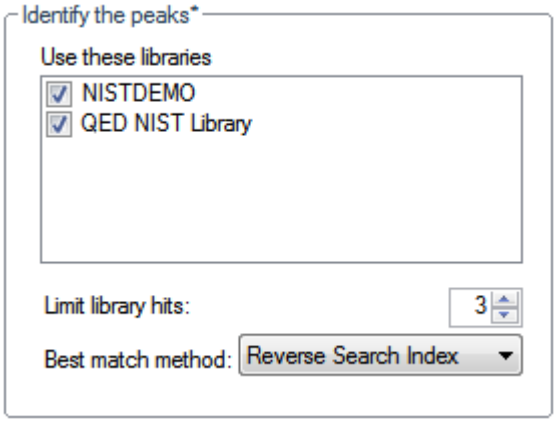
6. Click **Dismiss** to close the message box.

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



7. Click **Exit** in the Thermo Library Manager dialog box.
8. To confirm the library installation, do the following:
   a. Start the TraceFinder 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.

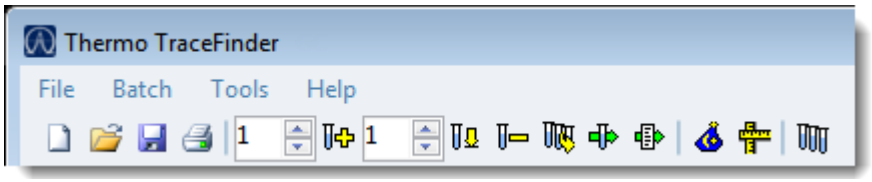


Launching the NIST Library Browser

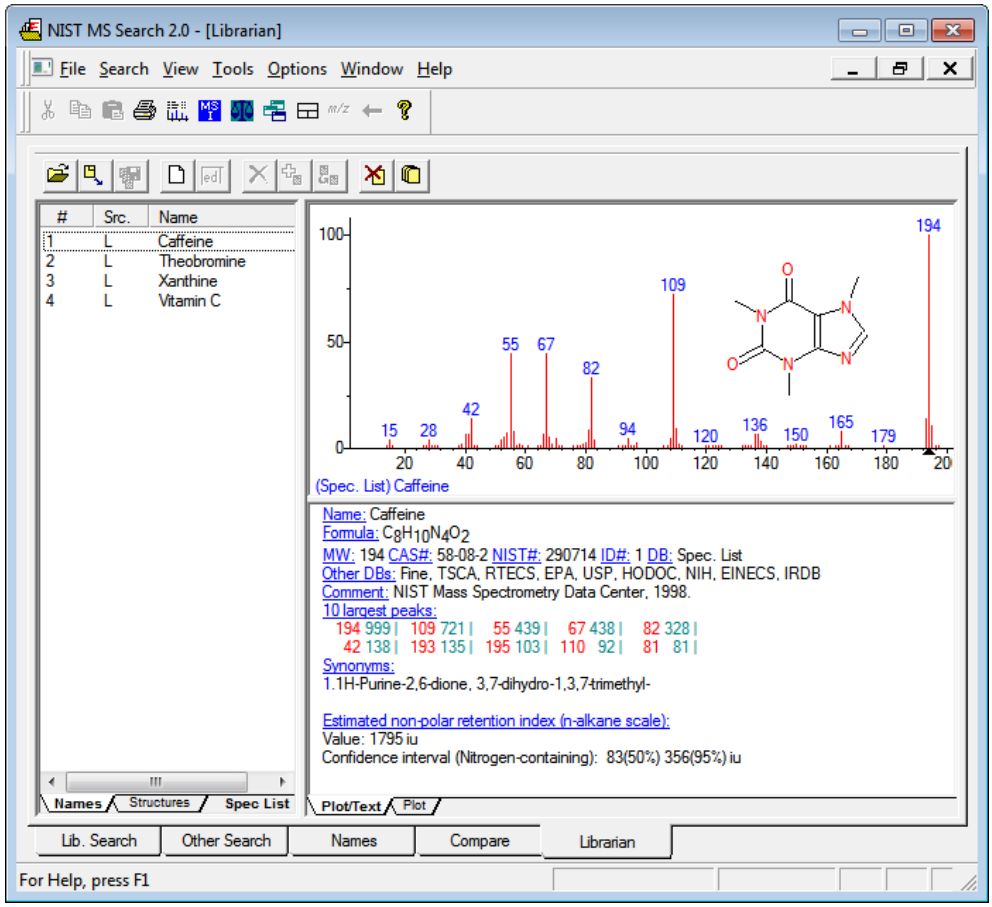
Use the NIST MS Search tool to search the NIST library.

❖ To open the NIST library browser

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



The NIST MS Search window opens.



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

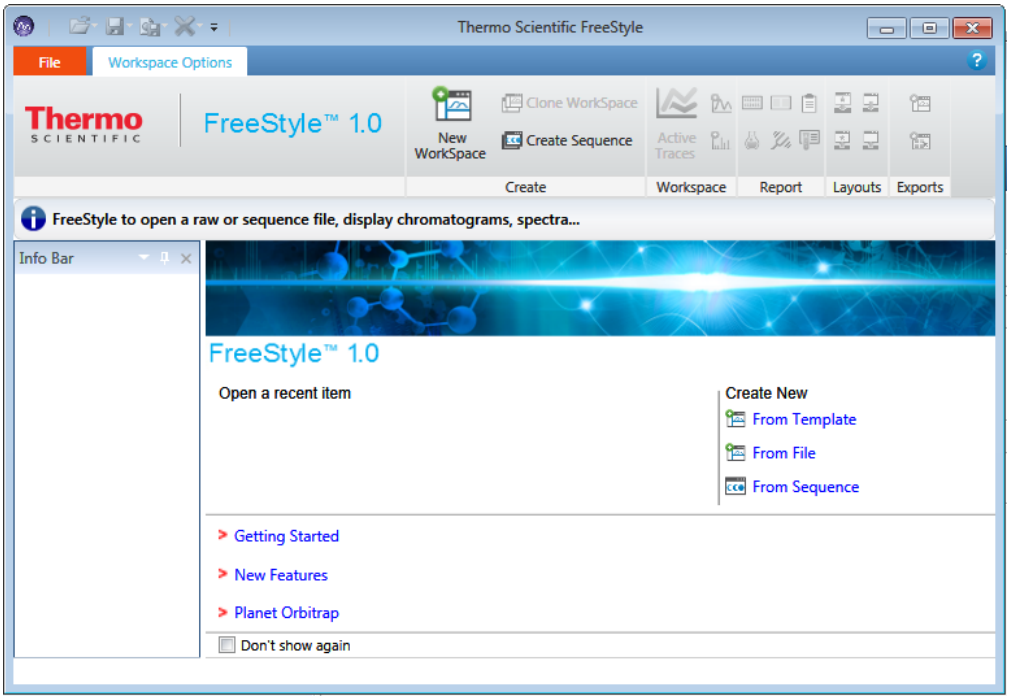
IMPORTANT The FreeStyle™ application is available only when you configure it as your default qualitative explorer in the Configuration Console. See Chapter 3, "Using the Configuration Console."

❖ 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

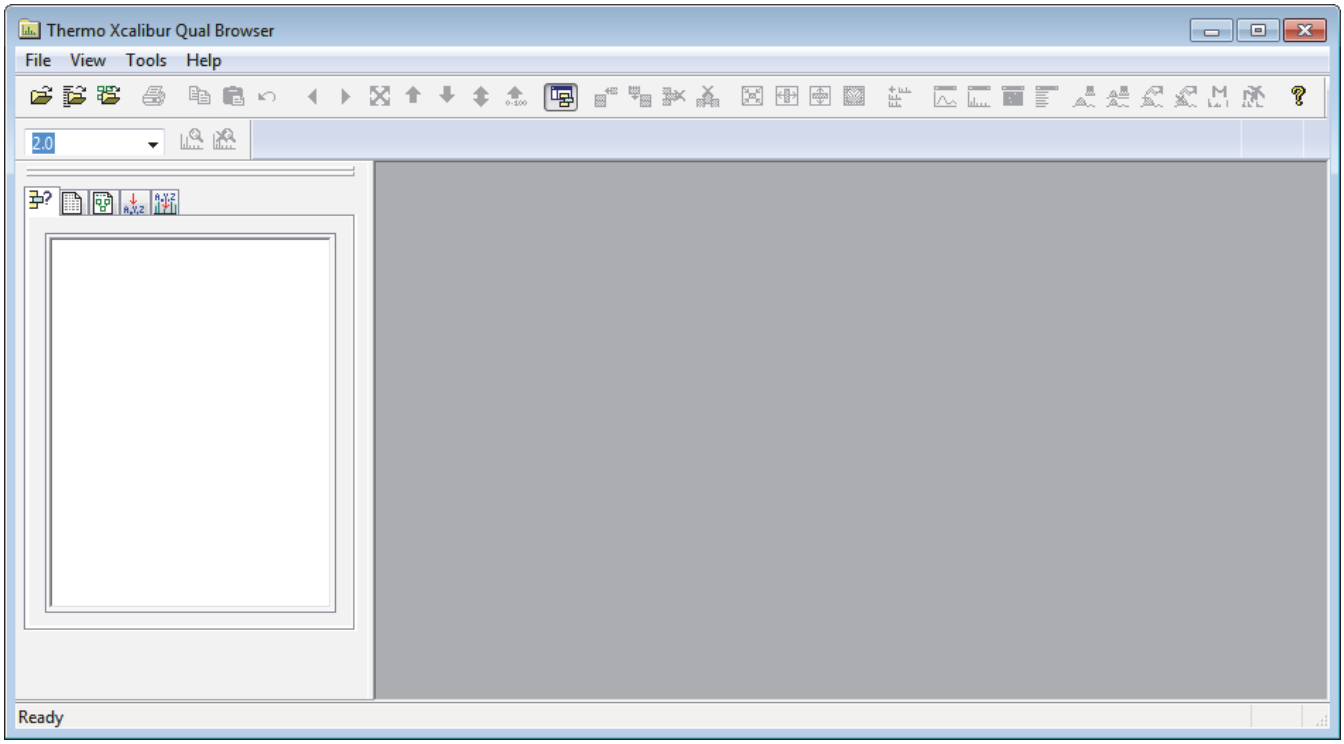
IMPORTANT The Qual Browser application is available only when you configure it as your default qualitative explorer in the Configuration Console. Chapter 3, "Using the Configuration Console."

❖ **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 Trace Finder Legacy Data Converter to convert methods, batches, method templates, or batch templates from the source versions to compatible TraceFinder 3.2 target configurations.

- You can convert legacy data from TraceFinder versions 2.0, 2.1, 3.0, or 3.1.
- You can convert data from TraceFinder 3.2 for general quantitation to another installed configuration of TraceFinder 3.2.

Version Compatibility

This table shows which source versions of methods, batches, method templates, or batch templates are compatible with TraceFinder 3.2 target configurations.

Table 3. Version compatibility

Source	TraceFinder 3.2 target			
	General	EFS*	Clinical Research	Forensic Toxicology
TraceFinder 3.2 General		✓	✓	✓
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			✓	✓
TraceFinder 2.0 General	✓	✓	✓	✓
TraceFinder 2.0 EFS		✓		
TraceFinder 2.0 Clinical Research			✓	✓

* Environmental and Food Safety

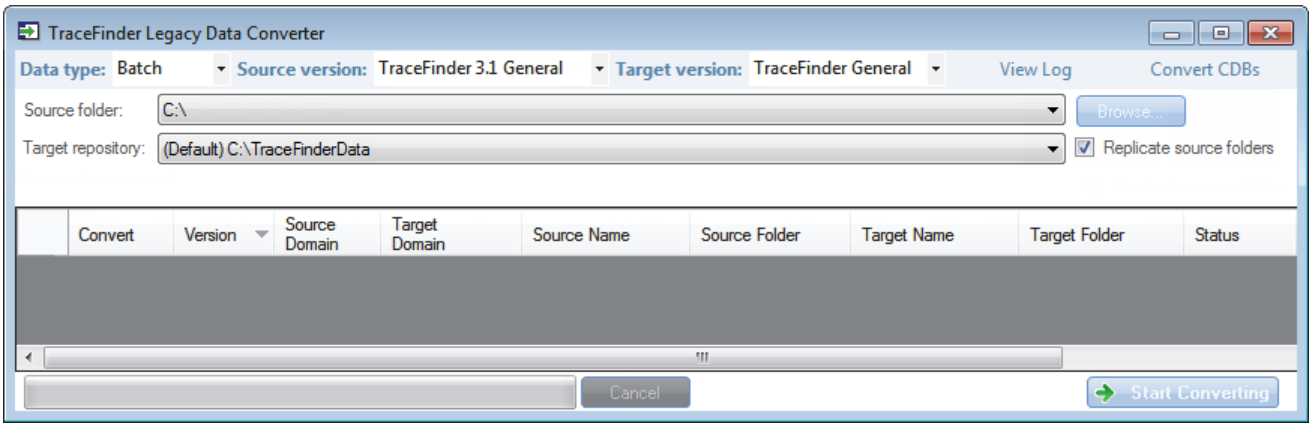
This section includes the following topics:

- Converting Methods
- Converting Batches
- Converting Method Templates
- Converting Batch Templates

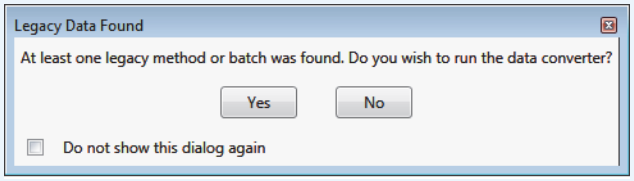
❖ **To open the TraceFinder Legacy Data Converter**

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

The TraceFinder Legacy Data Converter window opens.



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



Converting Methods

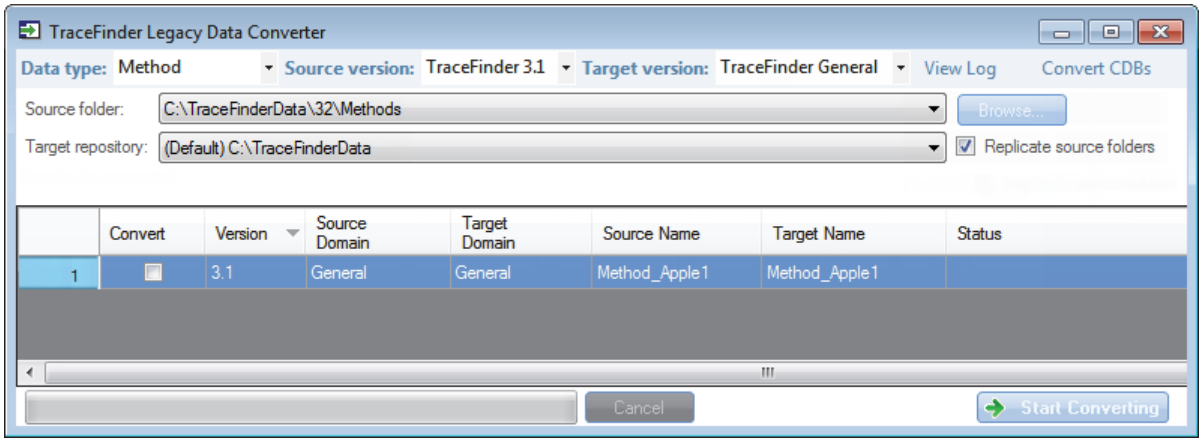
Use the data converter to convert legacy methods to TraceFinder 3.2 methods.

❖ 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 3.1 General configuration to the current General configuration. For a complete list of version compatibilities, see "Converting Methods" 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 "Converting Methods" 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 Start Converting.

   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 'QuanMethodData' from
XML file 'C:\TraceFinderData\32\Methods\Method_Apple1001\Metho
--- Saving master method
 --- Copying instrument method
--- Successfully converted master method from 'Method_Apple1'
 to 'C:\TraceFinderData\32\Methods\Method_Apple1\Method_Apple1.mmx'
-----------------------------------------------------------------------
========== Conversion completed. 1 total, 1 successful, 0 failed. =======
=======================================================================
```

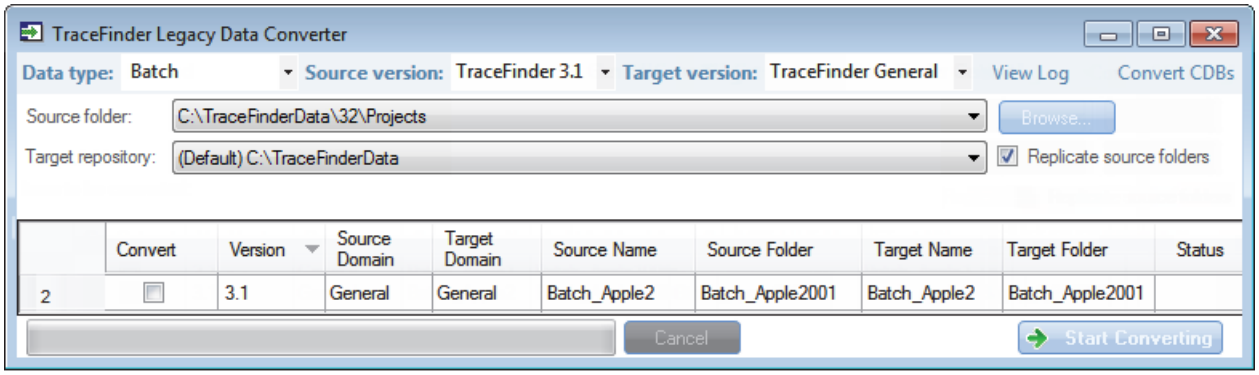
Converting Batches

Use the data converter to convert legacy batches to TraceFinder 3.2 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 3.1 General configuration to the current General configuration. For a complete list of version compatibilities, see "Converting Methods" 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 "Converting Methods" 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 Start Converting.

   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\32\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\32\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_Apple1\
--- 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\32\Projects\Batch_Appl
-----------------------------------------------------------------------------------------------
========== Conversion completed. 1 total, 1 successful, 0 failed. ==========
===============================================================================================
```

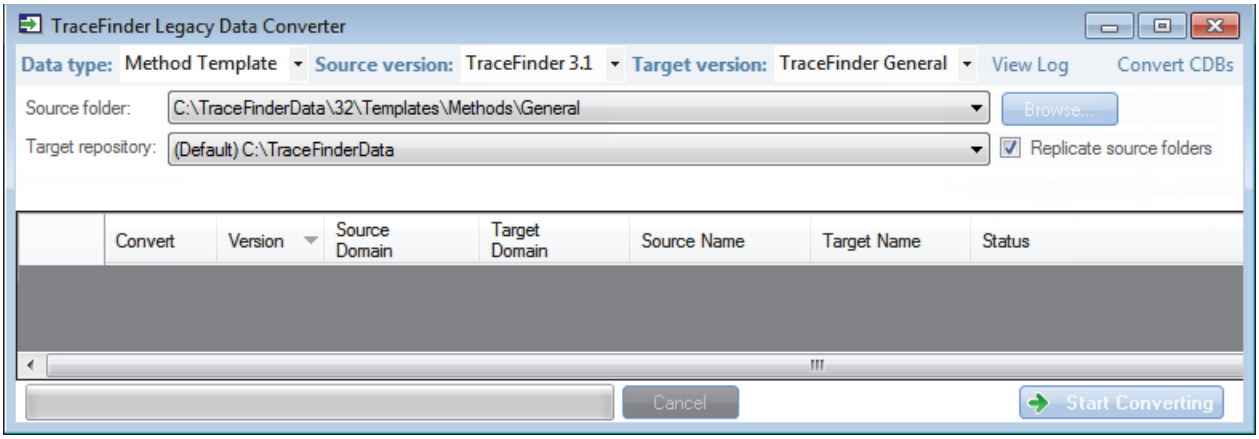
Converting Method Templates

Use the data converter to convert legacy method templates to TraceFinder 3.2 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 3.1 General configuration to the current General configuration. For a complete list of version compatibilities, see "Converting Methods" 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 "Converting Methods" 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

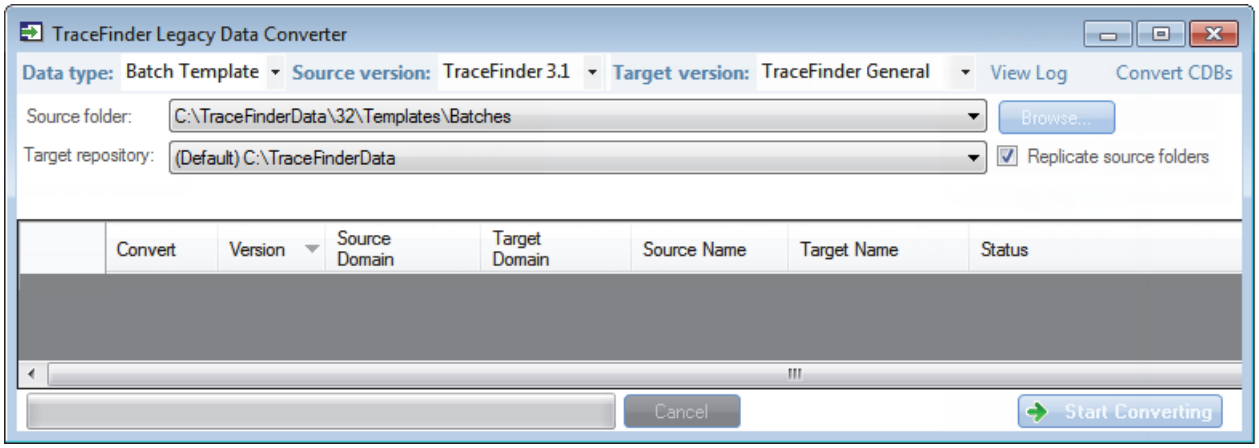
Use the data converter to convert legacy batch templates to TraceFinder 3.2 batch templates.

❖ To convert a batch template

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

   You can choose either LabForms batch templates or TraceFinder batch templates.

   The following example shows that you can convert batch templates from the TraceFinder 3.1 General configuration to the current General configuration. For a complete list of version compatibilities, see "Converting Methods" 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 "Converting Methods" 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 Start Converting.

   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\32\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 3.1 General to TraceFinder General
Archiving legacy batch template Apple as Apple_TF31
-- Converting batch template from 'C:\TraceFinderData\32\Templates\Batches\Apple\BatchData.l
-----------------------------------------------------------------------------------------
========= Conversion completed. 1 total, 0 successful, 1 failed. ==========
=================================================================================
```

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 7, "Using the Acquisition Mode."
Analysis	Opens the Analysis mode where you can review batches, batch data, reports, and local methods. See Chapter 8, "Using the Analysis Mode."
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 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."

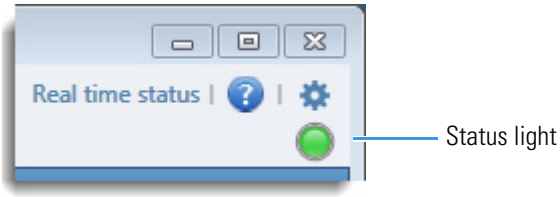
❖ To open the Administrator Console

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

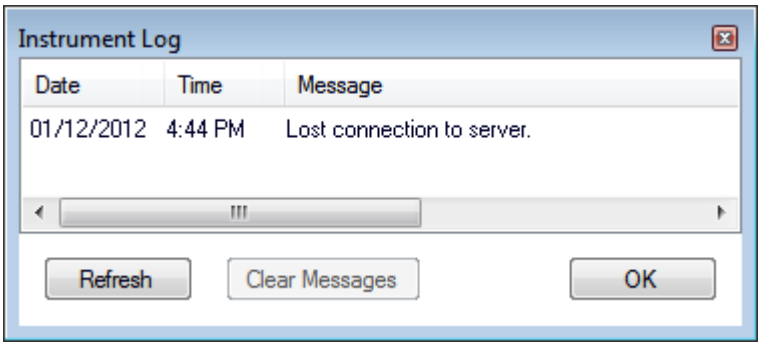
When user security is activated, you must have Administrator permissions to access the Administrator Console. Refer to the *TraceFinder Administrator Console User Guide*.

❖ 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 TraceFinder 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\3.2\Clinical\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.

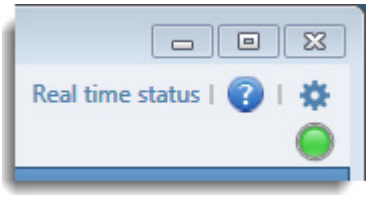
Green indicates that the instrument is ready.

Yellow indicates that the instrument is in standby mode.

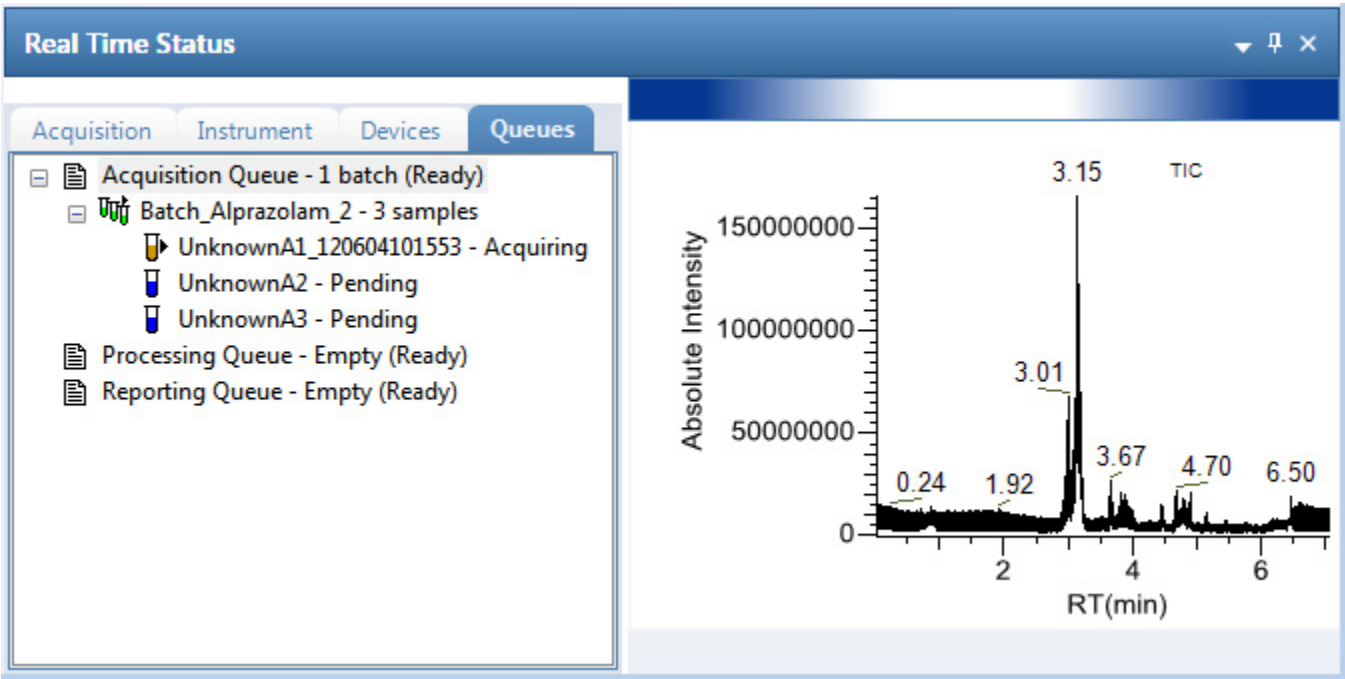
Red indicates that the instrument is turned off or no device is configured.

❖ 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 350.

TraceFinder Window Features

A TraceFinder window with user security for a user in the default LabDirector role has these functions.

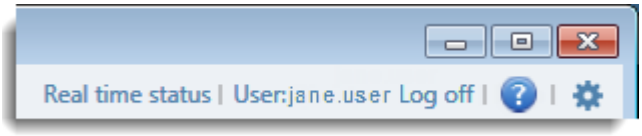


Table 5. TraceFinder window parameters

Parameter	Description
Real Time Status	Opens the Real Time Status pane for the current acquisition. The acquisition progress is displayed within the current mode window.
CurrentUserName	Displays the name of the current user. This is displayed only when user security is activated.
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.
Configuration Console	Opens the Configuration console where you can configure several options for using the TraceFinder application. See Chapter 3, "Using the Configuration Console."

3

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.

Contents

- Specifying Application Defaults
- Specifying Default Peak Detection Parameters
- Specifying Adducts
- Activating Optional Features
- Creating Custom Columns
- Creating Custom Flags
- Specifying the Reports

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 on 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.

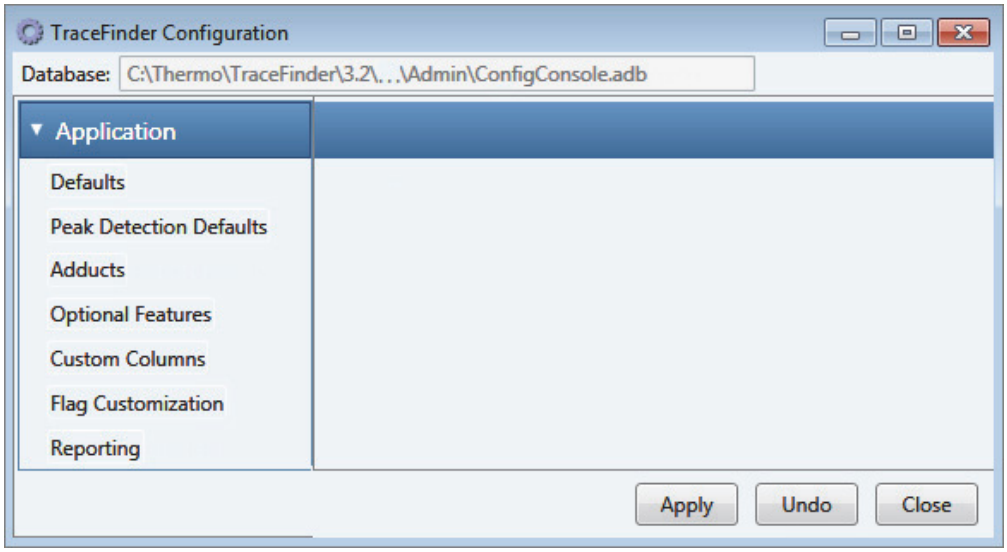


Table 6. Navigation pane functions in the Configuration console

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 35.
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 37.
Adducts	Use the Adducts view to specify the adducts that will be available for use in method development. See "Specifying Adducts" on page 52.
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 55.
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 66.
Reporting	Use the Reporting view to configure which reports are available to users. See "Specifying the Reports" on page 72.

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.

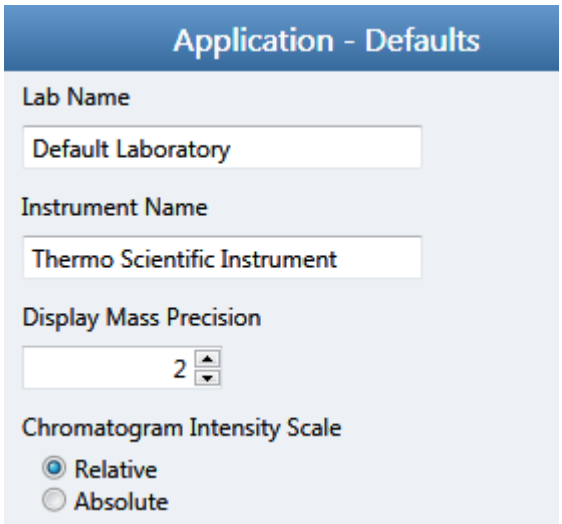
Follow these procedures:

- 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.



❖ 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 TraceFinder 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 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 TraceFinder 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.

This section includes 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 39.
- For parameter information about the Genesis detection algorithm, see "Genesis Detection Method" on page 42.
- For parameter information about the ICIS detection algorithm, see "ICIS Detection Method" on page 45.
- For parameter information about the Avalon detection algorithm, see "Avalon Detection Method" on page 48.

❖ 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 39.

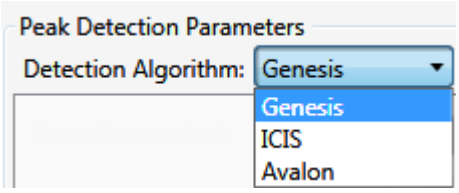
2. In the Mass Tolerance area, do the following:

   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. 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

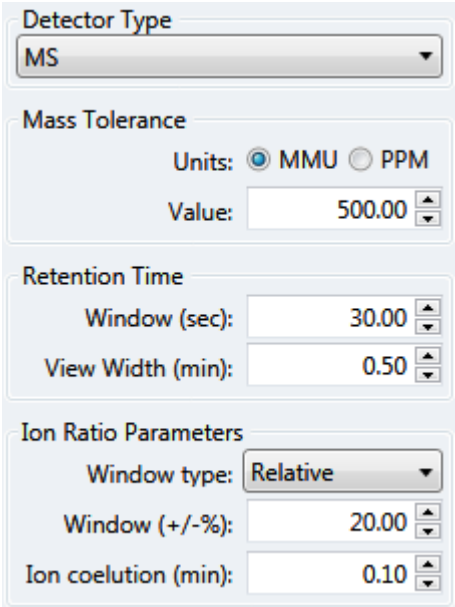


Table 7. Common peak detection parameters (Sheet 1 of 2)

Parameter	Description
Detector Type	MS: Mass spectrometer that ionizes sample molecules and then separates the ions according to their mass-to-charge ratio (m/z). 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. 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**. 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. 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.
Mass Tolerance	
Units	• (Default) MMU (millimass units) MMU is a static calculation to the extracted mass. • PPM (parts per million) PPM is a variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.
Value	Upper limit of MMU or PPM. Default: 500 Range: 0.1 through 50 000
Retention Time	
Window (sec)	Width of the window (in seconds) to indicate how far around the expected retention time the system will look for a peak apex.
View Width (min)	Viewable size (in minutes) of the ion chromatogram display. Changing the view width does not affect the process of peak detection; the TraceFinder application uses it only for graphical display.

Table 7. Common peak detection parameters (Sheet 2 of 2)

Parameter	Description
Ion Ratio Parameters	
Window Type	The absolute or relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	The acceptable ion ratio range.
Ion Coelution (min)	The maximum difference in retention time between a confirming ion peak and the quantification ion peak.

Genesis Detection Method

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

Figure 12. Genesis peak detection

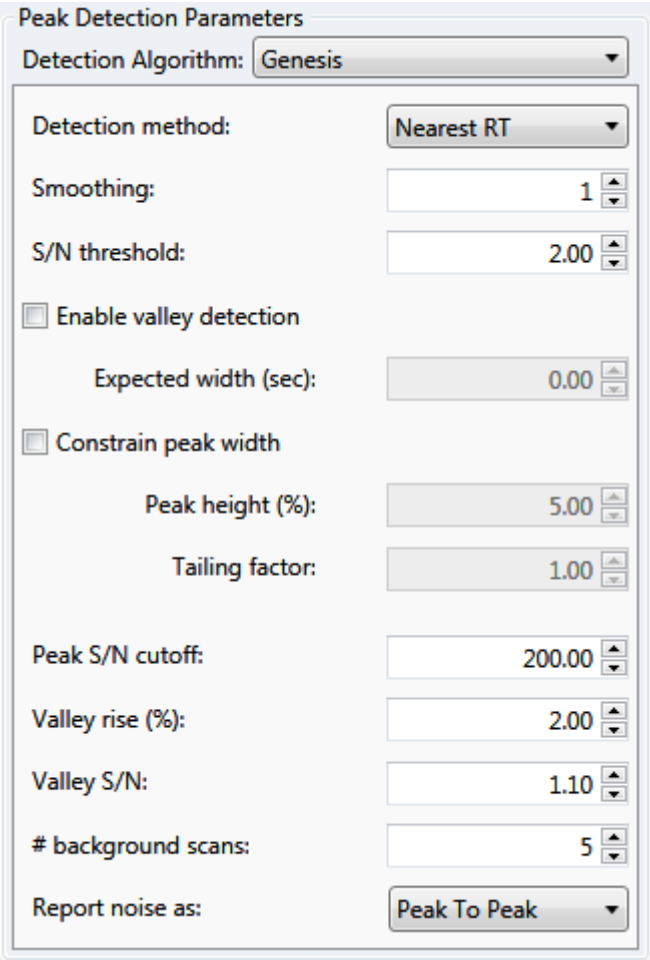


Table 8. Genesis peak detection parameters (Sheet 1 of 3)

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 8. Genesis peak detection parameters (Sheet 2 of 3)

Parameter	Description
Smoothing	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. Default: 1 Range: Any odd integer from 1 through 15 points
S/N threshold	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. Range: 0.0 to 999.0
Enable Valley Detection	Uses the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Expected Width (sec)	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. With valley detection enabled, any valley points nearer than the *expected width*/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the TraceFinder application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. Range: 0.0 to 999.0
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a 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. Range: 0.0 to 100.0%

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

Parameter	Description
Tailing Factor	Specifies the tailing factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0
Peak S/N Cutoff	Sets the peak edge to values below this signal-to-noise ratio. This test assumes it has found an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio. When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the TraceFinder application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 10000.0
Valley Rise (%)	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. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. When the trace exceeds rise percentage, the TraceFinder application applies valley detection peak integration criteria. This test is applied to both the left and right edges of the peak. Range: 0.1 to 500.0
Valley S/N	Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher. Default: 2.0 Range: 1.0 to 100.0
# Background Scans	Specifies the number of background scans performed by the TraceFinder application.
Report Noise As	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or peak-to-peak resolution threshold. Options are RMS or Peak To Peak.

ICIS Detection Method

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

Figure 13. ICIS peak detection

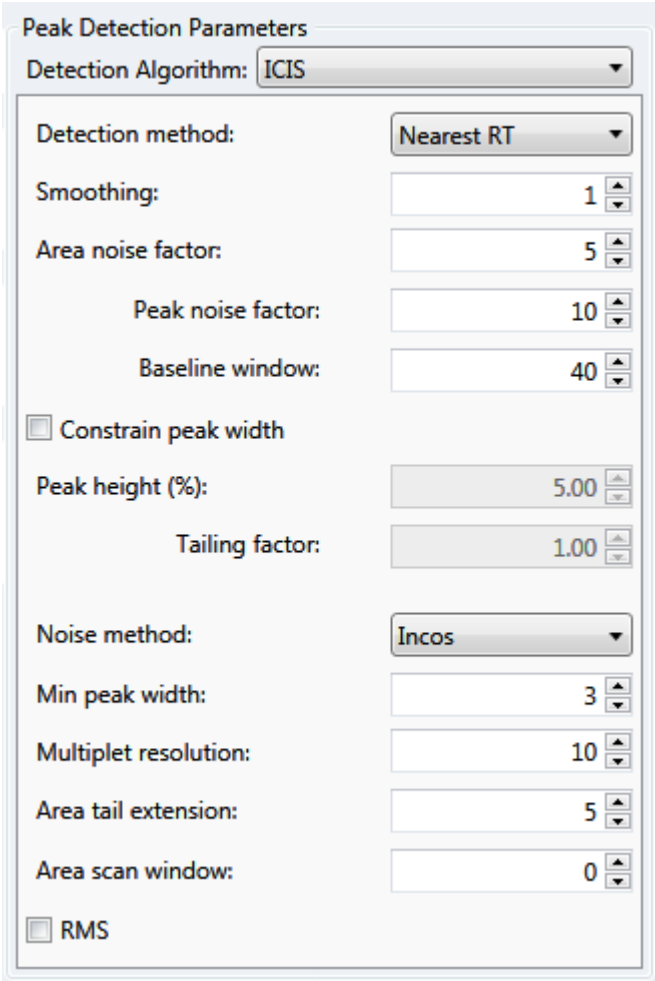


Table 9. ICIS peak detection parameters (Sheet 1 of 3)

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 9. ICIS peak detection parameters (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. The ICIS peak detection algorithm uses this value. Range: Any odd integer from 1 through 15 points Default: 1
Area Noise Factor	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. Range: 1 through 500 Default: 5
Peak Noise Factor	Specifies the noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value. Range: 1 through 1000 Default: 10
Baseline Window	Specifies that the TraceFinder application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 40
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box activates the Peak Height (%) and Tailing Factor options.
Peak Height (%)	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. Range: 0.0 to 100.0%
Tailing Factor	Specifies the tailing factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

Table 9. ICIS peak detection parameters (Sheet 3 of 3)

Parameter	Description
Noise Method	Specifies the noise method as INCOS or Repetitive. INCOS: Uses a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. Repetitive: Uses a multiple pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but the analysis takes longer.
Min Peak Width	Specifies the minimum number of scans required in a peak. The ICIS peak detection algorithm uses this value. Range: 0 to 100 scans Default: 3
Multiplet Resolution	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. Range: 1 to 500 scans Default: 10
Area Tail Extension	Specifies the number of scans past the peak endpoint to use in averaging the intensity. The ICIS peak detection algorithm uses this value. Range: 0 to 100 scans Default: 5
Area Scan Window	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. Range: 0 to 100 scans Default: 0
RMS	Specifies that the TraceFinder application calculate noise as RMS. By default, the application uses Peak To Peak for the noise calculation. RMS is automatically selected if you manually determine the noise region.

Avalon Detection Method

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

Figure 14. Avalon peak detection

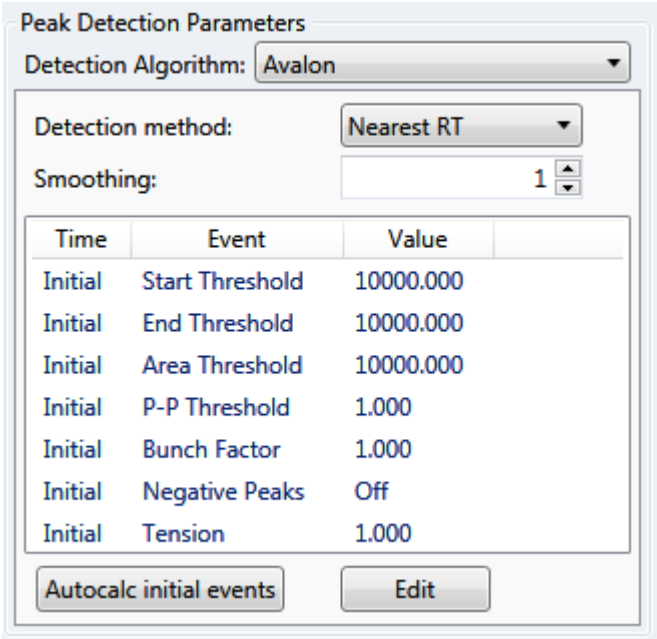


Table 10. Avalon peak detection parameters

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. Default: 1 Range: Any odd integer from 1 through 15 points
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

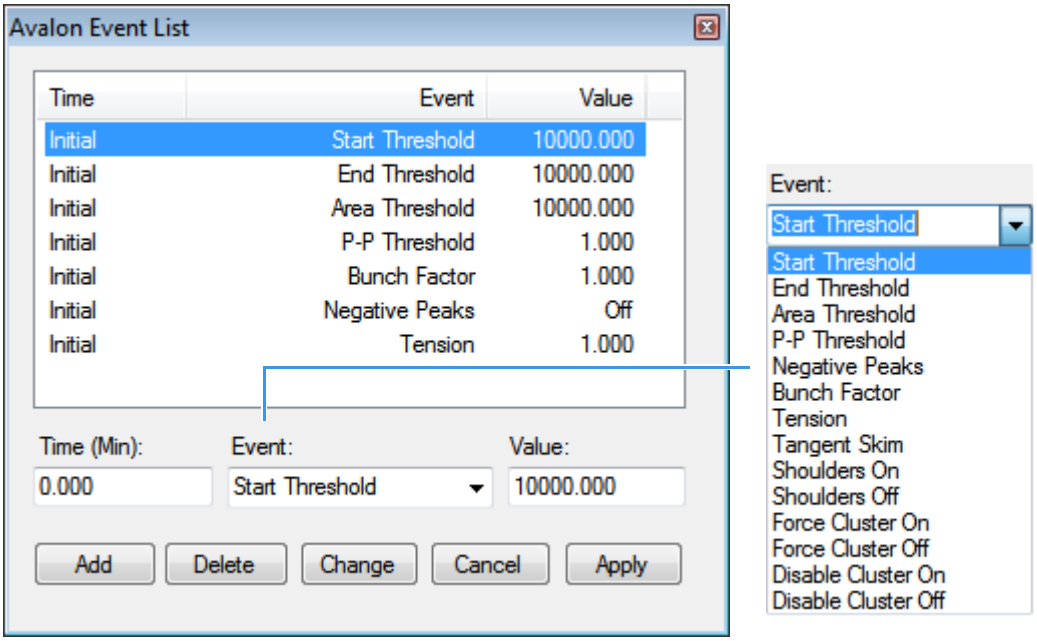


Table 11. Avalon Event List dialog box parameters

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

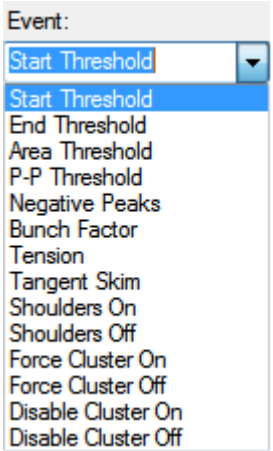


Table 12. Event type descriptions (Sheet 1 of 2)

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. Range: 0 to 999 999 999
End Threshold	Specifies the threshold at the end of a peak. The End Threshold is directly related to the RMS noise in the chromatogram. Range: 0 to 999 999 999
Area Threshold	Controls the area cutoff. Any peaks with a final area less than the area threshold will not be detected. This control is in units of area for the data. Range: 0 to 999 999 999
P-P Threshold	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. Range: 0.1 to 99.99
Negative Peaks	Permits detection of a negative going peak. Automatically resets after finding a negative peak. Valid values: On or Off
Bunch Factor	Specifies the number of points grouped together during peak detection. This event controls the bunching of chromatographic points during integration and does not affect the final area calculation of the peak. A high bunch factor groups peaks into clusters. Range: 0 to 999

Table 12. Event type descriptions (Sheet 2 of 2)

Event type	Description
Tension	Controls how closely the baseline should follow the overall shape of the chromatogram. A lower tension traces the baseline to more closely follow changes in the chromatogram. A high baseline tension follows the baseline less closely, over longer time intervals. Range: 0 to 999.99 minutes
Tangent Skim	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. Range: 0 to 1
Shoulders On	Allows peak shoulders to be detected (peaks which are separated by an inflection rather than a valley) Sets a threshold for the derivative.
Shoulders Off	Disables peak shoulder detection. Range: 0 to 50
Force Cluster On	Forces the following peaks to be treated as a cluster (single peak).
Force Cluster Off	Ends the forced clustering of peaks.
Disable Cluster On	Prevents any peaks from being clustered.
Disable Cluster Off	Permits clusters to occur again.

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.

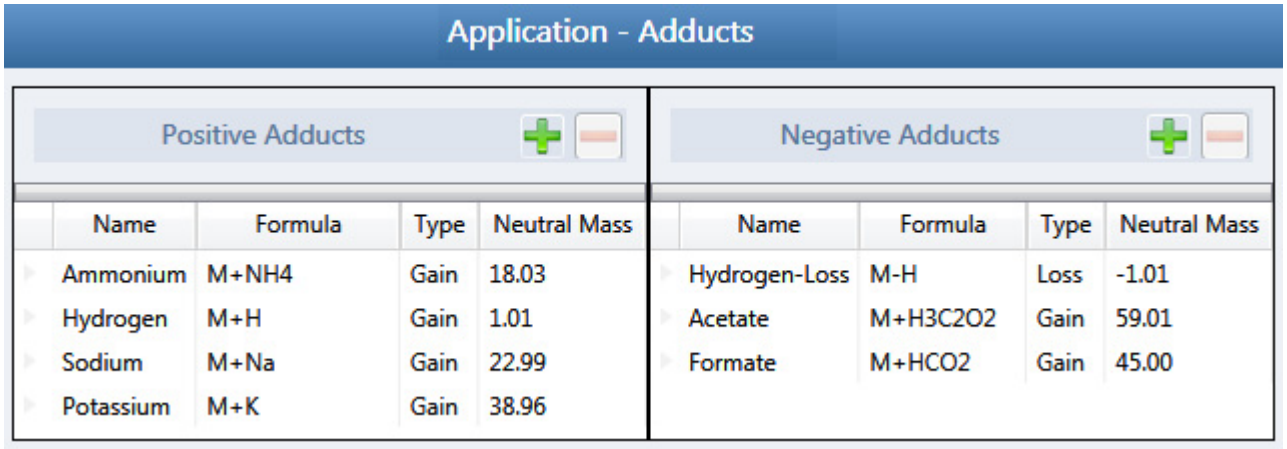
Follow these procedures:

- 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.



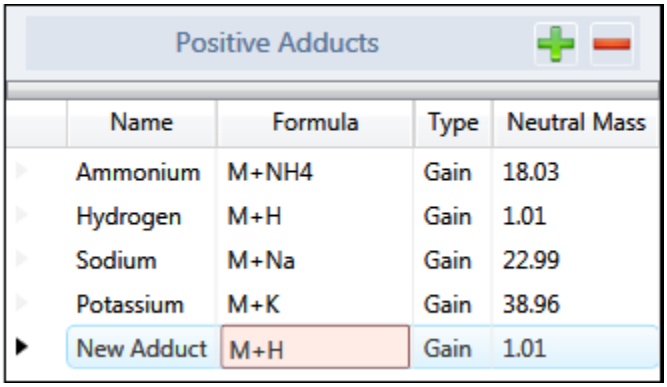
Name	Formula	Type	Neutral Mass
Ammonium	M+NH4	Gain	18.03
Hydrogen	M+H	Gain	1.01
Sodium	M+Na	Gain	22.99
Potassium	M+K	Gain	38.96

Name	Formula	Type	Neutral Mass
Hydrogen-Loss	M-H	Loss	-1.01
Acetate	M+H3C2O2	Gain	59.01
Formate	M+HCO2	Gain	45.00

❖ 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+H2O]+ 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 TraceFinder 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.

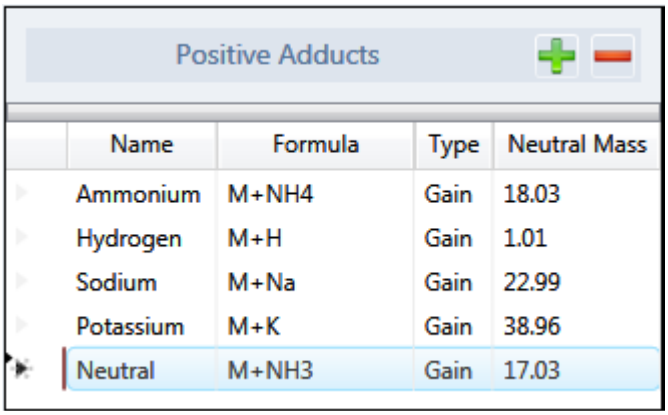
New Adduct	NH3	Gain	1.01

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

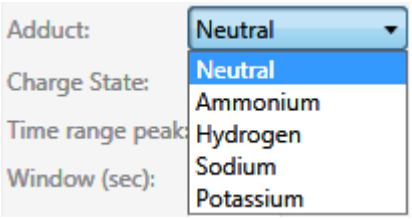
   You cannot change the type or neutral mass, but the application will correctly calculate these values later.

4. Press ENTER.

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



   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.

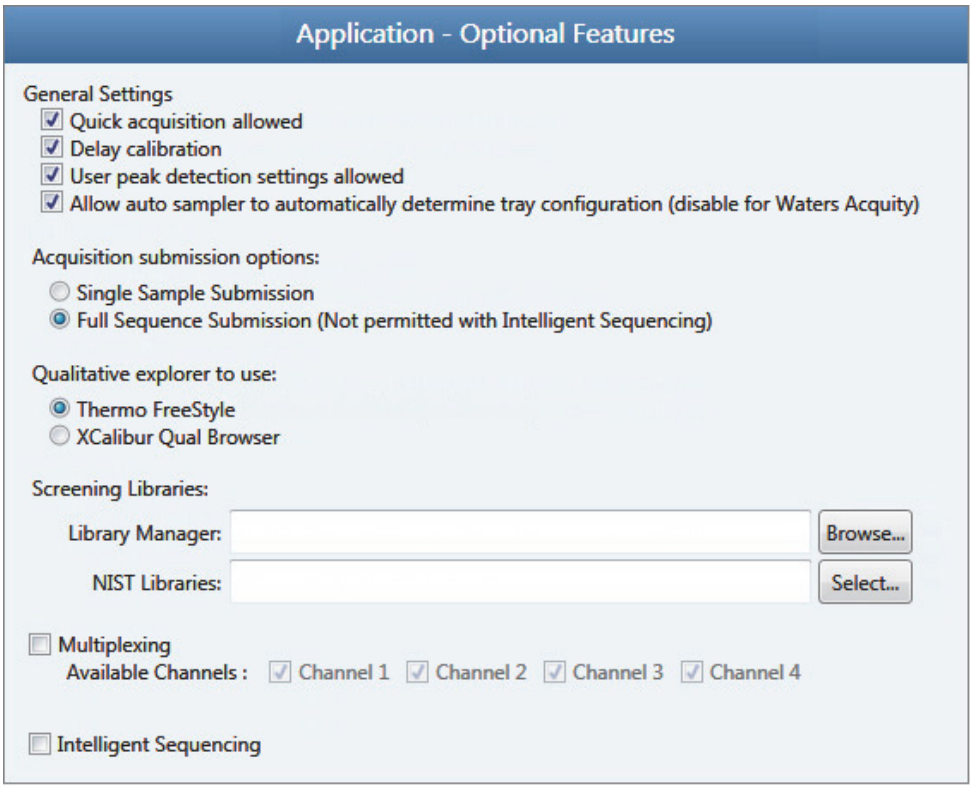
Use the Application – Optional Features view to activate the following features:

- Quick Acquisition
- Delay Calibration
- User Peak Detection Settings
- Auto Sampler Tray Configuration
- Acquisition Submission Options
- Qualitative Explorer
- Screening Libraries
- Multiplexing
- Intelligent Sequencing

❖ To open the Optional Features page

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

The Application – Optional Features page opens.



Quick Acquisition

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

Note The Quick Acquisition feature is not available when you activate Multiplexing. See "Multiplexing" on page 61.

❖ 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. For instructions about modifying the peak detection parameters, see "To modify the peak detection settings" on page 472.

❖ **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.

Auto Sampler 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 TraceFinder 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**.

   The application immediately applies 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 **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 16.

Screening Libraries

Use the screening libraries specified here 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. For more information about how you can use screening libraries in a target screening method, see Screening Libraries in a Target Screening Method.

When you specify the Library Search Type on the Processing page for a screening method, you choose either the Library Manager search type or the NIST search type. See "Editing the Acquisition Page" on page 275.

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

❖ To specify a Library Manager screening library

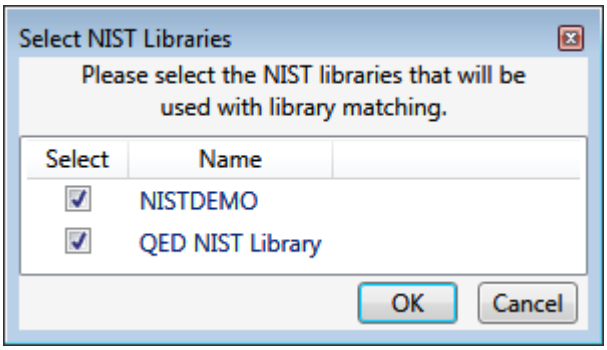
Click **Browse** and locate the library that you want to use for screening.

> **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, while 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 205. 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 279.

- 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.

Multiplexing

The application uses multiplexing features in the Acquisition mode when you specify channels for a sample in a batch (see "Defining the Sample List" on page 326) or monitor an acquisition (see "Devices Page" on page 354).

❖ **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 following optional features are not available:
- Quick Acquisition
- Single Sample Submission

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.

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 "Column Display" on page 373).

You can use the Field Chooser to display and change the order of these columns in the Data Review Samples pane (see "Samples Pane" on page 415).

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.

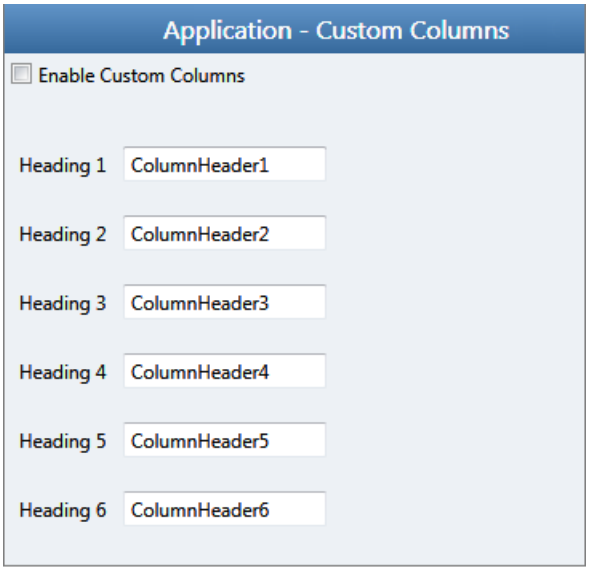
Follow these procedures:

- 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.



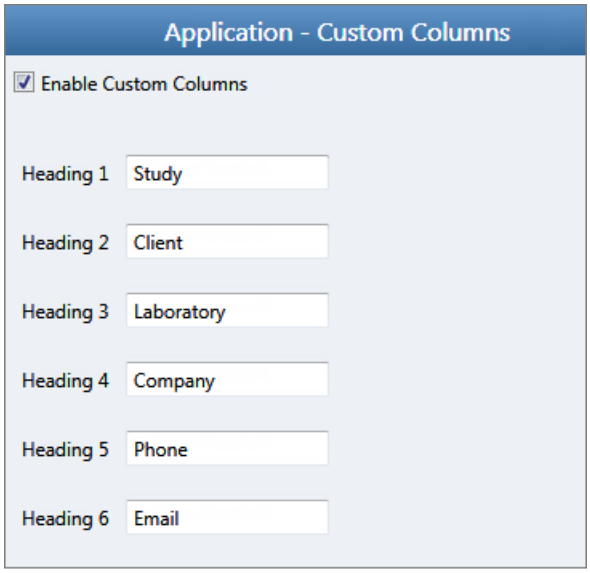
The Enable Custom Columns check box controls both the creation of custom columns on new batches and the display of custom columns on the Modify Columns dialog box in the Batch View and the Field Chooser in the Data Review Samples pane.

❖ 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.

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.**

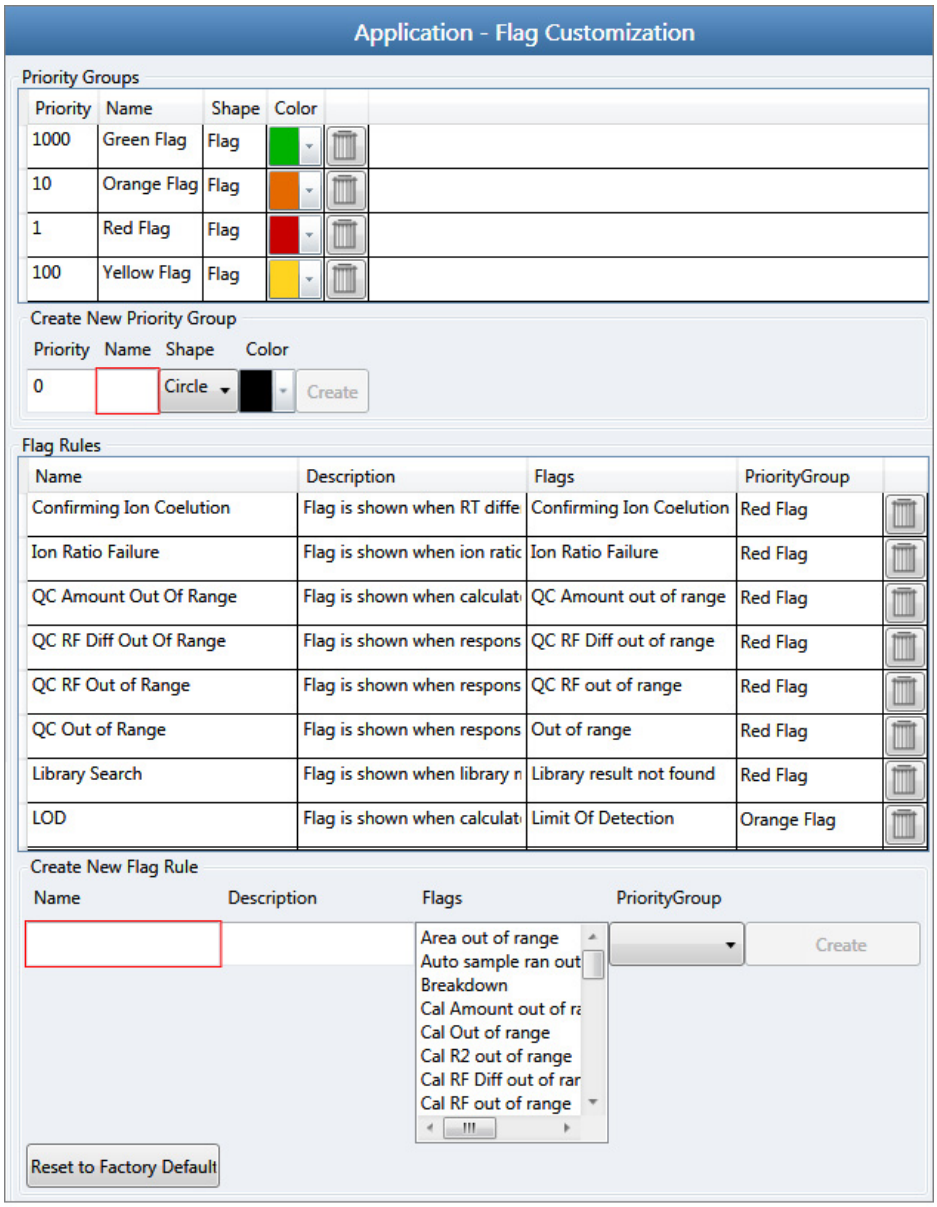
Creating Custom Flags

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.

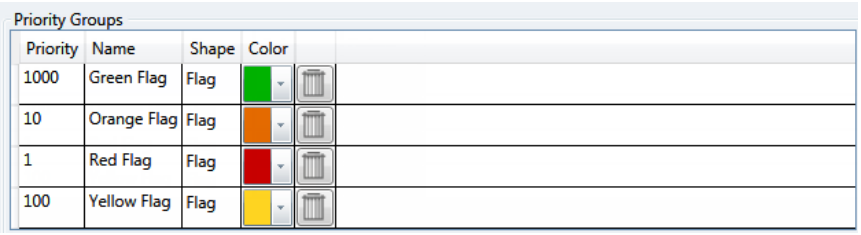


Follow these procedures:

- To edit priority groups
- To create a new priority group
- To edit flag rules
- To create a new flag rule
- To remove all customization

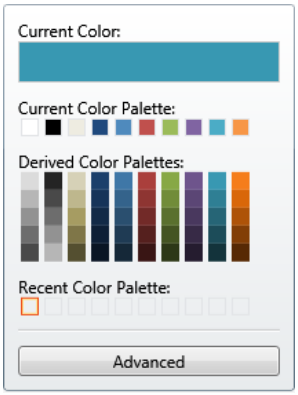
In the Priority Groups area, you can edit the priority, shape, or color of a flag. You can also delete a flag or create a new one. You cannot change the name of a flag.

❖ To edit priority groups



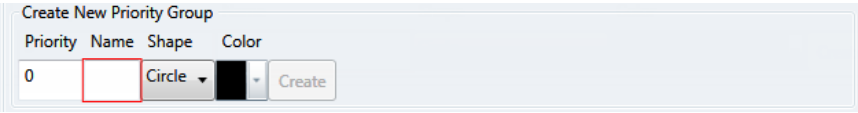
1. Do any of the following:
   - Select the default Priority value and type a new value.

     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.

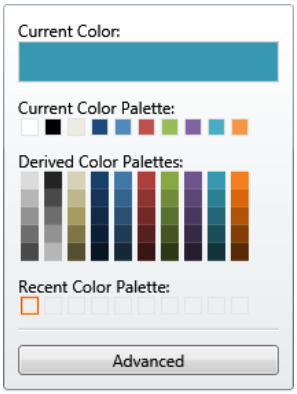
❖ To create a new priority group



1. In the Priority box, type a value.

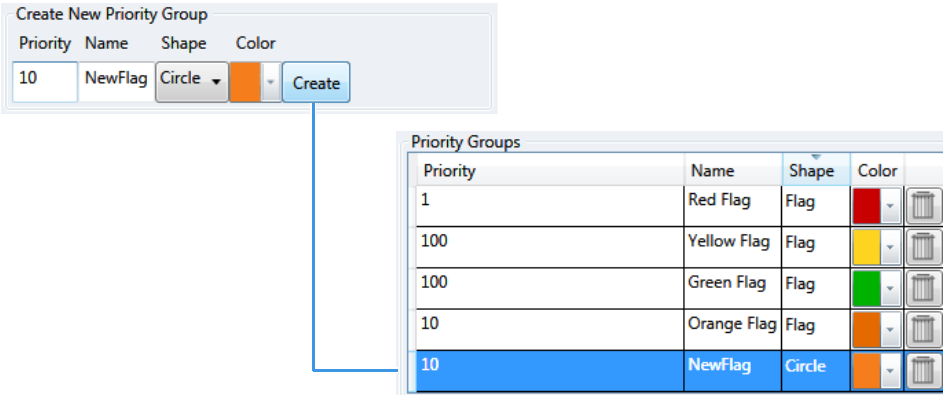
   You can enter positive or negative numbers. The lower the number, the higher the priority.

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 70.
6. Click **Create**.

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



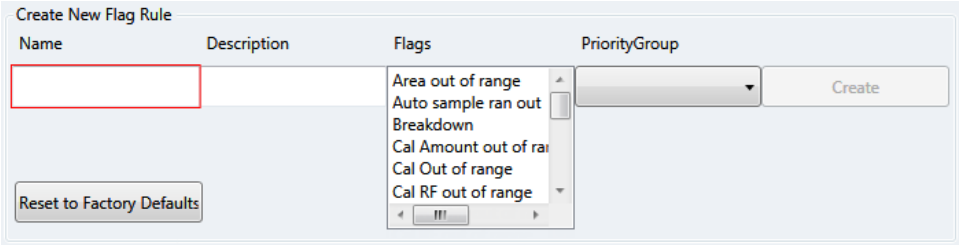
❖ To edit flag rules

> **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



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 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 68.
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.

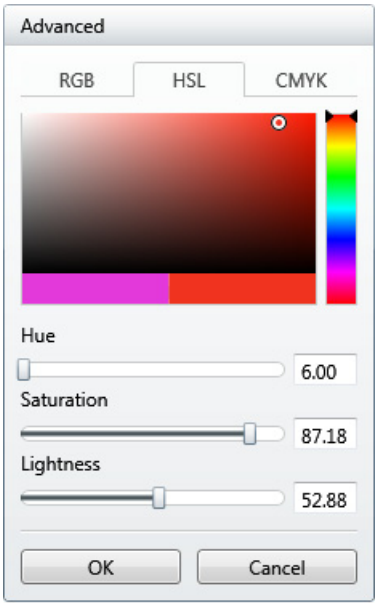
Advanced Dialog Box

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

Figure 17. Advanced RGB colors

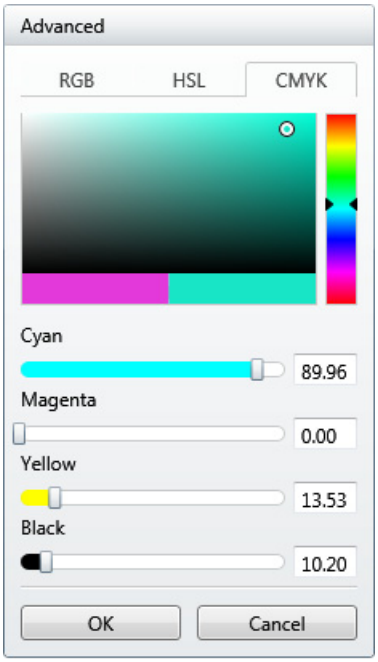
With the Red/Green/Blue (RGB) color palette, you can select a color with a specific RGB value, as displayed on a computer monitor.

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 – Reporting 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.

Follow these procedures:

- To open the Application – Reporting view
- To specify which reports are available

❖ To open the Application – Reporting view

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

The Application – Reporting view opens.

❖ 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 TraceFinder application.

Reports

The application can generate any of the following reports.

Figure 20. Reports

Application - Reporting

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

4

Using the Common Features of the Method Development Mode

This chapter includes method development tasks common to both quantitative and screening methods.

Contents

- Working with the Compound Database
- Working with Instrument Methods

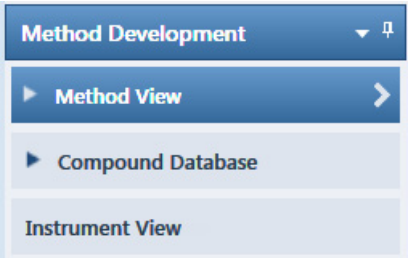
For information about creating either a quantitation method or a target screening method, see the appropriate chapter:

- Chapter 5, "Using the Method Development Mode for Quantitation Methods."
- Chapter 6, "Using the Method Development Mode for Screening Methods."

❖ To access the Method Development mode

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 for a quantitation method, see "Opening a Master Method" on page 122 (Chapter 5).

For descriptions of all the features in the Method Development navigation pane for a screening method, see "Opening a Master Method" on page 270 (Chapter 6).

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, this section also contains the following topics:

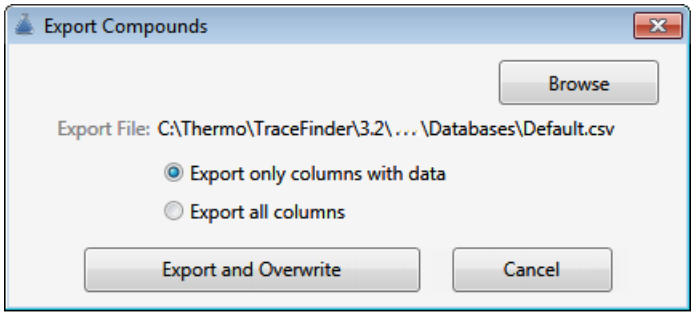
- Compound Database Names Mapped to CSV Column Names
- Data Columns with Default Values

❖ 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** to save the changes 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 112.

   - **Export All Columns**: Writes all columns to the CSV file, including columns that contain no data for any compound.

4. Click **Export and Overwrite**.

   The application stores the database as

   …\Thermo\TraceFinder\3.2\Clinical\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-acethyldeoxynivalenol	SRM	339.1
5	15-acethyldeoxynivalenol+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 109.

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 TraceFinder application replaces the data in that column with default values. For a list of default values, see "Data Columns with Default Values" on page 112.

❖ 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** to save the changes 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\32\Methods*Methodname**.xml

> **Note** If you have neither a TSQ, an ISQ, a Q Exactive, a TSQ Endura™, nor a 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.

For examples of exported mass lists, "Mass Data Formats" on page 81.

❖ 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** to save the changes 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 3.1 Legacy CDB
- ExactFinder™ 2.0 CDB
- .include-masses

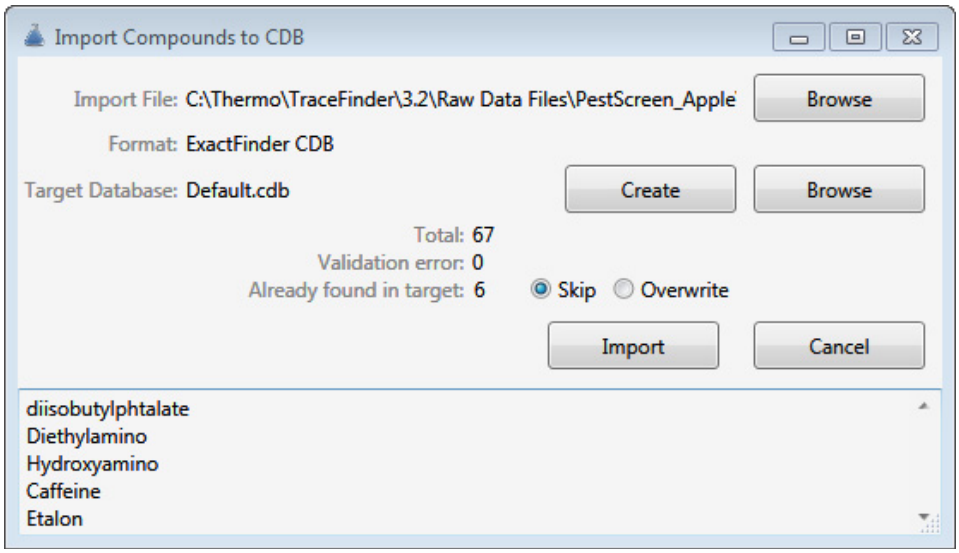
IMPORTANT Before you import data from a CSV file, verify that the following required columns have data for each compound. These columns have no default values and must have a value before you can import CSV data into the TraceFinder compound database:

- 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 83.

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**.

–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.

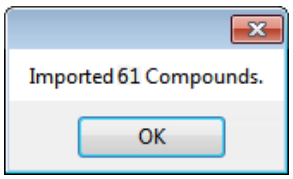
6. (Optional) Select one of these options:

   - **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 TraceFinder 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 TraceFinder application writes the mass data to the following file:

…\TraceFinderData\32\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 TraceFinder application writes the mass data to the following file:

…\TraceFinderData\32\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 TraceFinder application writes the mass data to the following file:

…\TraceFinderData\32\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 TraceFinder 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 TraceFinder application writes the mass data to the following file:

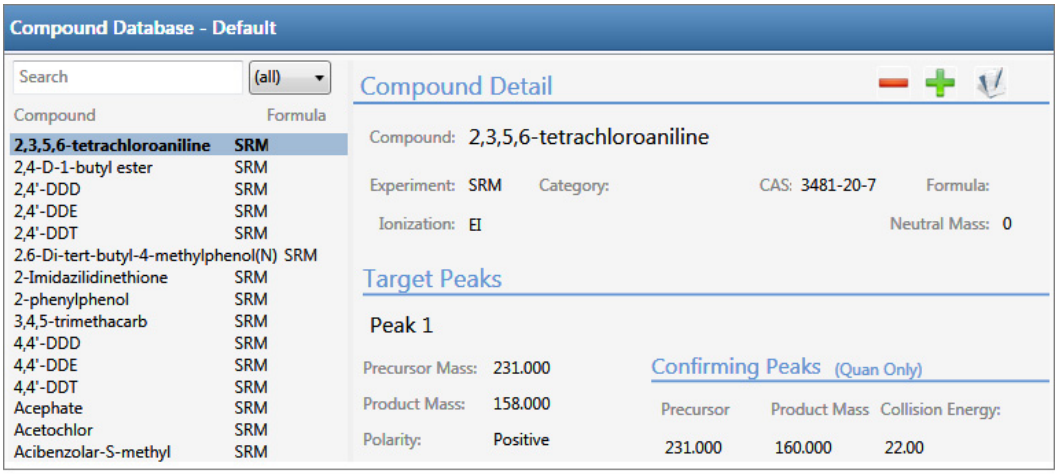
…\TraceFinderData\32\Methods*Methodname**Methodname*.xml

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 TraceFinder 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 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

This section includes the following topics:

- Sorting Compounds in the Database
- Editing Compounds in the Database

Figure 22. Compound Detail page for SRM experiments

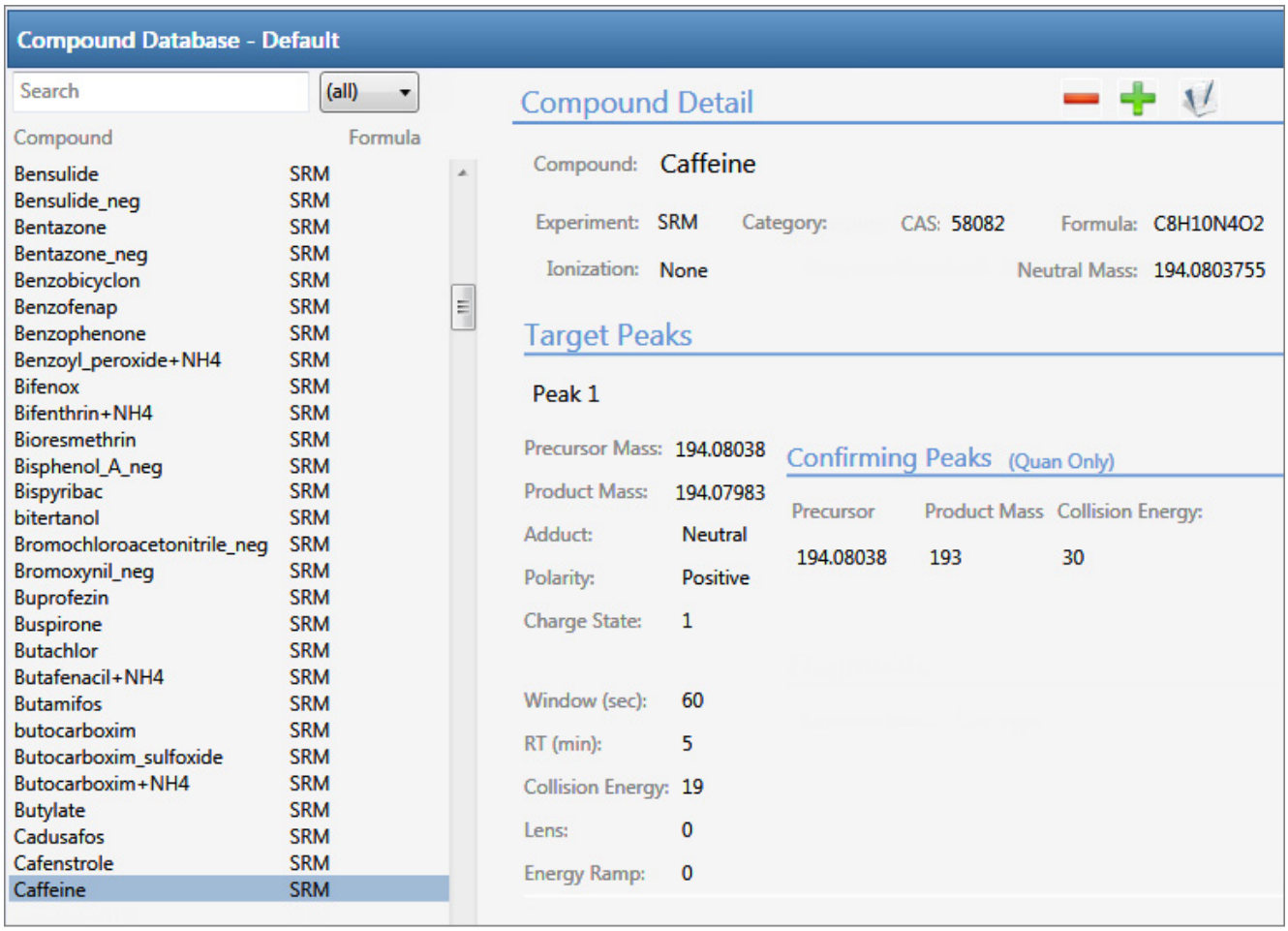


Figure 23. Compound Detail page for SIM experiments

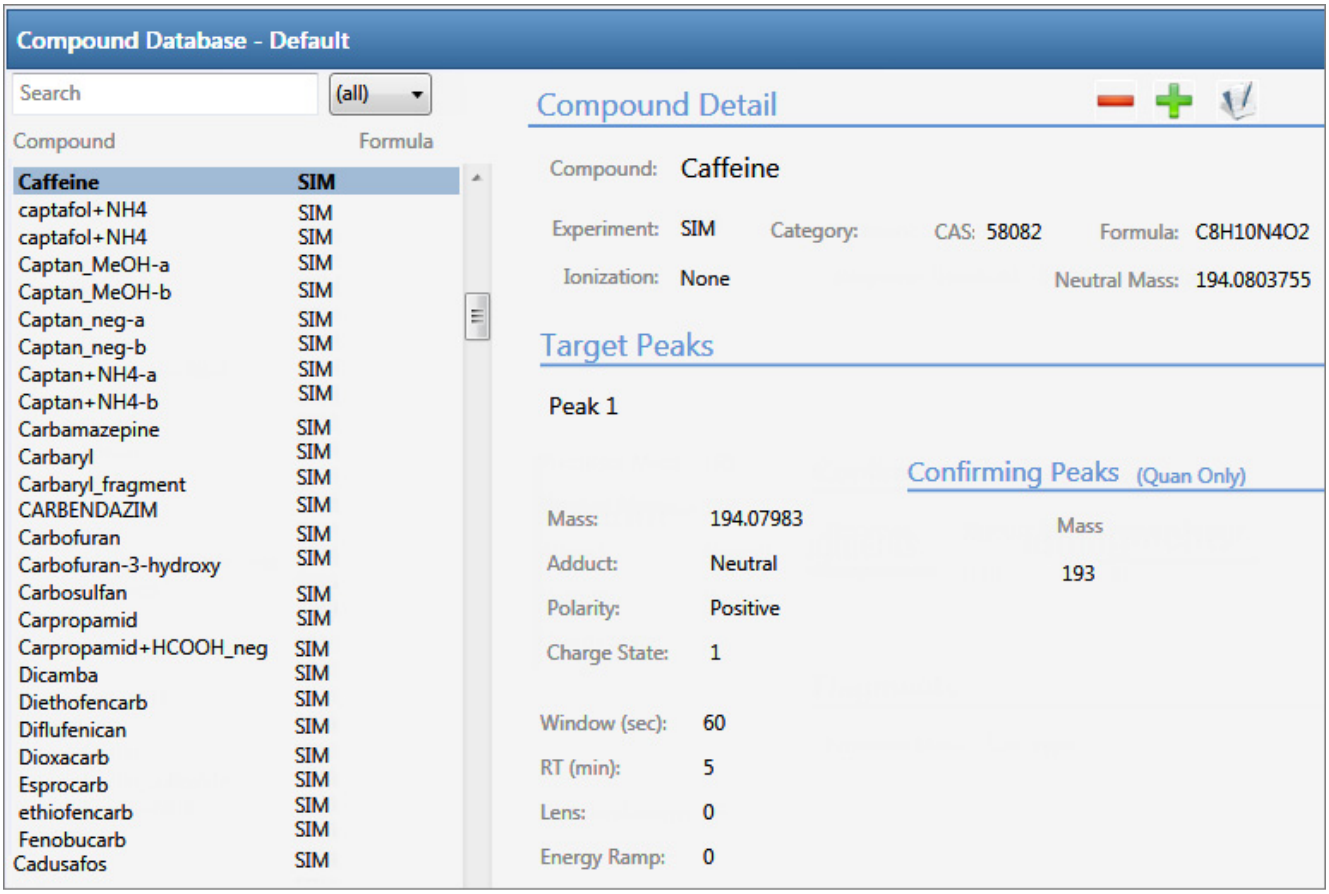
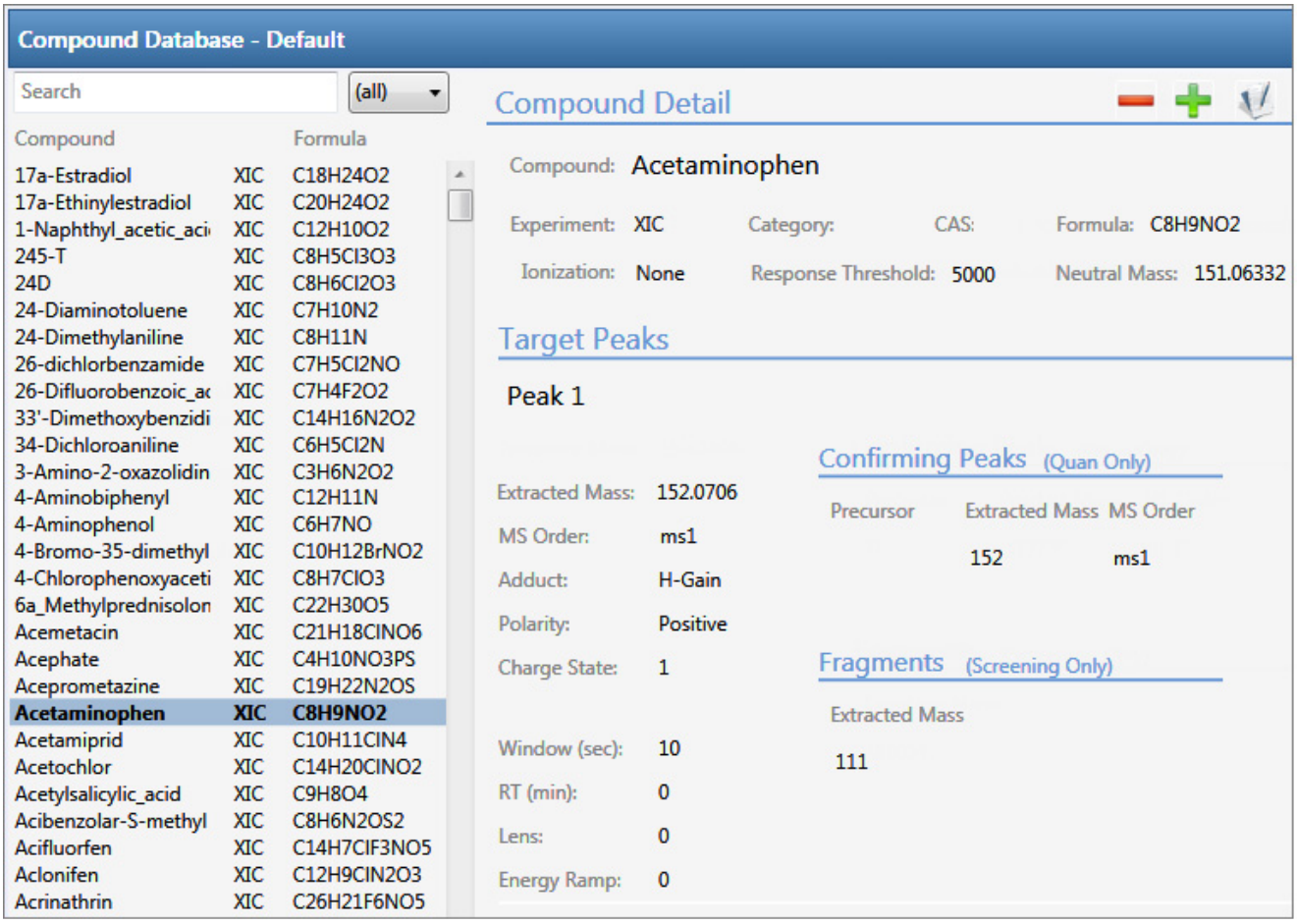
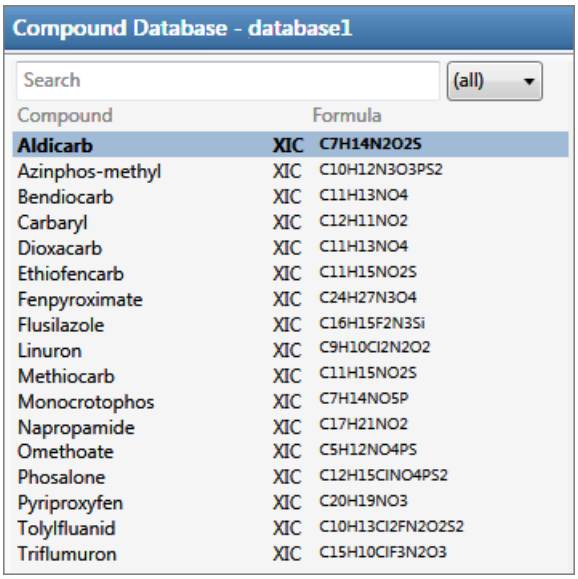


Figure 24. Compound Detail page for XIC experiments



Sorting Compounds in the Database

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



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 (all) list.

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

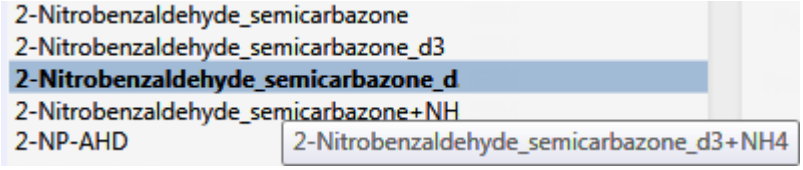
- SRM: Selected Reaction Monitoring
- XIC: Extracted Ion Chromatogram
- SIM: Single Ion Monitoring

For detailed descriptions of each experiment type, see “Experiment Types” on page 106.

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

In 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 106.

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 101.
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, .

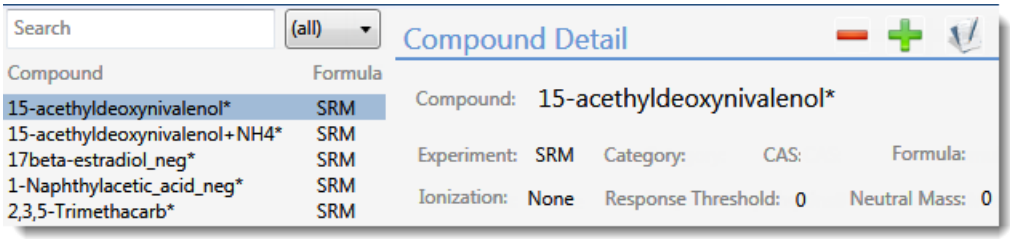
IMPORTANT After you complete the edits for the compounds, the header in the Compound Database page marks the database name with an asterisk, indicating that the database is not saved. To save the database with your compound changes, choose **File > Save Compound Database** from the main menu.

❖ 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



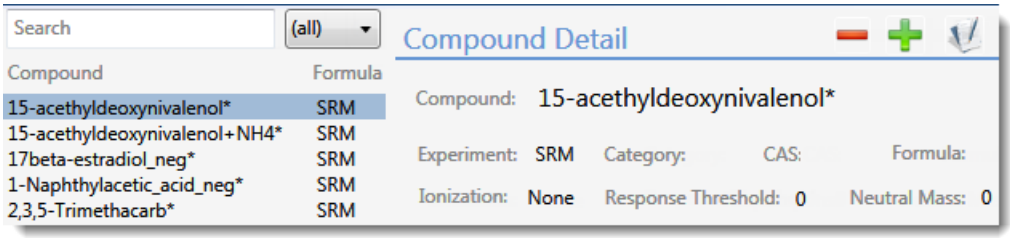
2. Click the **Delete Selected Compounds** icon, .

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.



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

   The application makes the compound parameters editable and displays the

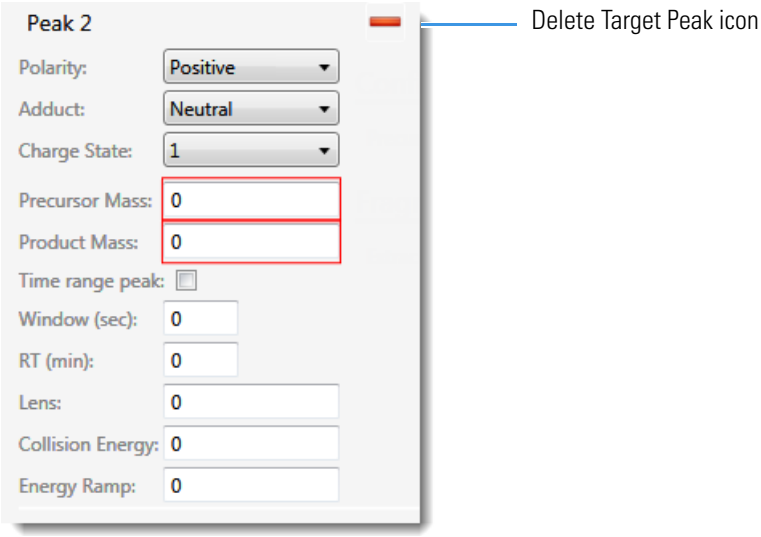
   Add icon, , so that you can add target peaks, confirming peaks, and fragments to the compound details.

> **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 106.

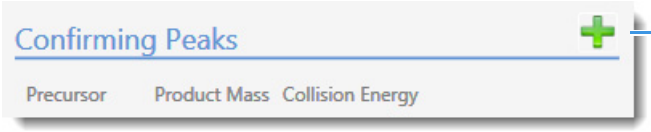
   For a list of required and optional parameters, see the list of "Compound Parameters" on page 101.

   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.

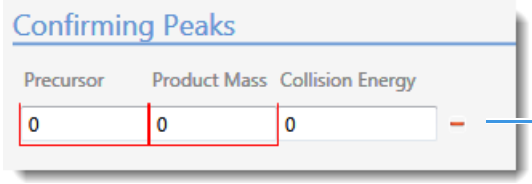
❖ To add a confirming peak to a target peak

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



Add Confirming Peak icon

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



Delete Confirming Peak icon

2. Type the required values for the confirming peak.

   The required confirming peak values differ for each experiment type. See "Experiment Types" on page 106.

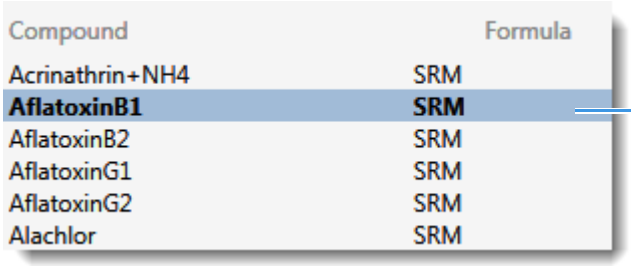
   For a list of required and optional parameters, see "Compound Parameters" on page 101.

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.

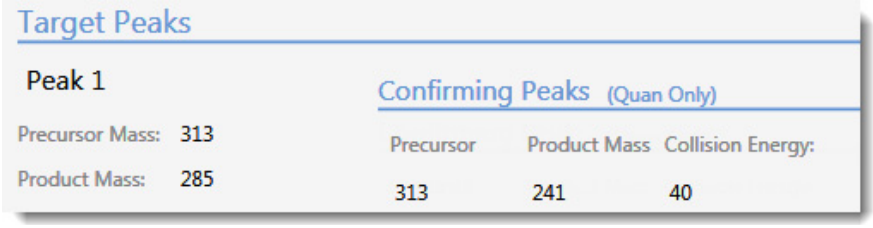
❖ To copy target peaks from one compound to another

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

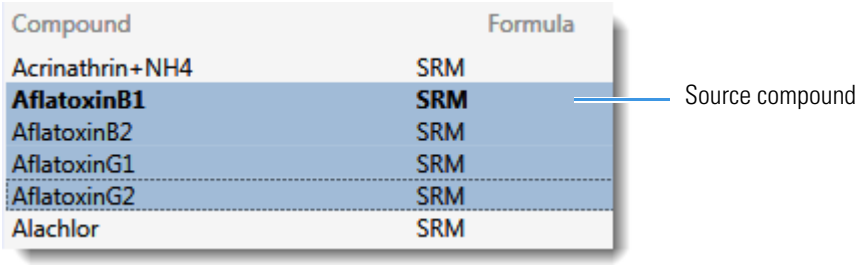


Source compound

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

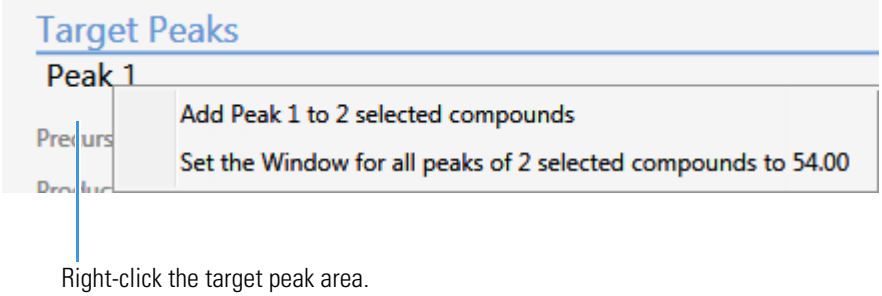


3. In the compounds list, keep the source compound selected and use the SHIFT or CTRL keys to select the compounds that you want to copy the target peak to.



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.



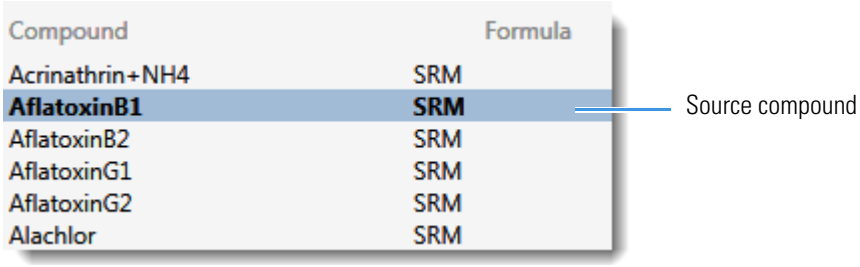
The application reports that the peak was copied to the specified number of compounds.

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

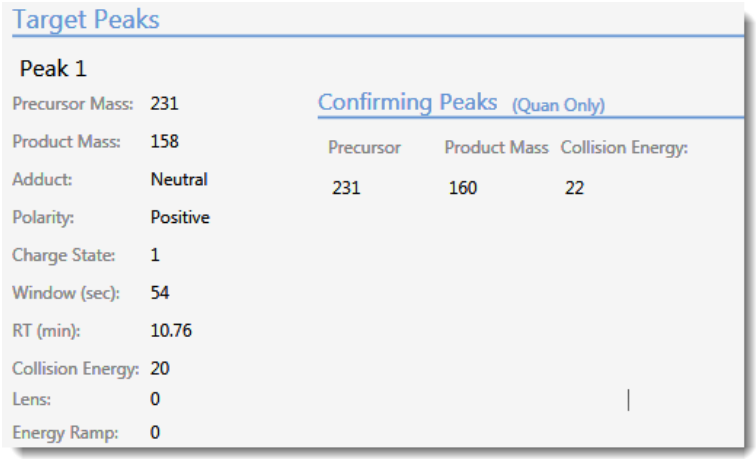
5. Click **OK**.

❖ To copy window values from one peak to another

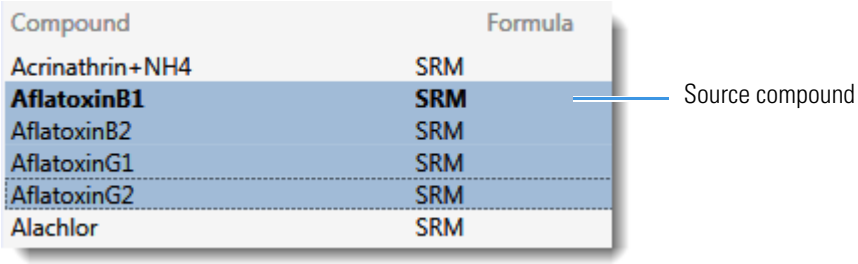
1. In the compounds list, select the compound with the window value that you want to copy.



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

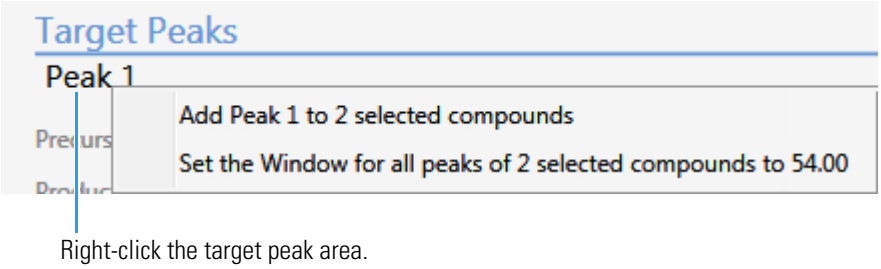


3. In the compounds list, keep the source compound selected and use the CTRL key to select the compounds that you want to copy the window to.



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 **Set the Window for All Peaks of *selectedCompounds* to *windowValue*** from the shortcut menu.



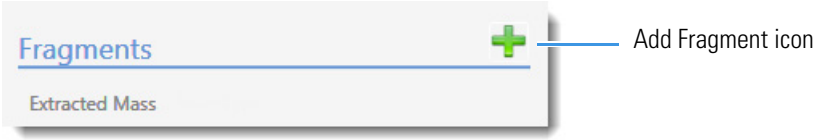
The application reports that the retention time and window were copied to the specified number of compounds, including the source compound when it has multiple peaks.

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.

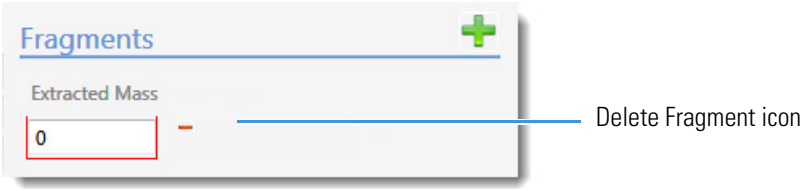
5. Click **OK**.

❖ 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.

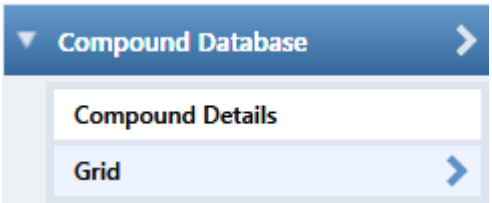
- There must be at least one compound in the compound database to view the Grid page.
- There are no empty columns on the Grid page. There must be at least one value for a parameter in the compound database or that parameter column is not displayed.

> **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.

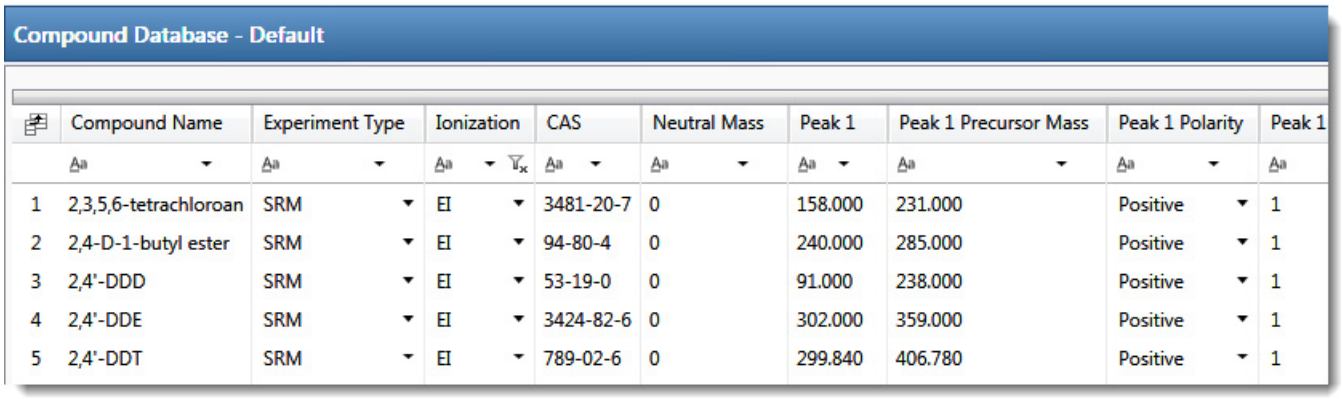
On the Grid page, you can import compounds into the database, add compounds to or remove compounds from the database, add target or confirming peaks to a compound, or remove target or confirming peaks from a compound.

❖ 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 101.

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.

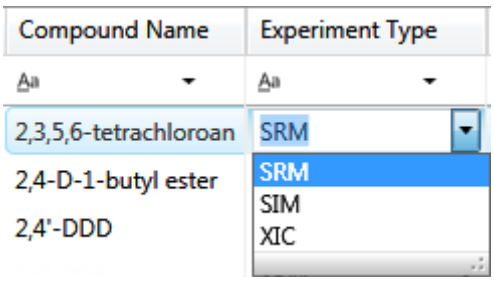
When you edit a value in the Formula column, the application calculates the *m/z* for the precursor and product masses.

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.



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.

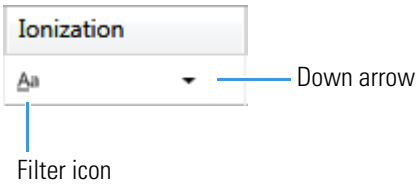
   The application sorts the grid by ascending column values (alphabetically or numerically).

> **Note** Columns with alphanumeric values sort from 1–*n* and then A–Z.

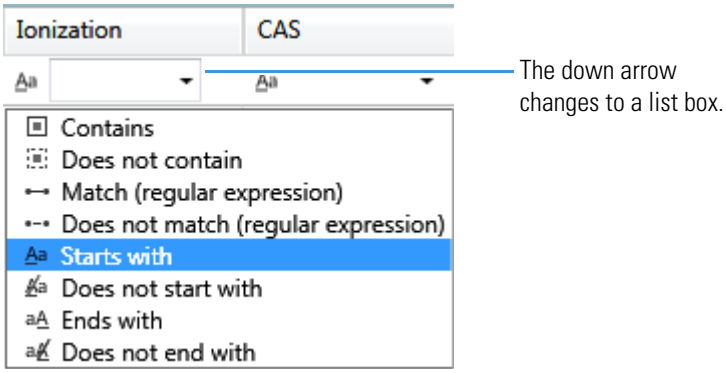
2. Click the header a second time to sort by descending column values.

❖ To organize compounds by column data

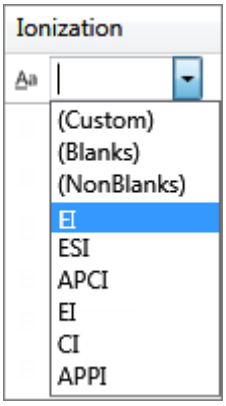
1. In the banner at the top of the column, click the filter icon.



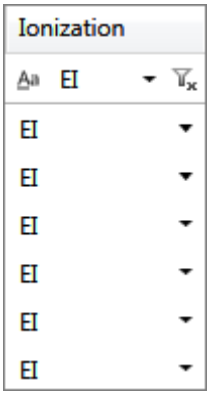
2. Select one of the filtering options, for example, **Starts With**.



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.



Compound Parameters

The Compound Detail page and the Grid page occasionally use different names for the same parameter. The Parameter column in Table 13 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 13. Compound parameters (Sheet 1 of 5)

Parameter	Description
(Compound Detail page) Compound (Grid page) Compound Name	Alphanumeric name assigned to the compound.
(Compound Detail page) Experiment (Grid page) Experiment Type	Experiment type: SRM, XIC, or SIM. For details about the differences, see "Experiment Types" on page 106.
Category	(Optional) Alphanumeric identifier.
CAS	The Chemical Abstract Service (CAS) number that the TraceFinder application matched with the compound.
(Compound Detail page) Formula (Grid page) Chemical Formula	Chemical formula for the compound. Used to calculate the neutral mass for the compound.
Ionization	Alphanumeric identifier. Valid values: None, ESI, APCI, EI, CI, or APPI Default: None
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. Available only for XIC experiments. Default: 5000 Range: 1000 or greater
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.

Table 13. Compound parameters (Sheet 2 of 5)

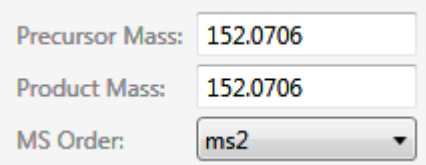
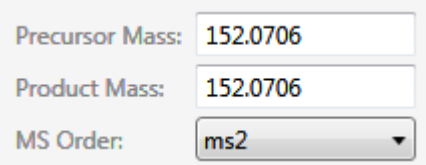
Parameter	Description
Target Peaks	
(Compound Detail page) Precursor Mass (Grid page) Peak *n* Precursor Mass	The mass-to-charge ratio (*m/z*) of a target peak. The location of the center of a target precursor ion peak in mass-to-charge ratio units. In confirming peaks, the precursor mass is the same as the target peak precursor mass. Default: 0.0 Range: 10.000 to 2999.999 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 (Grid page) Peak *n*	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. Default: 0.0 Range: 10.000 to 2999.999 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) Mass (Grid page) Peak *n* 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.

Table 13. Compound parameters (Sheet 3 of 5)

Parameter	Description
(Compound Detail page) Extracted Mass (Grid page) Peak *n* 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. Default: 0.0 Range: 10.000 to 2999.999 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 (Grid page) Peak *n* Polarity	Positive or Negative
(Compound Detail page) Adduct (Grid page) Peak *n* Adduct	The adducts specified in the configuration file. To add or remove adducts from the default lists, see "Specifying Adducts" on page 52. 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, NH4, H, Na, K Default Negative valid values: Neutral, H, H3C2O2, HCO2 Default: Neutral
(Compound Detail page) Charge State (Grid page) Peak *n* 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. Valid values: 1 through 10 Default: 1
MS Order	The confirming peaks come from the same scan (MS1) or are fragments from an adjacent scan (MS2). Available only for XIC experiments.

Table 13. Compound parameters (Sheet 4 of 5)

Parameter	Description
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. Range: 0.00 to 499.50 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
(Compound Detail page) RT (min) (Grid page) Peak *n* RT	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. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
(Compound Detail page) Lens (Grid page) Peak *n* Lens	Range: –400 to 400
(Compound Detail page) Collision Energy (Grid page) Peak *n* Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00
(Compound Detail page) Energy Ramp (Grid page) Peak *n* Energy Ramp	Range: 0.00 to 200.00
Confirming Peaks	Confirming peak parameters are used only in quantitative methods.
(Compound Detail page) Precursor (Grid page) Peak *n* Confirming *n* 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. Default: 0.0 Range: 10.000 to 2999.999

Table 13. Compound parameters (Sheet 5 of 5)

Parameter	Description
(Compound Detail page) Product Mass (Grid page) Peak *n* Confirming *n*	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. Default: 0.0 Range: 10.000 to 2999.999
(Compound Detail page) Mass (Grid page) Peak *n* Confirming *n* Extracted 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.
(Compound Detail page) Extracted Mass (Grid page) Peak *n* Confirming *n* 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. Default: 0.0 Range: 10.000 to 2999.999
(Compound Detail page) Collision Energy (Grid page) Peak *n* Confirming *n* Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00
(Compound Detail page) MS Order (Grid page) Peak *n* Confirming *n* MS Order	Specifies whether the confirming peaks or fragments come from the same scan (MS1) or an adjacent scan (MS2). Available only for XIC experiments.
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 (*m/z*) units. Available only for XIC experiments. Default: 0.0 Range: 10.000 to 2999.999

Experiment Types

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

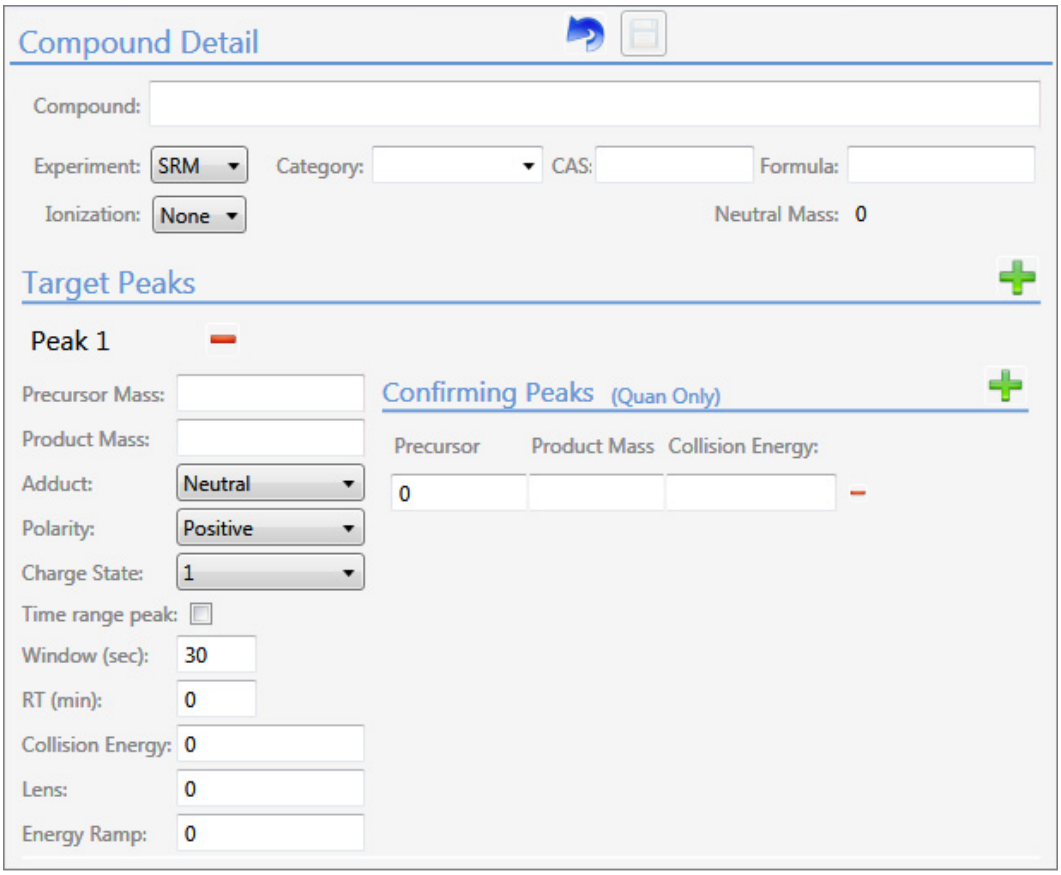
Each of these experiment types uses a different structure for the mass filter. The target peak and confirming peak parameters for each experiment type are defined in the "Compound Parameters" on page 101.

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.

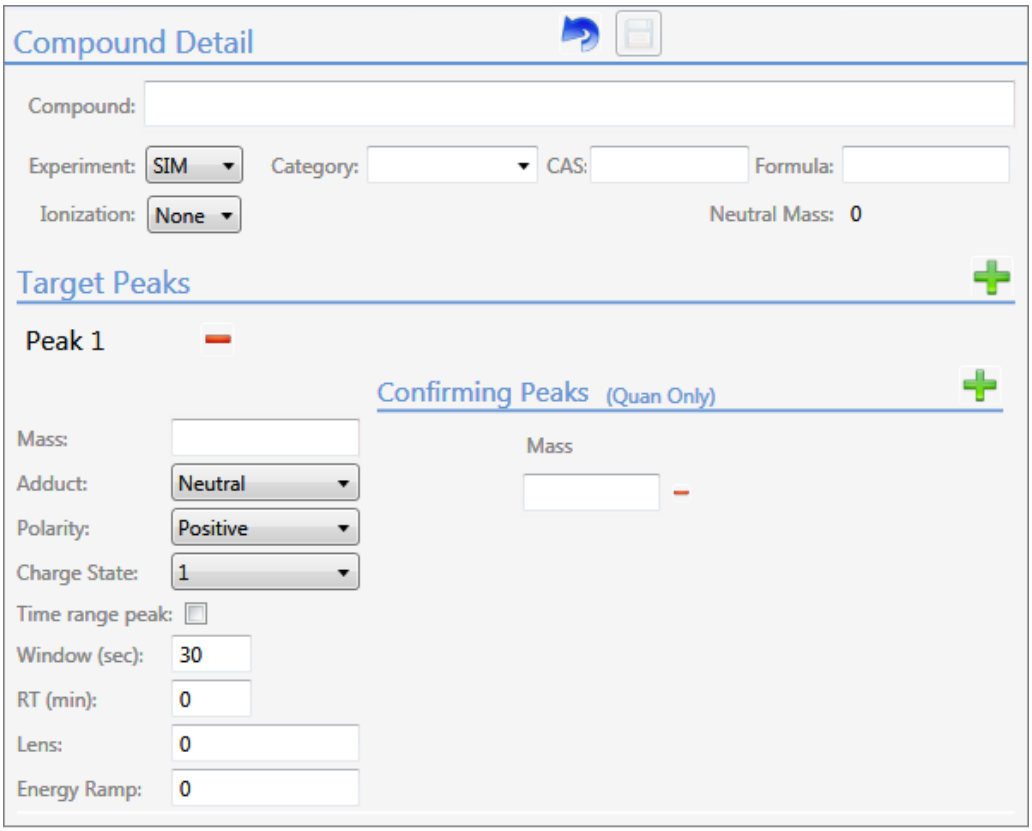
Confirming peaks include values for precursor mass, product mass, and collision energy.



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.

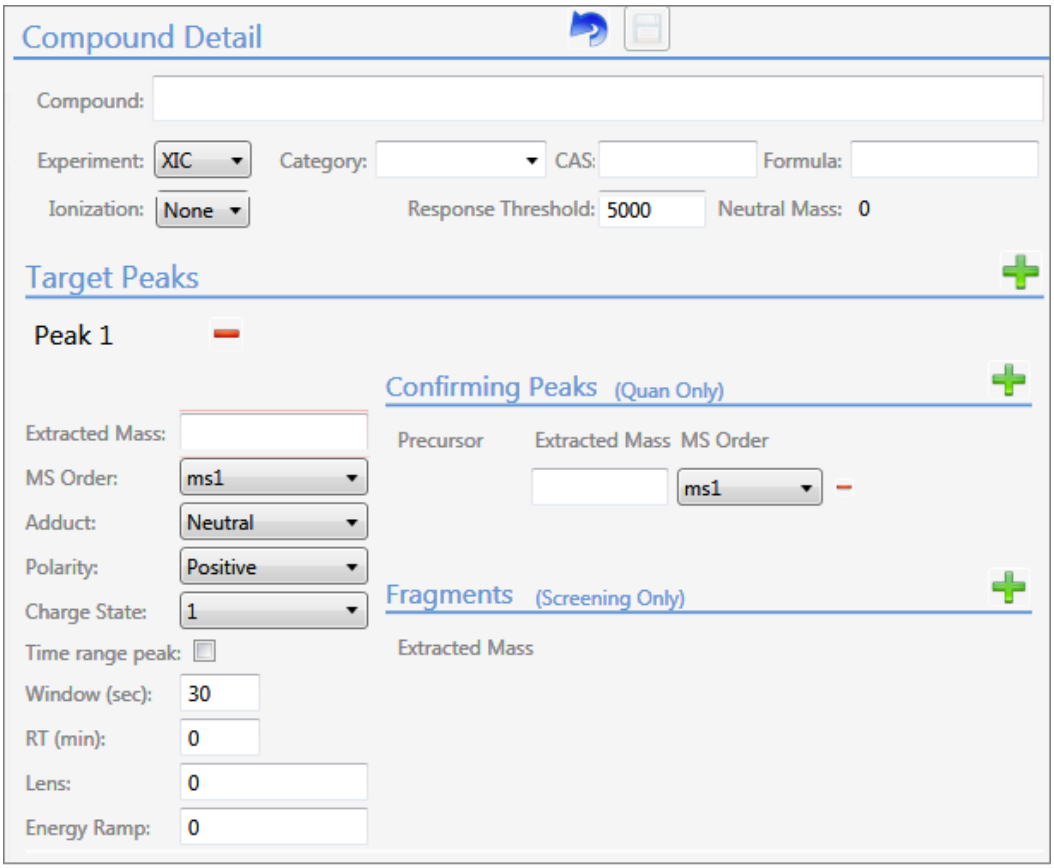
Confirming peaks include an extracted mass value.



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

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

Table 14. 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 (Grid page) Peak *n* Adduct	Adduct
Polarity	Polarity
(Compound Detail page) Charge State (Grid page) Peak *n* Charge State	ChargeState
Window	Window
(Compound Detail page) RT (min) (Grid page) Peak *n* RT	RT
(Compound Detail page) Collision Energy (Grid page) Peak *n* Collision Energy	CollisionEnergy (SRM only)
(Compound Detail page) Lens (Grid page) Peak *n* Lens	Lens
Energy Ramp	EnergyRamp
Confirming Peaks	
(Compound Detail page) Precursor (Grid page) Peak *n* Confirming *n* Precursor	Confirm Precursor (SRM and XIC only)

Table 14. CSV column names for compound parameters (Sheet 3 of 3)

Compound database parameter	CSV column heading
(Compound Detail page) Product Mass (Grid page) Peak *n* Confirming *n*	Confirm Product (SRM only)
(Compound Detail page) Mass (Grid page) Peak *n* Confirming *n* Extracted Mass	Confirm Product (SIM only)
(Compound Detail page) Extracted Mass (Grid page) Peak *n* Confirming *n* Extracted Mass	Confirm Extracted (XIC only)
(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 (Grid page) Peak *n* Confirming *n* Collision Energy	Confirm Energy (SRM only)
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 15. 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 import an instrument method

❖ To open the Instrument View

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

   The Method Development navigation pane opens.

2. Click **Instrument View**.

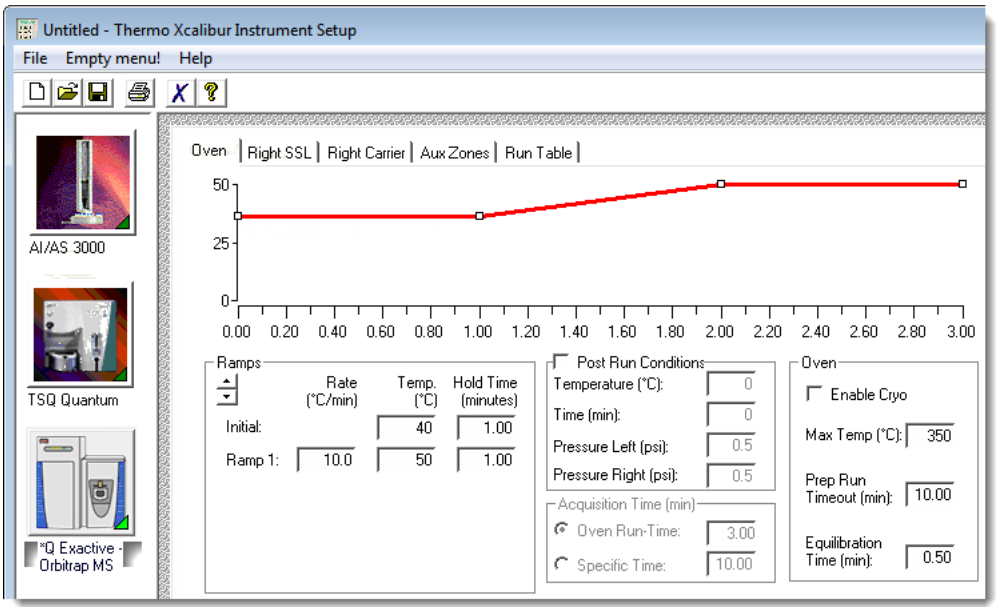
   The Instrument View opens.

❖ 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

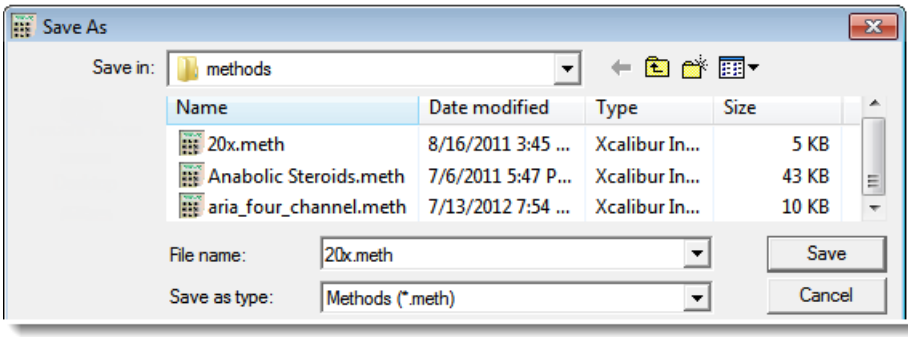


2. Click the icon for the instrument that you want to use for the method.

3. Edit the values on the instrument page.

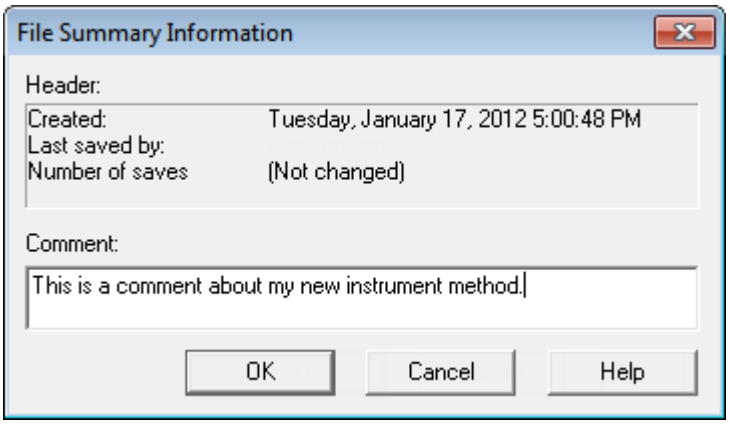
4. From the main menu in the Thermo Xcalibur Instrument Setup window, choose **File > Save As**.

   The Save As dialog box opens.



5. Select an instrument method name to overwrite, or type a new name for the instrument method, and click **Save**.

   The File Summary Information dialog box opens.



6. (Optional) Type a comment about the new instrument method.
7. Click **OK**.

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

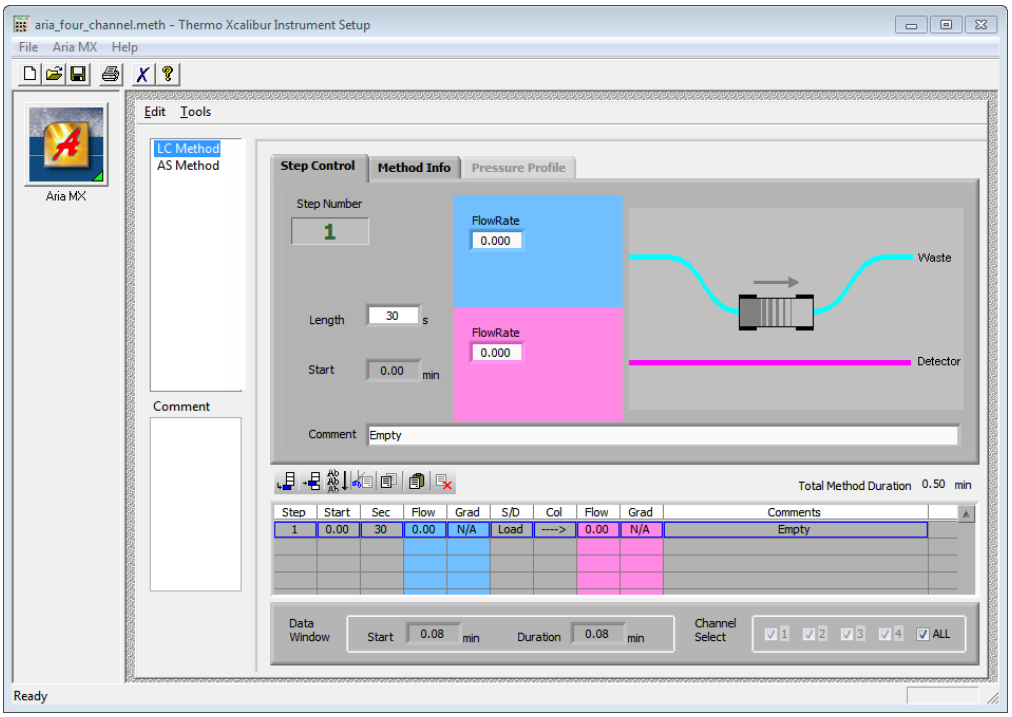
   …\Xcalibur\methods

❖ To create a new multiplexing instrument method

1. 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.

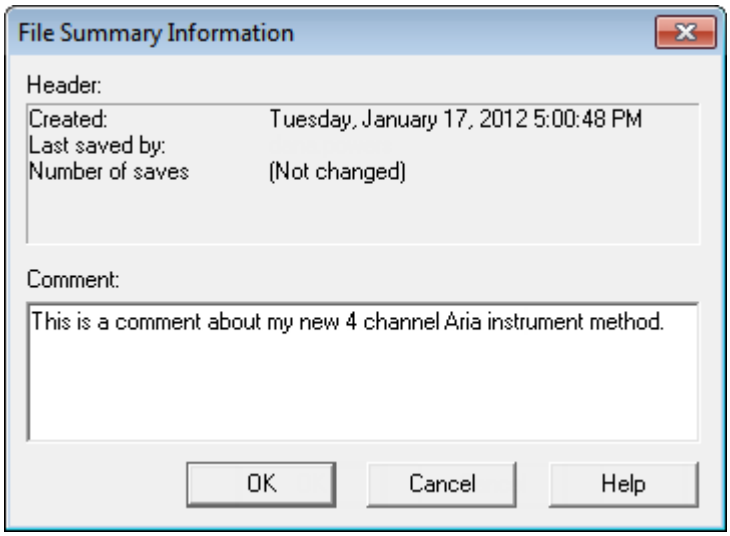
4. Specify the channels that you want to use for acquisition, as in this example:

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

   …\Xcalibur\methods

❖ To open an instrument method

1. Click **Open Instrument Method** in the Instrument View navigation pane.

   An instrument method browser opens.

2. In the browser, do one of the following:
   - Select an instrument method from the list and click **Open**.
   - Click **Xcalibur Instrument Method**, select a method from the list of recent methods, and click **Open**.

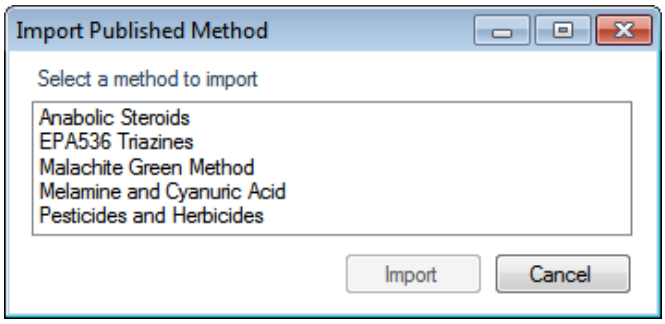
   The selected method opens in the Thermo Xcalibur Instrument Setup window. You can edit this method and save the changes, or you can save this method with another name.

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

❖ To import an instrument method

1. From the main menu, choose **Instrument View > Import Published Method**.

   The Import Published Method dialog box opens. This dialog box lists the master methods in the Published Master Methods folder. You can import instrument methods that are associated with these published master methods.



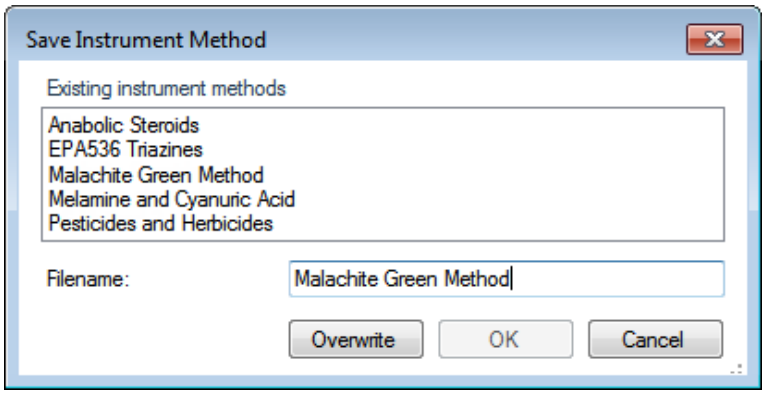
2. Select a method that includes the instrument method that you want to import.

   For instructions about importing the master methods for a quantitation method, see "Importing Published Master Methods" on page 267.

   For instructions about importing the master methods for a screening method, see "Importing Published Master Methods" on page 311.

3. Click **Import**.

   The Save Instrument Method dialog box opens.



4. Do one of the following:

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

   –or–

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

   The application reports that the method successfully imported.

You can use any of the Open Instrument Method commands to open this method just as you would an instrument method that you created.

5

Using the Method Development Mode for Quantitation Methods

This chapter includes method development tasks for creating and editing a quantitative method. When user security is activated, you must have Method Development Access permission before accessing these features.

Contents

- Opening a Master Method
- Starting a New Master Method
- Editing a Master Method
- Saving a Master Method to a New Name
- Creating a Method Template
- Importing Published Master Methods
- 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 settings for detecting, processing, and reporting those compounds.

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

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

To speed up the creation of master methods, you can create a method template. Using a method template helps you to develop methods faster because the TraceFinder application saves all of your commonly used method settings in a template, such as the number of confirming ions or the use of data-dependent scans.

Figure 27. Method Development navigation pane

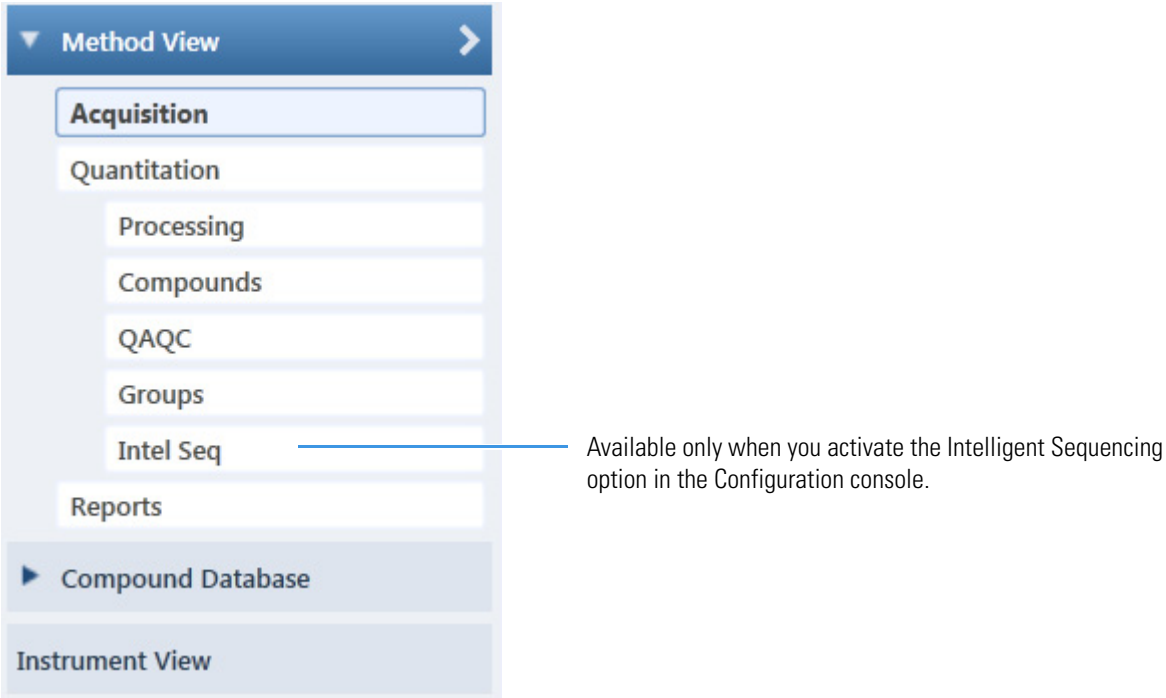


Table 16. Method Development navigation pane commands

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 146.
Quantitation	
Processing	Displays the Processing page of the Method View. See "Editing the Processing Page" on page 151.
Compounds	Displays the Compounds page of the Method View. See "Editing the Compounds Page" on page 155.
QAQC	Displays the QAQC page of the Method View. See "Editing the QAQC Page" on page 230.
Groups	Displays the Groups page of the Method View. See "Editing the Groups Page" on page 241.
Intel Seq	Displays the Intelligent Sequencing page of the Method View. See "Editing the Intelligent Sequencing Page" on page 244. 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 249.
Compound Database	See "Working with the Compound Database" on page 76.
Instrument View	See "Working with Instrument Methods" on page 113.

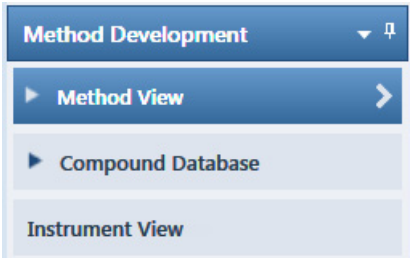
Opening a Master Method

Use the TraceFinder application to open a master method that was created and saved in the current TraceFinder application or converted from previous versions of TraceFinder. To convert legacy methods, see "Converting Legacy Data" on page 18.

❖ 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 Master Method" on page 124.

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.

Figure 28. Open Master Method dialog box

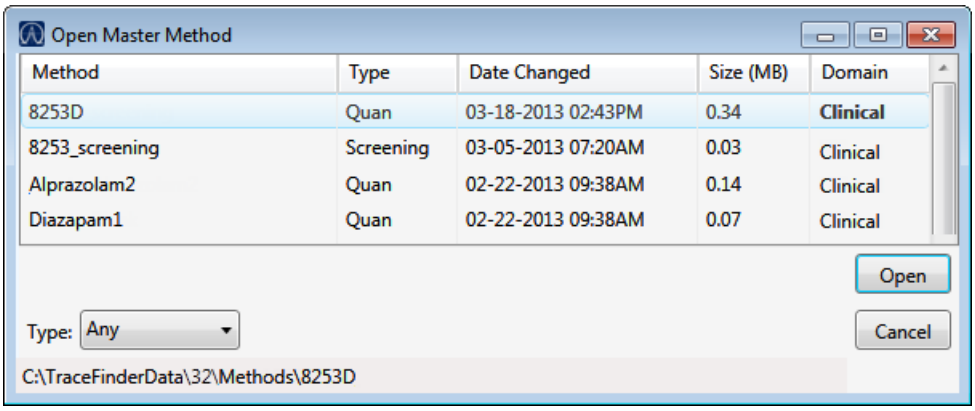
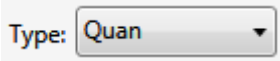


Table 17. Open Master Method dialog box parameters

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan or Screening.
Date Changed	Date the method was last updated.
Size	Size in megabytes.
Domain	TraceFinder domain for which the method was created.
Type	Type of method to display: Quan, Screening, or Any.
Path	Path to the selected method in the TraceFinderData\32\Methods folder.

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 149.

Starting a New Master Method

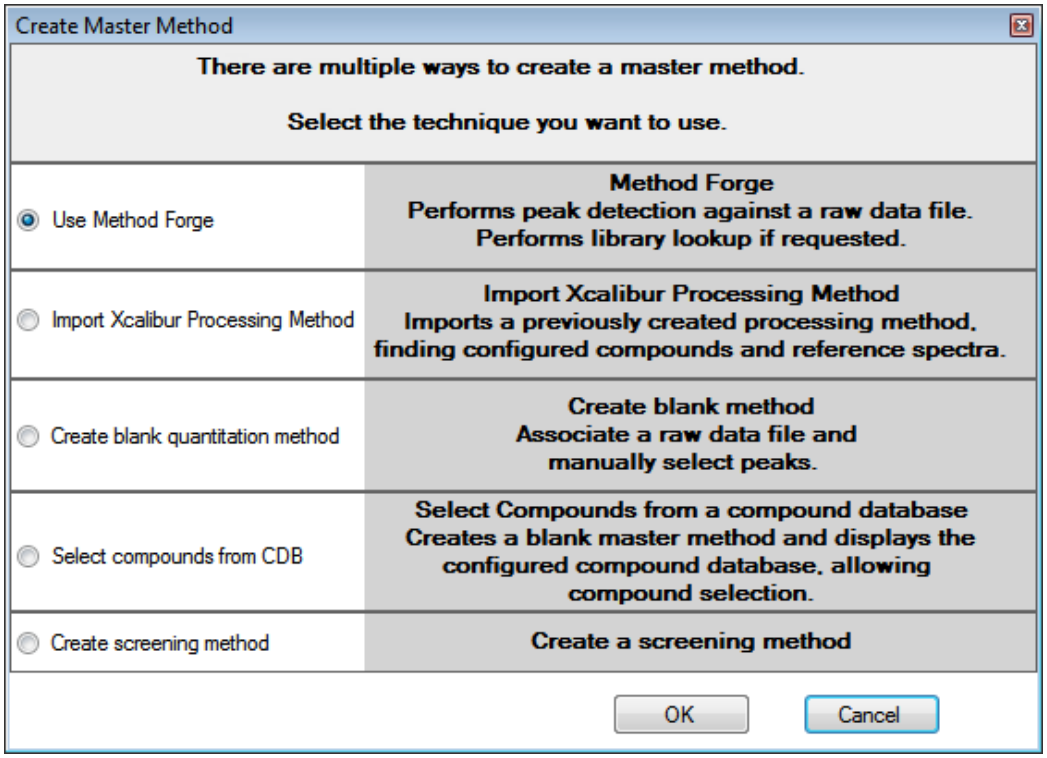
To create or start a specific method, select as applicable from one of the four different quantitation method procedures (or techniques) in the Create Master Method dialog box:

- 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



Creating a New Method with Method Forge

With Method Forge, you can create a new master method by manually selecting peaks, selecting multiple compounds, renaming peaks, or comparing mass spectra from the library searches. You can also choose to let the TraceFinder application automatically create a master method for you. For detailed descriptions of all the Method Forge parameters, see "Method Forge Dialog Box" on page 133.

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

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

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 124.

2. Select the **Use Method Forge** option and click **OK**.

Use 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 "Method Forge Dialog Box" on page 133.

   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:

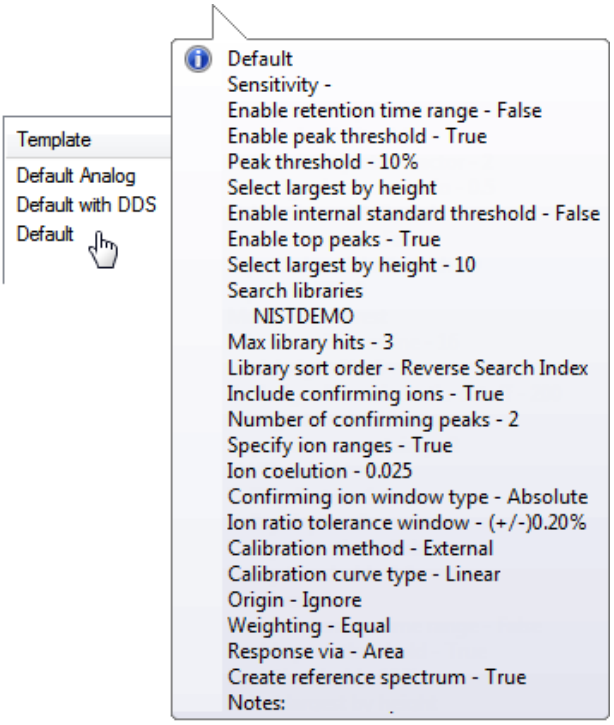
   - Click **Open Method Template Editor** to create and save a new method template.

     See "Creating a Method Template" on page 257.

   - 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 TraceFinder 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.

c. In the Raw Filename box, type the name of the file where the TraceFinder application will write the raw data file.

d. In the Path box, type a path or click the browse button and locate a folder where the application will save the raw data file.

e. (Optional) Type a comment about the acquired sample or the data file.

7. 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.

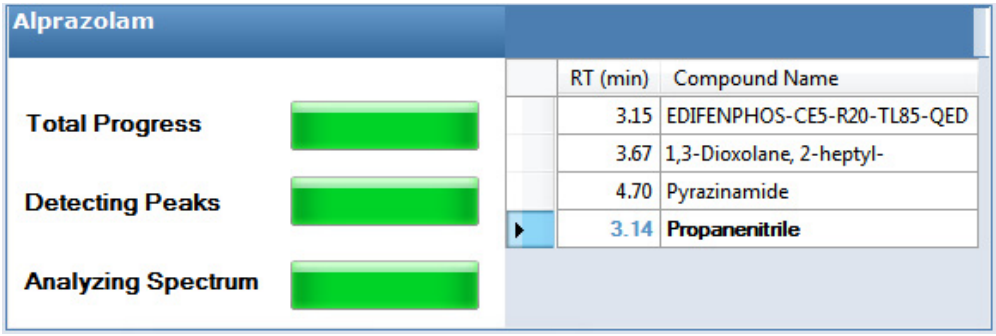
   b. In the Vial Position box, type a vial position.

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

      Range: 0.1 to 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:



- 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 quantitative samples following target compound analysis.

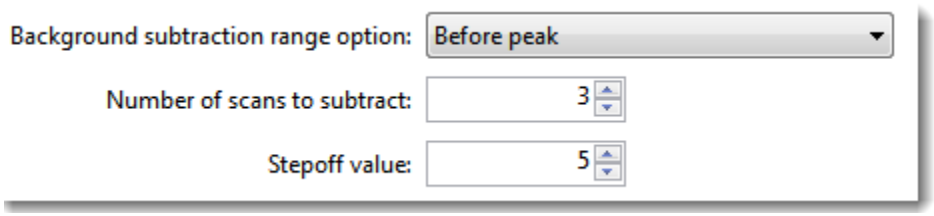
11. (Optional) From the Background Subtraction Range Option list, select how you want the background subtraction range determined from one of these options:

    - **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 Stepoff Value box, enter a number.

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



    If you entered 3 in the Number of Scans To Subtract box and the stepoff value is 5, the TraceFinder application ignores the first 5 scans to the left of the peak and applies the averaging and subtraction to the 6th, 7th, and 8th scans to the left of the peak.

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 144.

❖ 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 124.

2. Select the **Use Method Forge** option and click **OK**.

Use 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 135.

   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

3. 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 257.

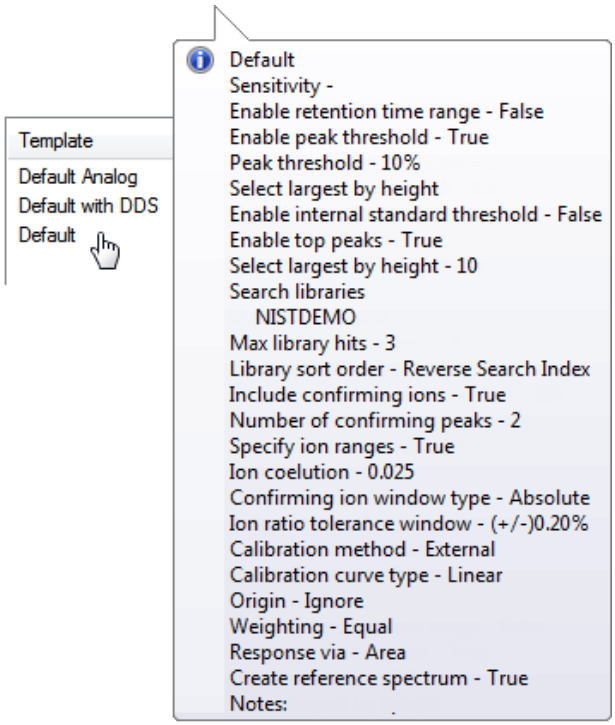
   - Select a method template from the template list, and click **Open Method Template Editor** to edit and save the method template. The application saves the methods to the following folder:

     …\TraceFinderData\32\Templates\Methods\Clinical folder

   - 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 TraceFinder 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 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.

5. Ensure that the **Automatically Create the Master Method** check box is cleared.

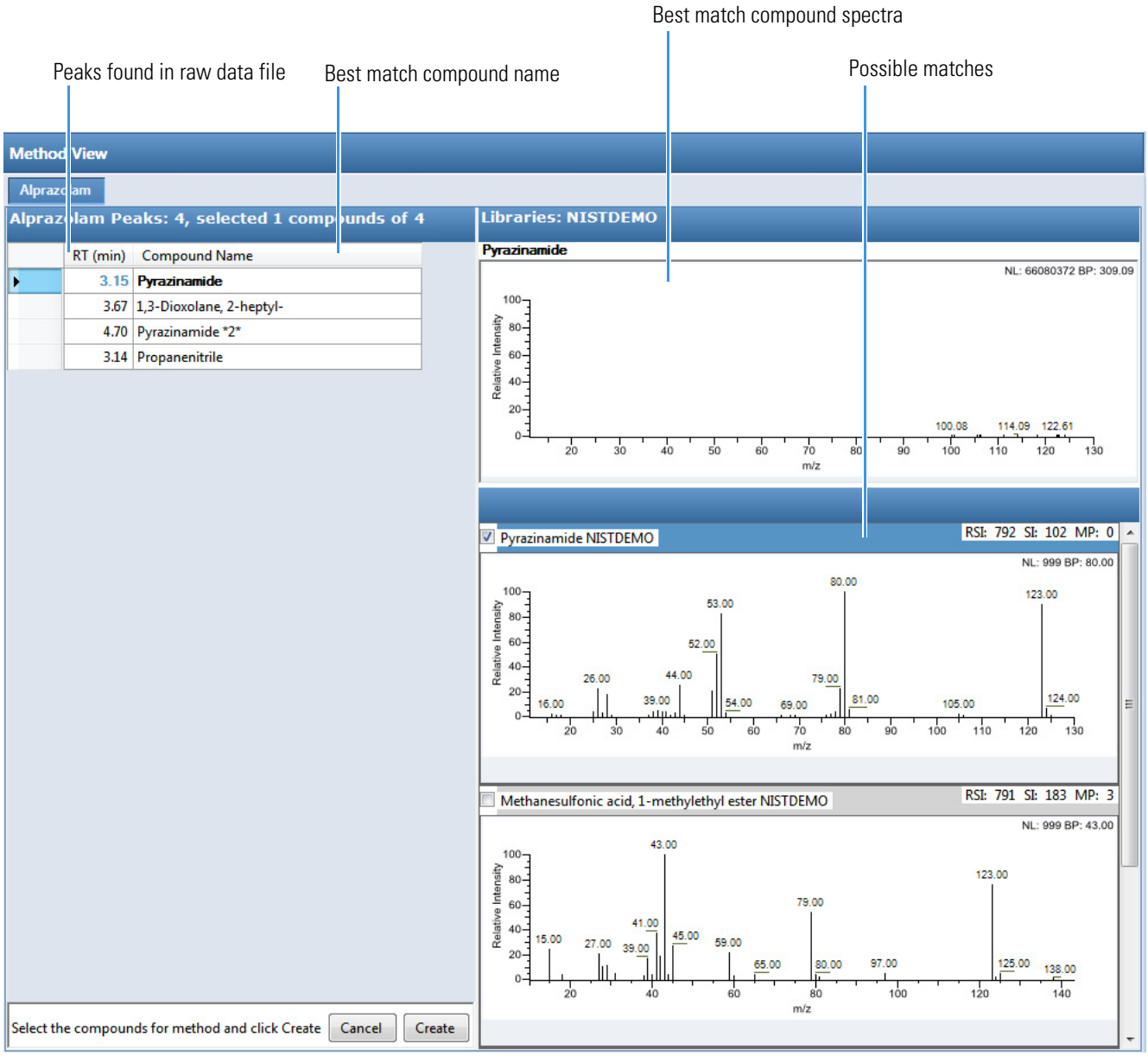
6. To select a raw data file, browse to the file location.

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

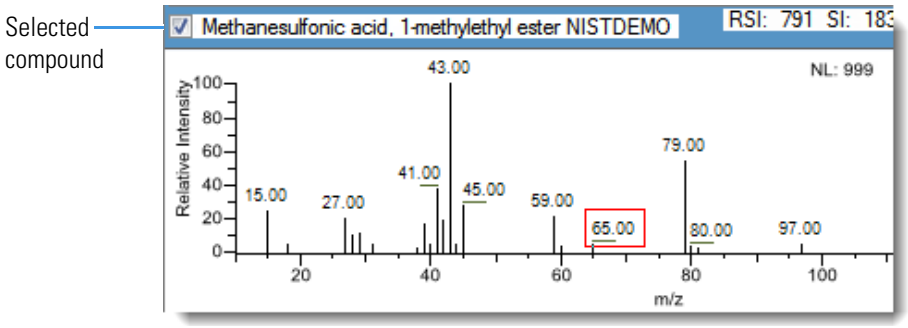
   The method forge results view opens, listing all peaks found in the raw data file.

   For each peak listed in the RT column, the application displays a list of possible matches in the Libraries pane. The TraceFinder 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



8. (Optional) To use a library compound other than the compound chosen by the TraceFinder 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.



   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 TraceFinder 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 149.

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 144.

Method Forge Dialog Box

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

Figure 31. Method Forge dialog box

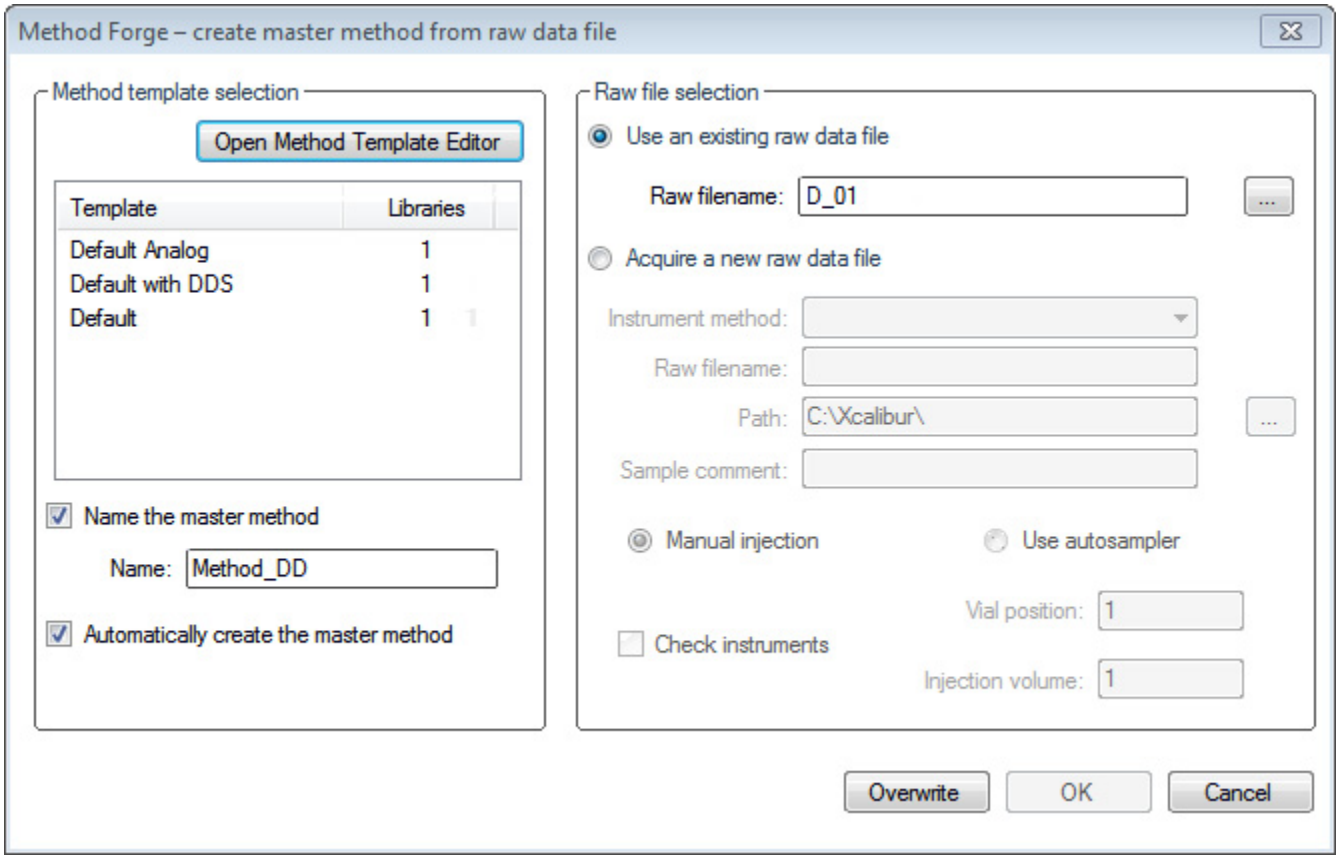


Table 18. Method Forge dialog box parameters (Sheet 1 of 2)

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 257.
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 125.
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 18. 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 TraceFinder application writes the raw data.
Path	Specifies the location where the TraceFinder 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

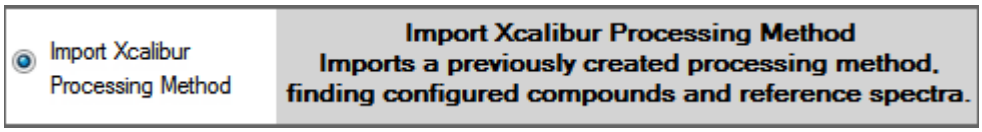
You can create a new master method from an existing Xcalibur processing method.

❖ To import an Xcalibur master method

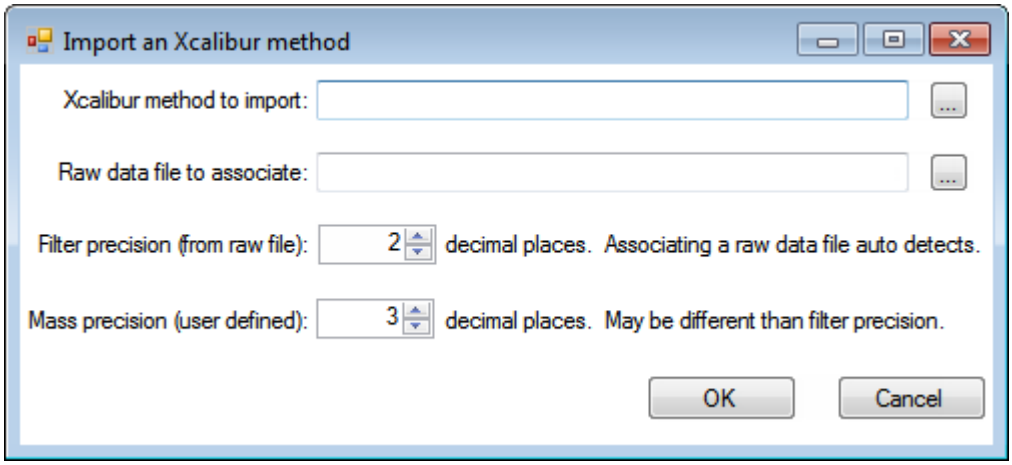
1. Choose **File > New > Master Method** from the main menu.

   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 124.

2. Select the **Import 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 TraceFinder 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\32\Methods*Methodname*

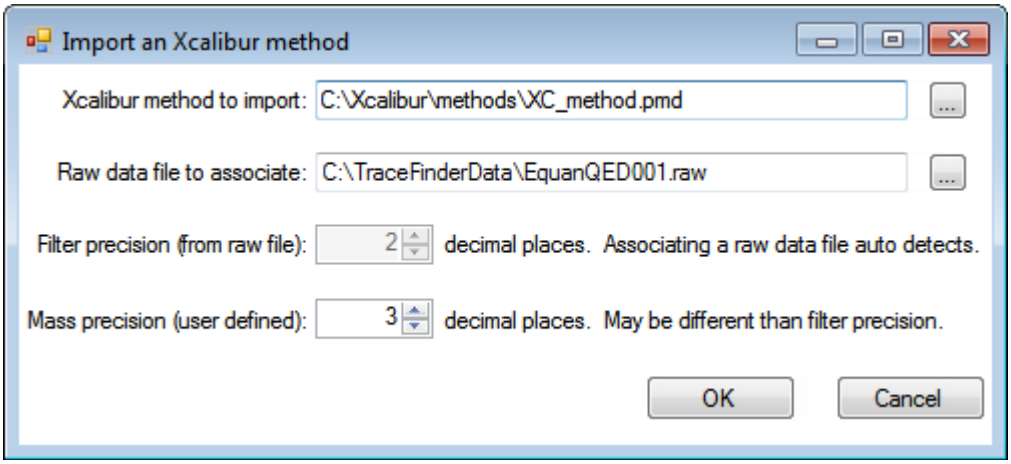
5. (Optional) Change the number of decimal places in the Filter Precision box.

   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 TraceFinder 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 149.

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 144.

Creating a Blank Method

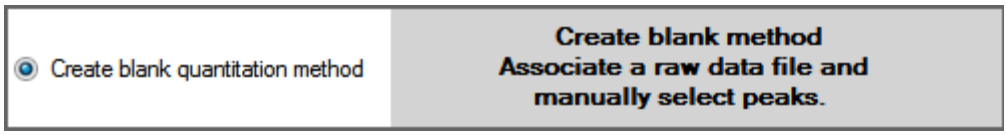
You can use the compounds in a previously acquired raw data file to create a new blank master method.

❖ 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 124.

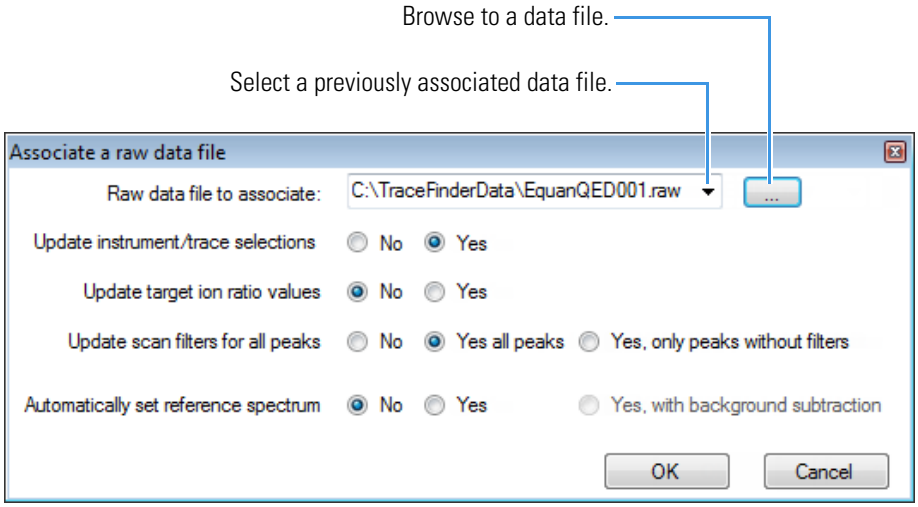
2. Select the **Create Blank Quantitation Method** option and click **OK**.



   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\32\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 176.

   - **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 146.

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

6. Click **OK**.

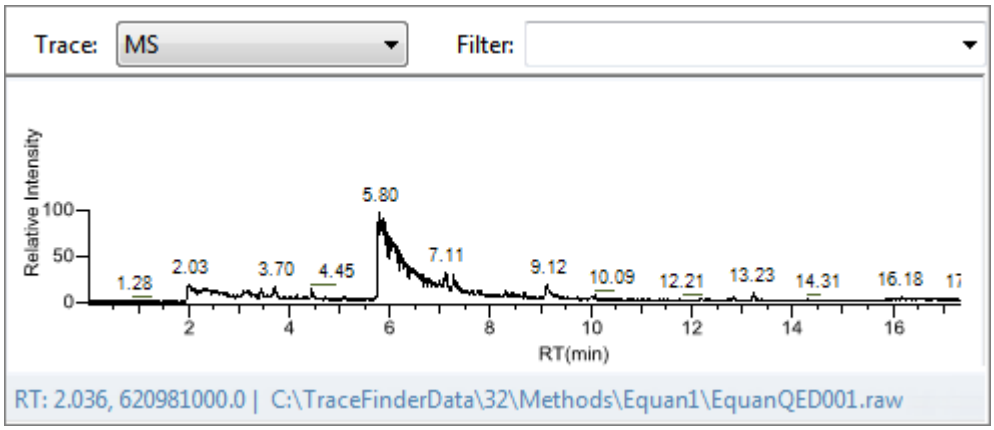
   The TraceFinder application displays the Acquisition page of the Method View.

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

   The method must include at least one compound.

8. Click the **Detection** tab.

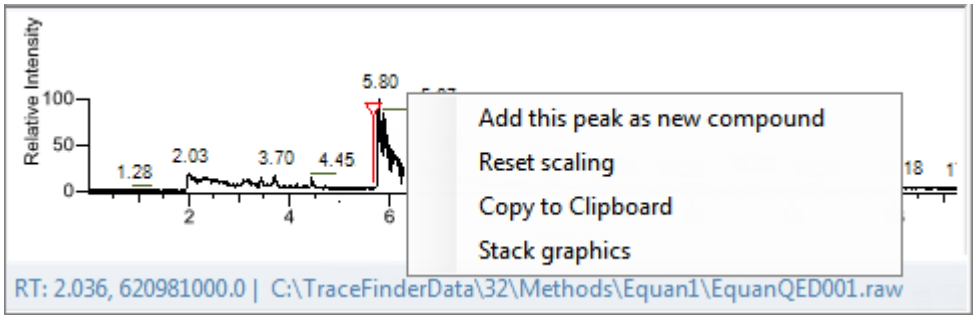
   The Detection page shows an empty Compound list and displays the chromatographic data for the compounds in the raw data file.



9. Select a filter from the Filter list.

10. Select the peak in the chromatogram that represents the compound that you want to add to the method.

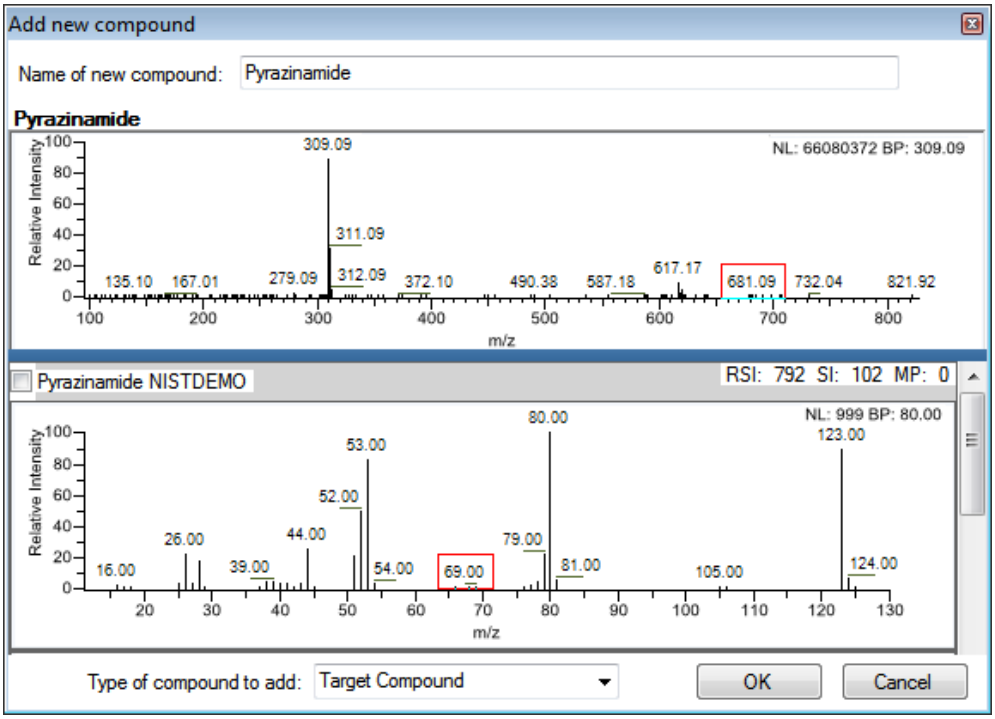
11. Right-click and choose **Add This Peak as New Compound** from the shortcut menu.



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

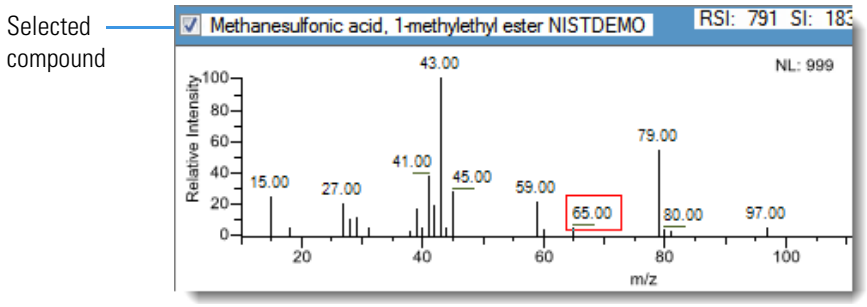
   Note When the peak is from an analog trace, the application does not perform a library search and does not identify any confirming ions.

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



12. (Optional) Do the following:

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



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

    c. Click **OK**.

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 155.

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 149.

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 144.

Selecting Compounds from the Compound Database

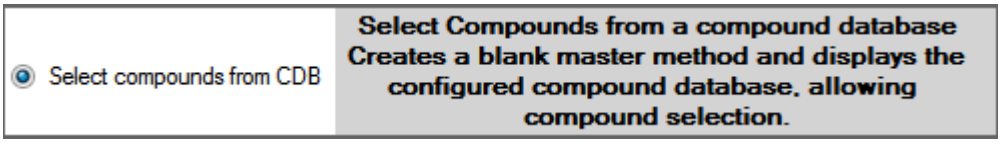
You can select compounds from the compound database to create a new master method.

❖ To select compounds from the compound database

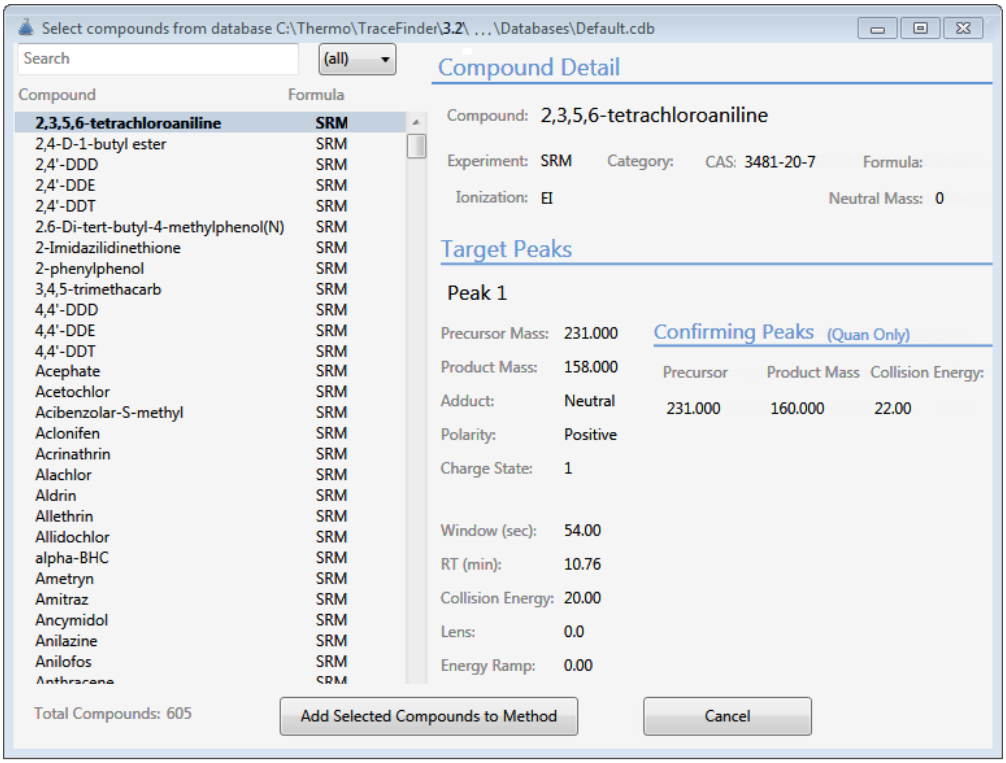
1. Choose **File > New > Master Method** from the main menu.

   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 124.

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



   The Select Compounds from Database dialog box opens, listing all the compounds defined in the compound database.



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**.

   The TraceFinder application adds the selected compounds to the method.

6. 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 149.

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.

   For a detailed description of how to modify a master method, see "Editing a Master Method" on page 144.

Editing a Master Method

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

This section includes instructions for the following tasks:

- Modifying Retention Times
- 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 Reports Page

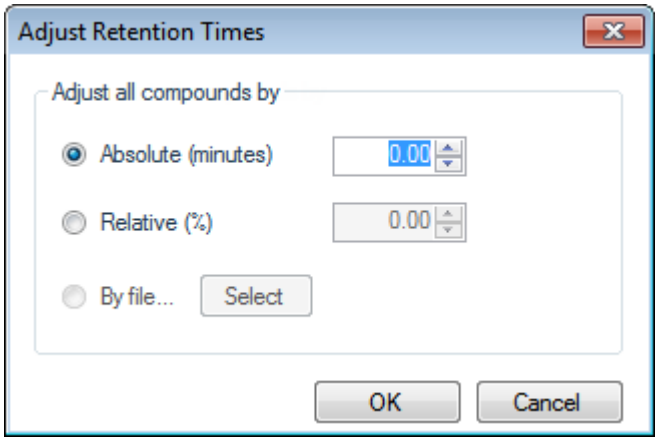
Modifying Retention Times

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 values: –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 values: –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.

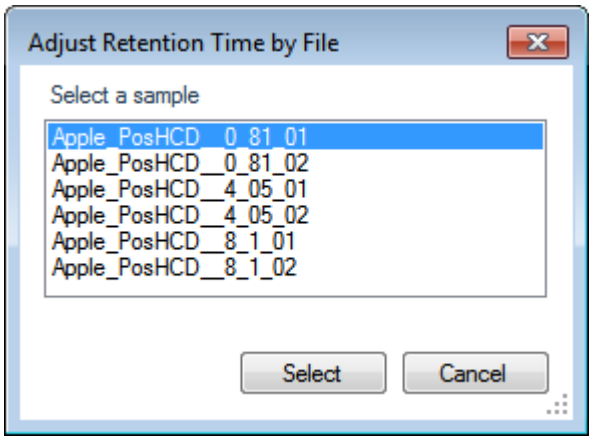
   –or–

   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.

Editing the Acquisition Page

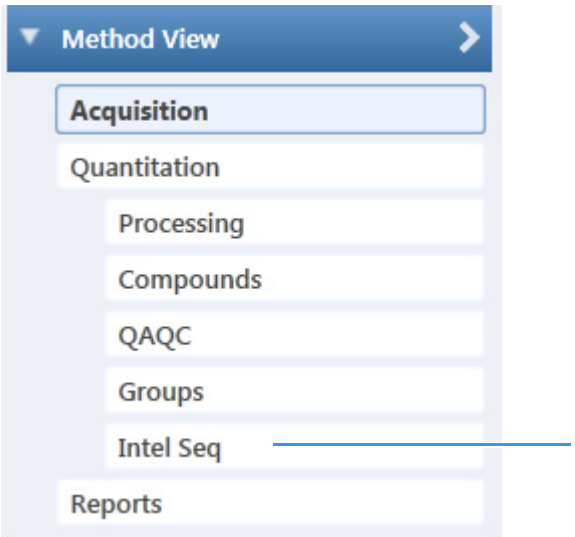
The Acquisition page defines basic information about the master method. For detailed descriptions of all the features, see "Acquisition Page for a Quantitation Method" on page 149.

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 on the top of each printed, saved, or exported report.

   The default name is Default Laboratory.

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

3. From the Injection Volume box, select an injection volume (between **0.1** and **2000** µL) to be used for sample injection.

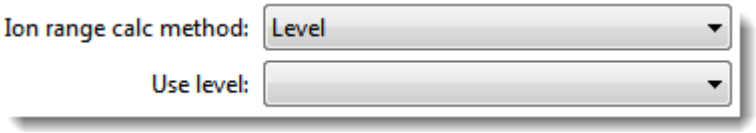
   Use the up/down arrows to change the volume in increments/decrements of 1 µL, or use the keyboard to enter non-integer injection volumes.

   IMPORTANT The TraceFinder 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 TraceFinder 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 155.



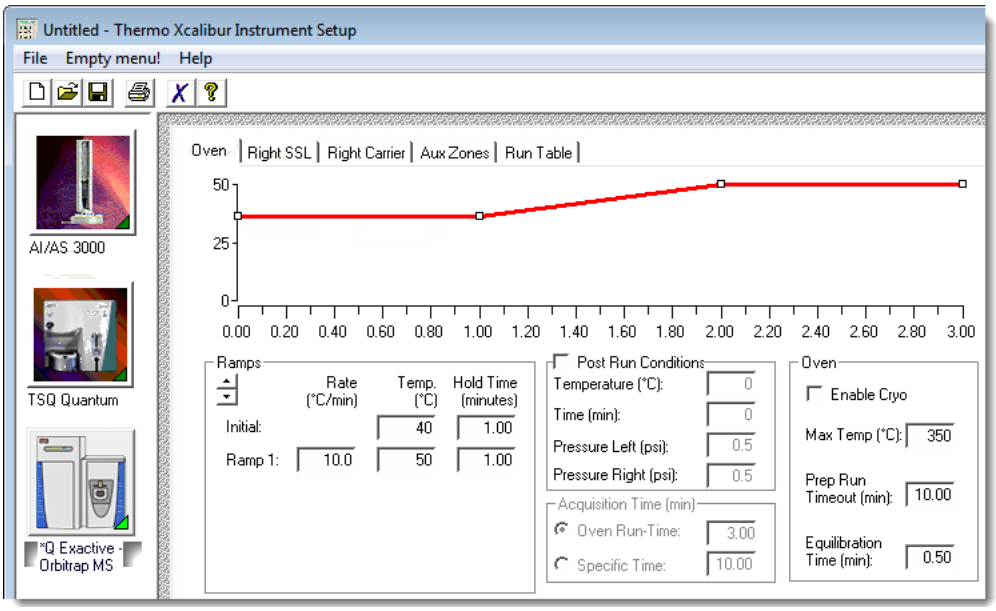
❖ To edit an instrument method

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 Xcalibur Instrument Setup dialog box opens. This example of an instrument setup shows multiple configured instruments.

Figure 32. Thermo Xcalibur Instrument Setup window



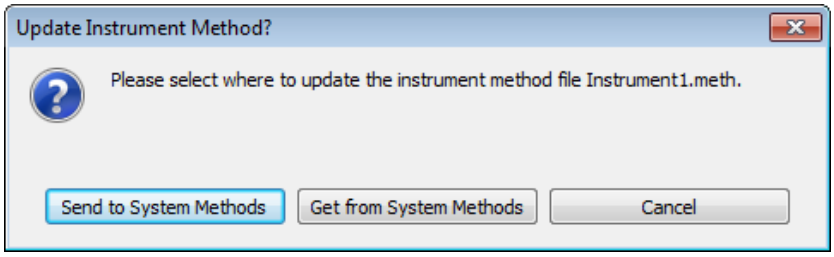
3. Edit the values on the instrument page for your instrument.

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

   The TraceFinder 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\32\Methods folder with the current instrument method.
   - **Get from System Method**: Overwrites the current instrument method with the instrument method in the C:\TraceFinderData\32\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 33. Acquisition page for a quantitation method

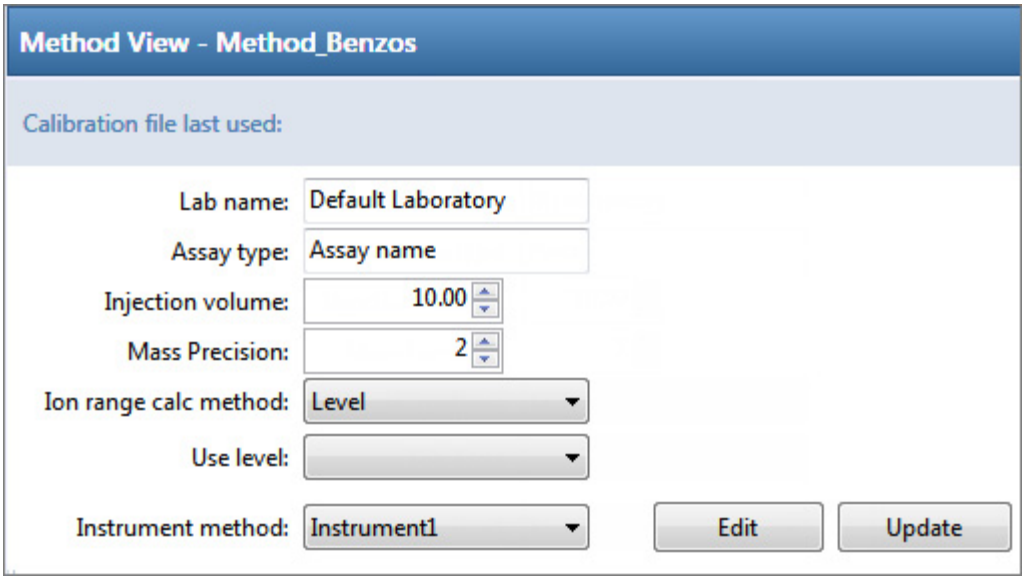


Table 19. Acquisition page parameters (Sheet 1 of 2)

Parameter	Description
Lab Name	Specifies the laboratory name to be displayed on the top of each printed, saved, or exported report. Default: Default Laboratory To specify this default laboratory name, see "Specifying Application Defaults" on page 35.
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. Range: 0.1 to 2000 µL
Mass Precision	Specifies the number of decimal places used in reports and in peak and spectrum displays. Valid values: Integers from 2 to 6, inclusive.

Table 19. Acquisition page parameters (Sheet 2 of 2)

Parameter	Description
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 155.
Instrument Method	Specifies the instrument method used for acquiring samples.
Edit	Opens the Thermo Xcalibur Instrument Setup dialog box 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\32\Methods folder with the current instrument method. **Get from System Methods**: Overwrites the current instrument method with the system method in the C:\TraceFinderData\32\Methods folder.

Editing the Processing Page

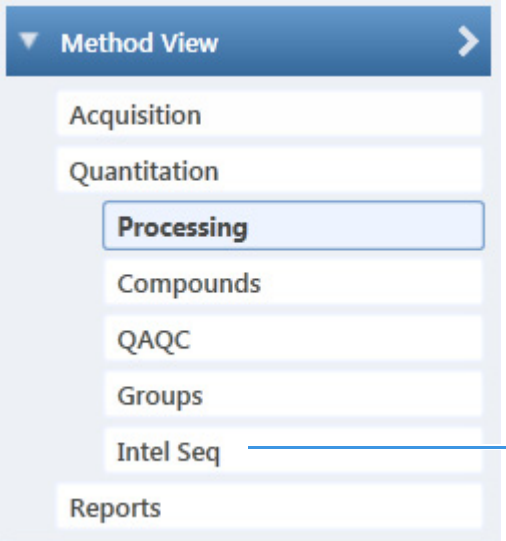
The Quantitation – Processing page defines basic information about the master method. For detailed descriptions of all the features, see "Processing Page for a Quantitation Method" on page 154.

Follow these procedures:

- To select a qualitative peak processing template
- To set automated background subtraction options
- To specify mass tolerance
- To include data-dependent filters
- To specify a threshold override

❖ 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 select a qualitative peak processing template

In the Qualitative Peak Processing Template list, select the template that you want to use to perform peak detection on quantitative samples after compound analysis is complete.

The application uses the libraries in this template to identify compounds for the method. If there is no library selected in the method template, the application identifies found peaks as peak@*RT* on the Compounds page. To specify the libraries that are including in a qualitative peak processing template, open the template in the Method Template Editor, and then follow the instructions "To identify the peaks" on page 259.

The application lists all method templates (.pmtx file extensions) in the following folder:

…\TraceFinderData\32\Templates\Methods\Clinical

❖ 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.

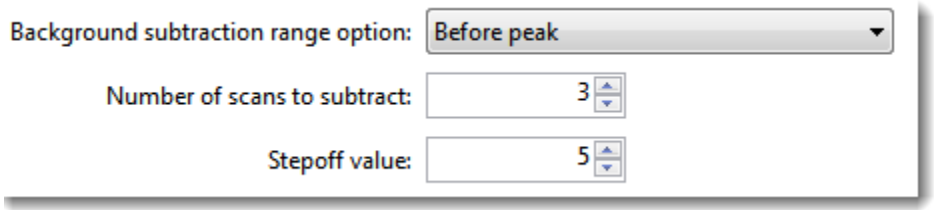
   When you create a reference spectrum with background subtraction, the TraceFinder application uses the selected method to conduct background subtraction of peak spectra during quantitative processing. The application then reports the background-subtracted reference spectrum (indicated with BS in the 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 TraceFinder 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 Stepoff Value box, enter a number.

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



   Before Peak example:

   When the Number of Scans to Subtract equals 3 and the Stepoff Value equals 5, the TraceFinder application ignores the first 5 scans to the left of the peak and applies the averaging and subtraction to the 6th, 7th, and 8th scans to the left of the peak.

   After Peak example:

   When the Number of Scans to Subtract equals 3 and the Stepoff Value equals 5, the TraceFinder 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 Stepoff Value equals 5, the TraceFinder 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* ± tolerance value.

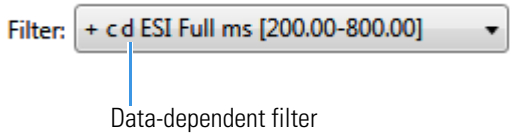
   The application applies this mass tolerance to the extracted chromatograms.

❖ 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 176.

Data-dependent filters are indicated with a "d".



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 MS^n scan.

❖ To specify a threshold override

1. Select the **Threshold Override** check box.
2. In the box, type a value for creating a threshold guide to overlay on compounds in the Comparative View in the Data Review mode.

   This threshold value overrides the Threshold value specified on the QAQC – Threshold page. See "Threshold" on page 237.

Processing Page for a Quantitation Method

Use the features on the Processing page to define basic information about the master method.

Figure 34. Processing page for a quantitation method

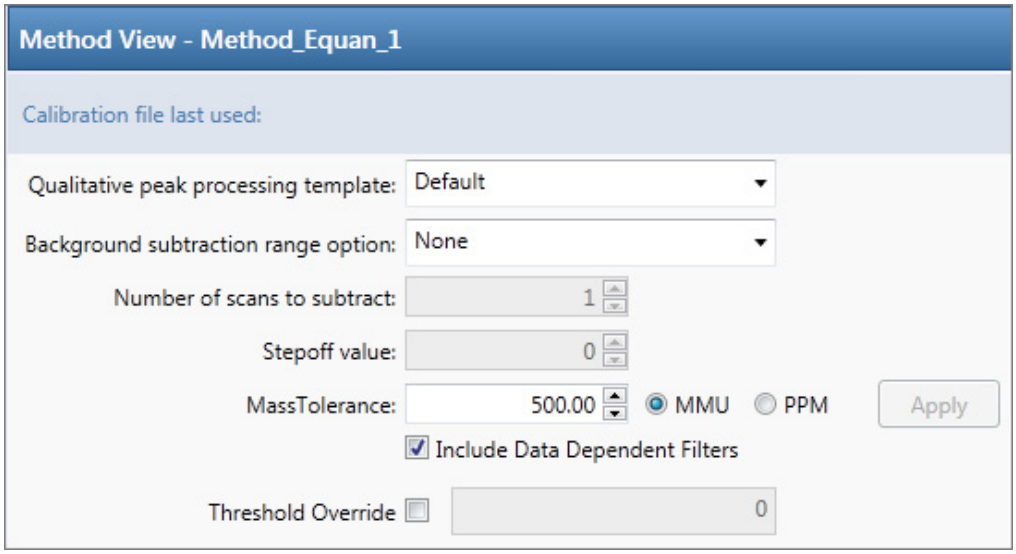


Table 20. Processing page parameters

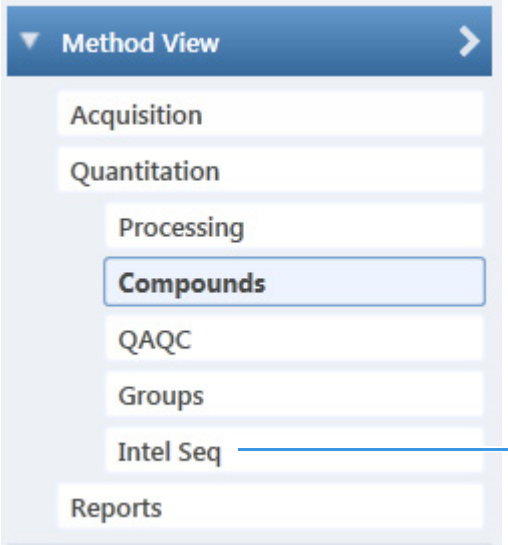
Parameter	Description
Qualitative Peak Processing Template	Specifies the template used to perform peak detection on quantitative samples following compound analysis.
Background Subtraction Range Option	Specifies the range used for background subtraction. Valid values: None, Before Peak, After Peak, Both Sides of Peak Default: None
Number of Scans To Subtract	Valid values: Even numbered integers Default: 0
Stepoff Value	Offset from the selected peak to the first subtracted peak.
Mass Tolerance	Specifies the upper limit of MMU or PPM. Default: 500 Range: 0.1 through 50 000 • (Default) MMU (millimass units): MMU is a static calculation to the extracted mass. • PPM (parts per million): PPM is a variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.
Include Data Dependent Filters	Specifies that the method includes data-dependent filters. Available only for quantitation methods.
Threshold Override	Overrides the Threshold value specified on the QAQC – Threshold page.

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.
Identification	See also Identification page parameters.
Detection	See also Detection page panes.
Calibration	See also Calibration page parameters.
Calibration Levels	See also Calibration Levels page parameters.
QC Check Levels	See also QC Check Levels page parameters.
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 225.

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 76.

❖ 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

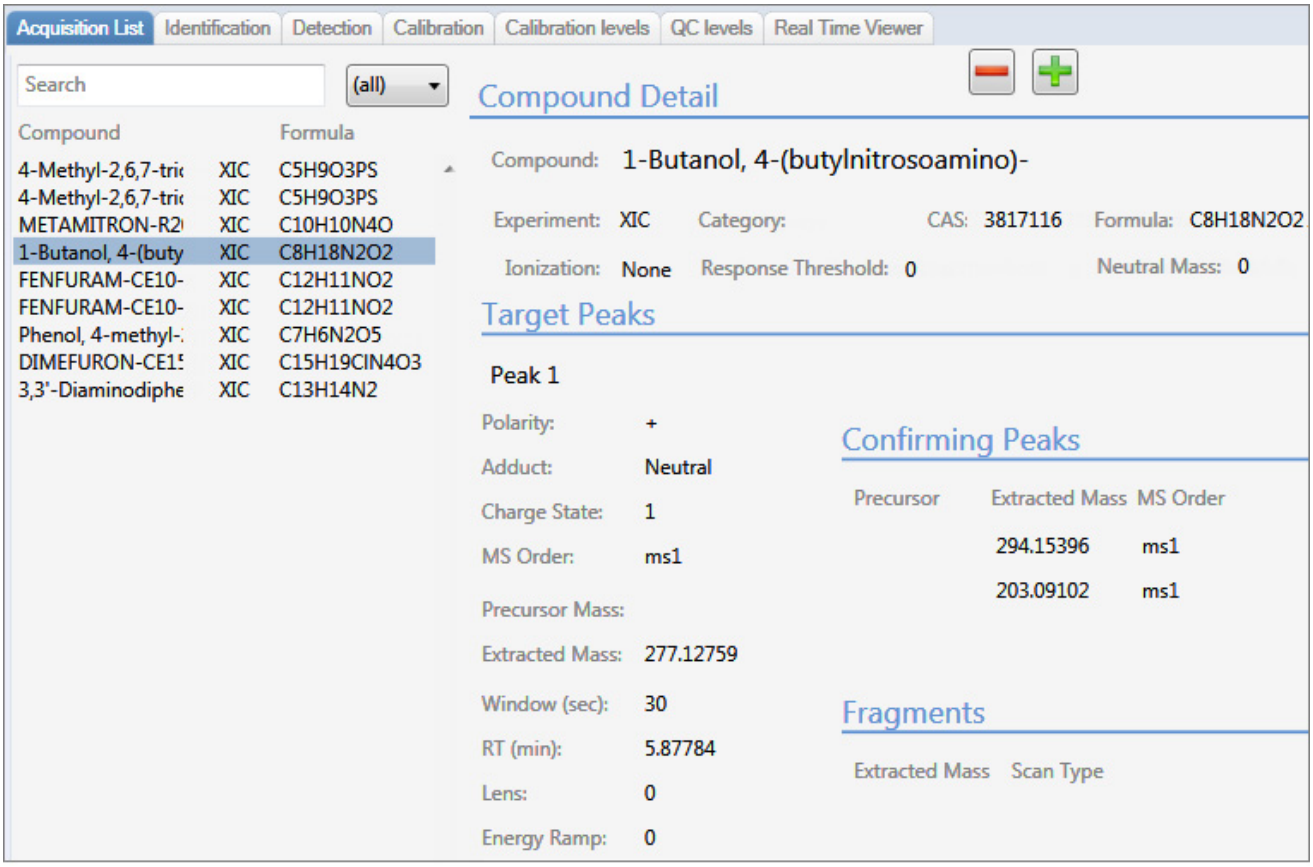
1. Click the **Add Compound from Compound Database** icon, .

   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 TraceFinder application adds the selected compounds to the acquisition list for the method.

Figure 35. Acquisition List page

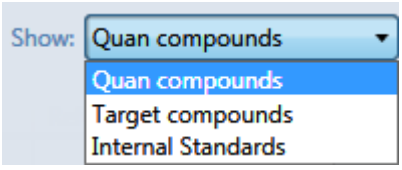


Identification

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."

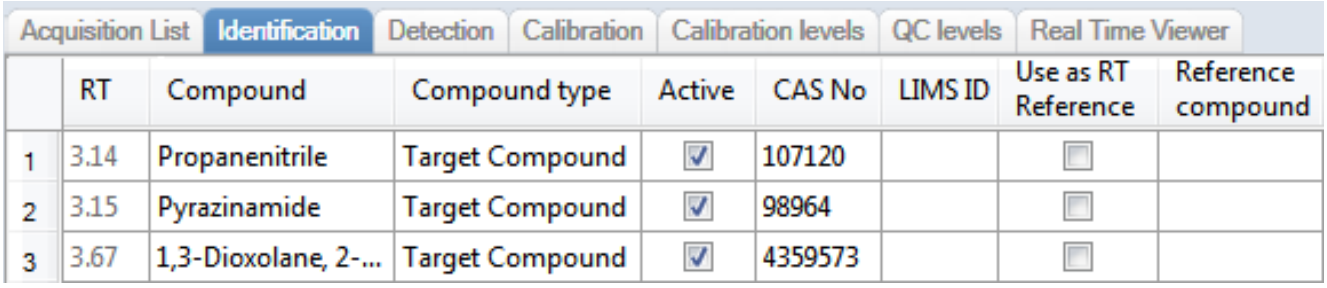
❖ To filter the displayed compounds

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.

Figure 36. Identification page



	RT	Compound	Compound type	Active	CAS No	LIMS ID	Use as RT Reference	Reference compound
1	3.14	Propanenitrile	Target Compound	☑	107120		☐	
2	3.15	Pyrazinamide	Target Compound	☑	98964		☐	
3	3.67	1,3-Dioxolane, 2-...	Target Compound	☑	4359573		☐	

Table 21. Identification page parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column. The TraceFinder application uses the RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Compound	A list of 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.

Table 21. Identification page parameters (Sheet 2 of 2)

Parameter	Description
Compound Type	Compound types are Target Compound and Internal Standard. The TraceFinder 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 TraceFinder 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 TraceFinder application first identifies those compounds identified as retention time standards and then uses their observed retention times to adjust any associated target compound.
Reference Compound	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 225.

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 172), 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 TraceFinder 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.

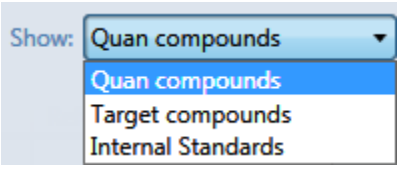
Follow these procedures:

- 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

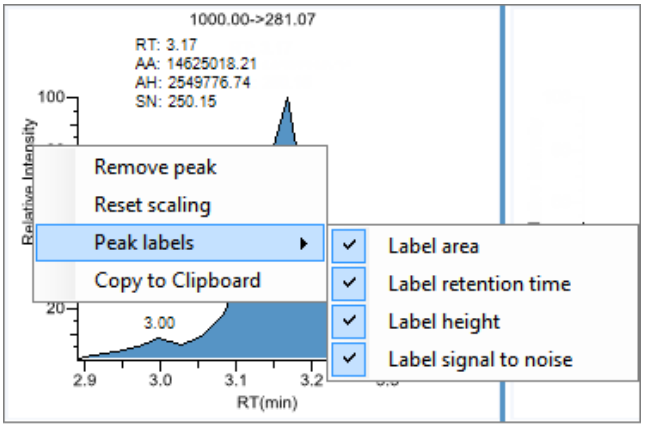
From the Show list, select the type of compounds that you want to display in the compounds list.



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, select the label type again and clear it.

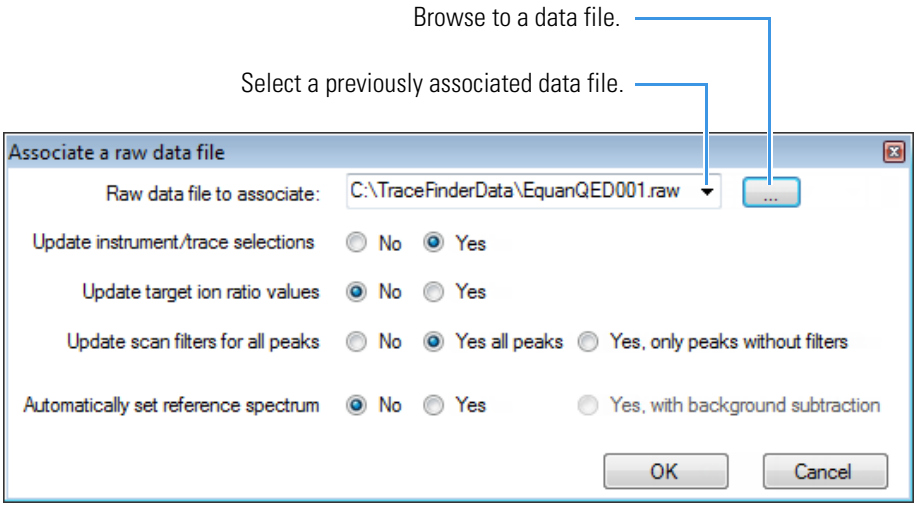
The application globally applies these label settings to all quantitative peaks, confirming peaks, and internal standard peaks in the method.

❖ 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\32\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–

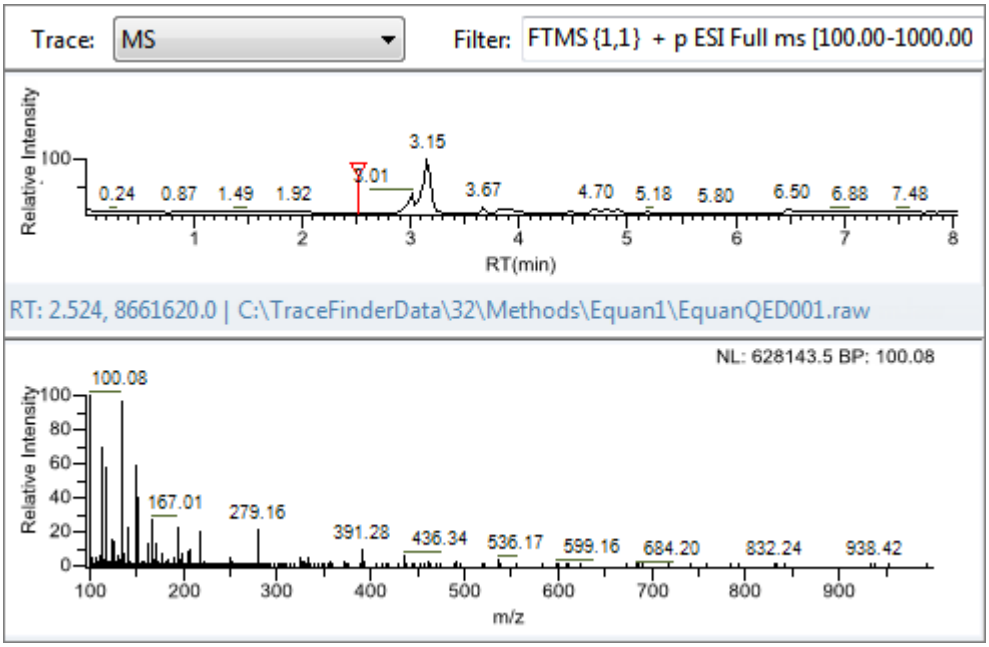
   Select the **Yes, with Background Subtraction** option.

   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 146.

6. Click **OK**.

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

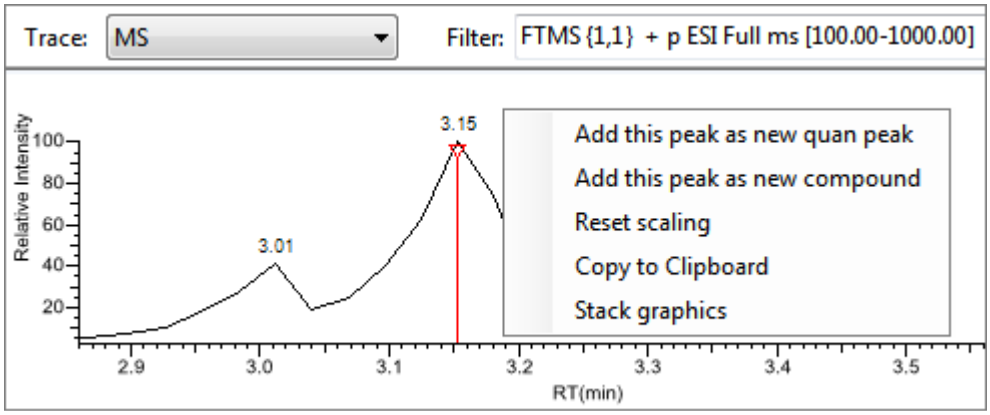


IMPORTANT While the spectra pane displays the associated raw data file, you cannot display peak information for an original compound in the Compound list. You can display peak information only for compounds in the associated raw data file. To return the display functionality for all compounds in the 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.

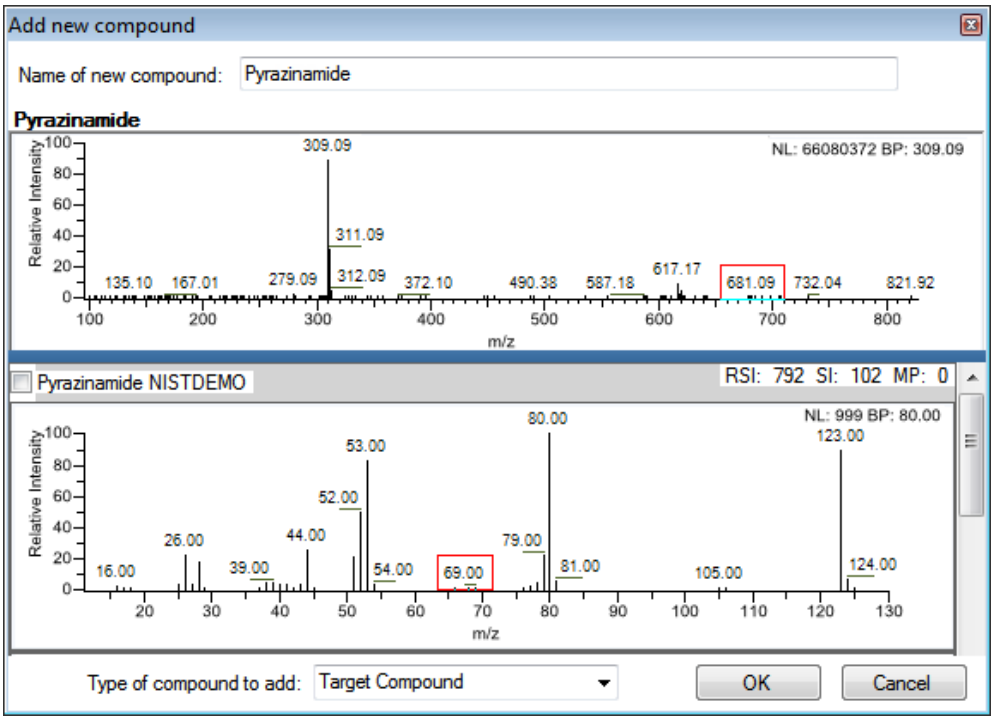
9. Right-click and choose **Add This Peak as New Compound** from the shortcut menu.



The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the 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. 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 37. Add New Compound dialog box



10. Do one of the following:

    - Type a new name for the first matched compound.

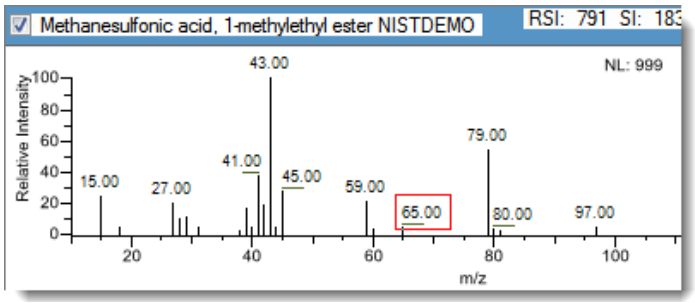
      The application displays a red warning when the selected compound name already exists in the method. You cannot overwrite the compound name, and you cannot create a duplicate name in the method. You must type a unique name.

      Name of new compound: Pyrazinamide

    –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.

      Selected compound

11. In the Type of Compound To Add list, select a compound type.

12. Click **OK**.

❖ To change the compound reference spectrum

1. In the chromatogram pane, click a peak.

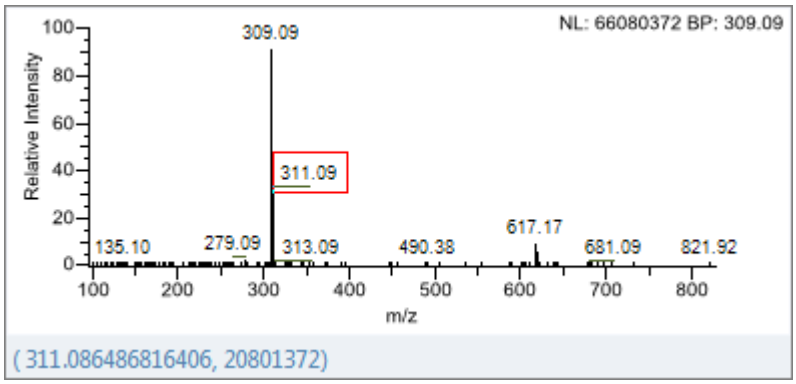
   The TraceFinder application displays the spectrum for the selected peak in the spectrum pane.

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

❖ To replace a quantitation mass

1. Click the data pane for the quantitation mass that you want to replace.
2. In the 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 Quan Value** from the shortcut menu.
4. Choose either **Don't Update Ion Ratios** or **Update Ion Ratios Using This Spectrum**.

   You can see the updated ion ratios on the Ratios page for the confirming ion peaks. See "Ratios" on page 213.

❖ 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 TraceFinder 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 213.

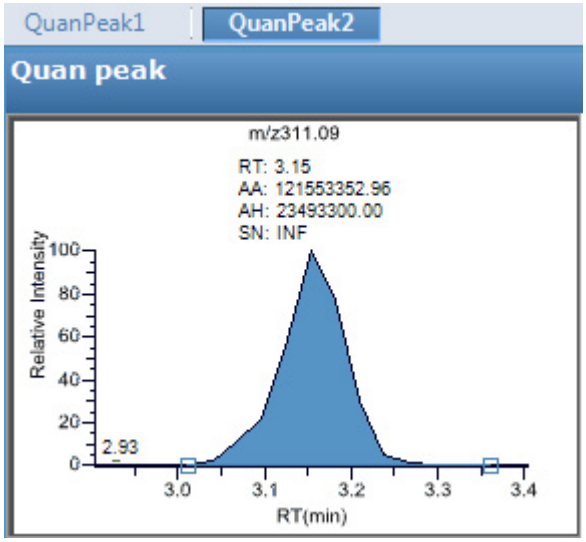
❖ To add a quantitative peak

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.

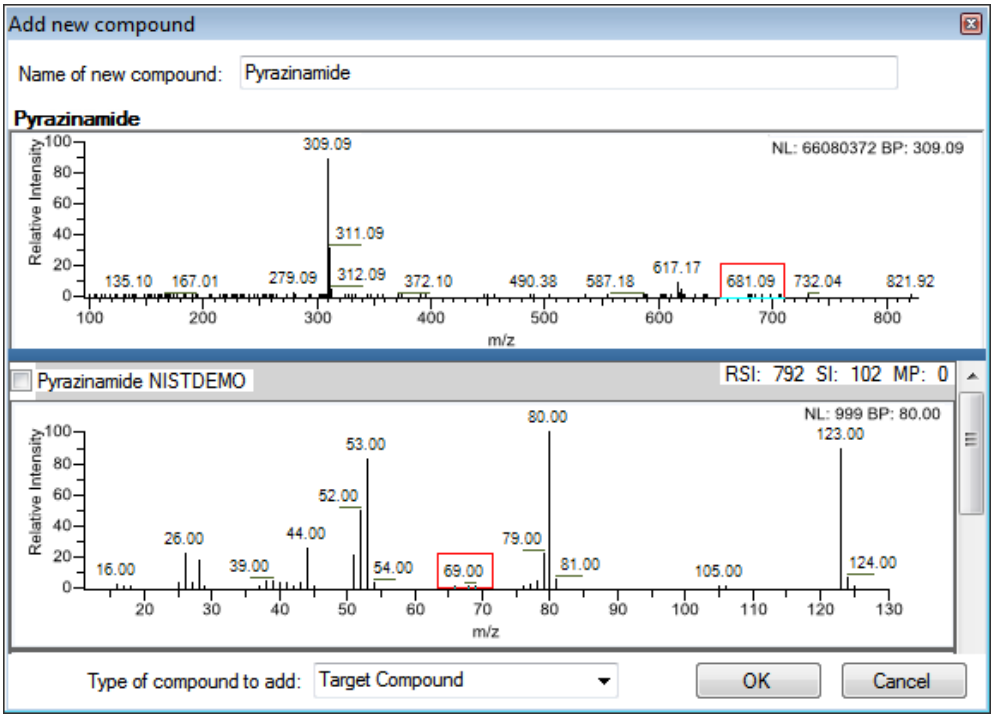
   The red box indicates the selected peak.

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

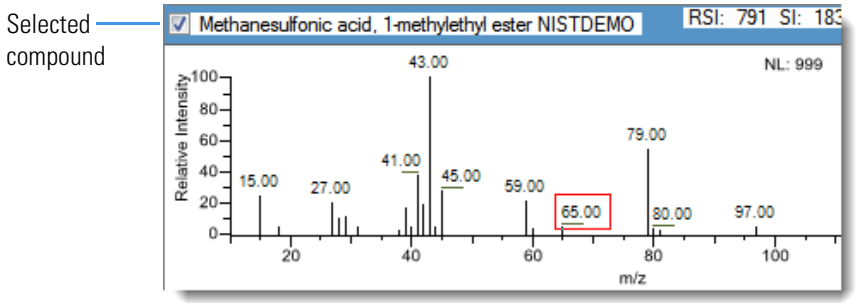
   The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quantitative peak, and the second and third largest ions as the confirming ion peaks.

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

Figure 38. 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 TraceFinder 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.

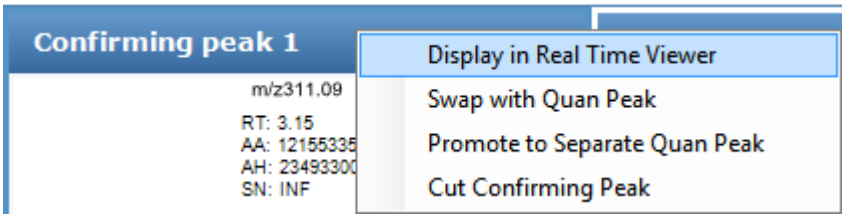
❖ To set a confirming ion peak as an additional quantitative peak

Right-click the header bar for the confirming ion peak and choose **Promote to Separate Quan Peak** from the shortcut menu.

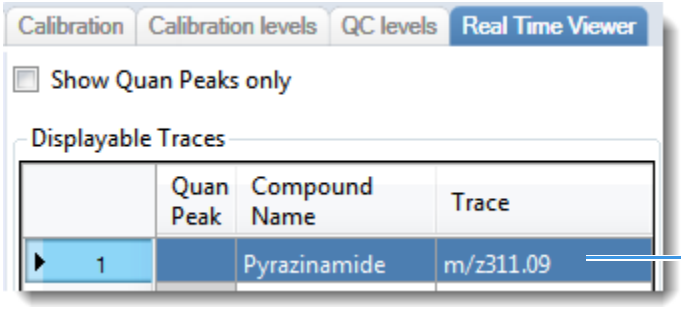
The application creates a new quantitative peak, using information from the confirming ion peak. This includes the expected retention time that the confirming ion peak inherited from the original quantitative peak. The application removes all references to the confirming ion peak from the method.

❖ 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.

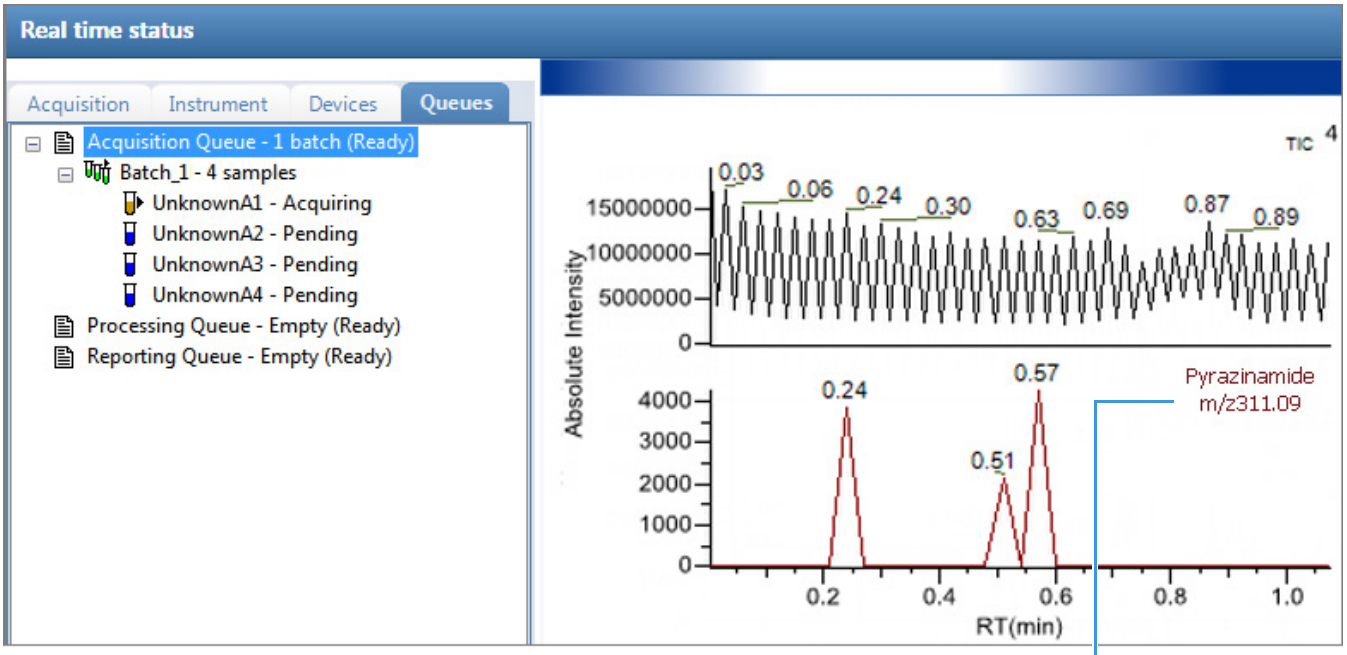


The application moves the peak to the Traces To Display in Real Time Viewer pane on the Real Time Viewer page. See "Real Time Viewer" on page 223.



Trace *m/z* 311.09 added to Real Time Viewer

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.



Trace *m/z* 311.09 added to Real Time Status display

❖ 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.

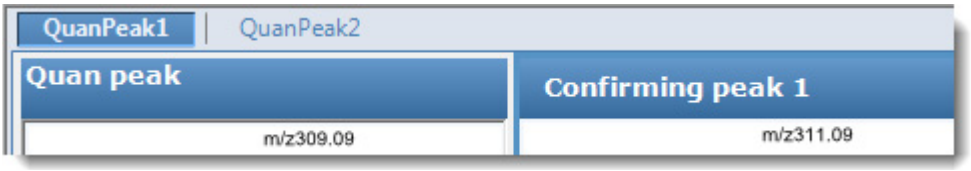
   The TraceFinder application replaces the confirming ion peak with the selected mass.

❖ 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 TraceFinder application adds the confirming ion peak to the quantitative peak.



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

   …\TraceFinderData\32\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 39. Detection page

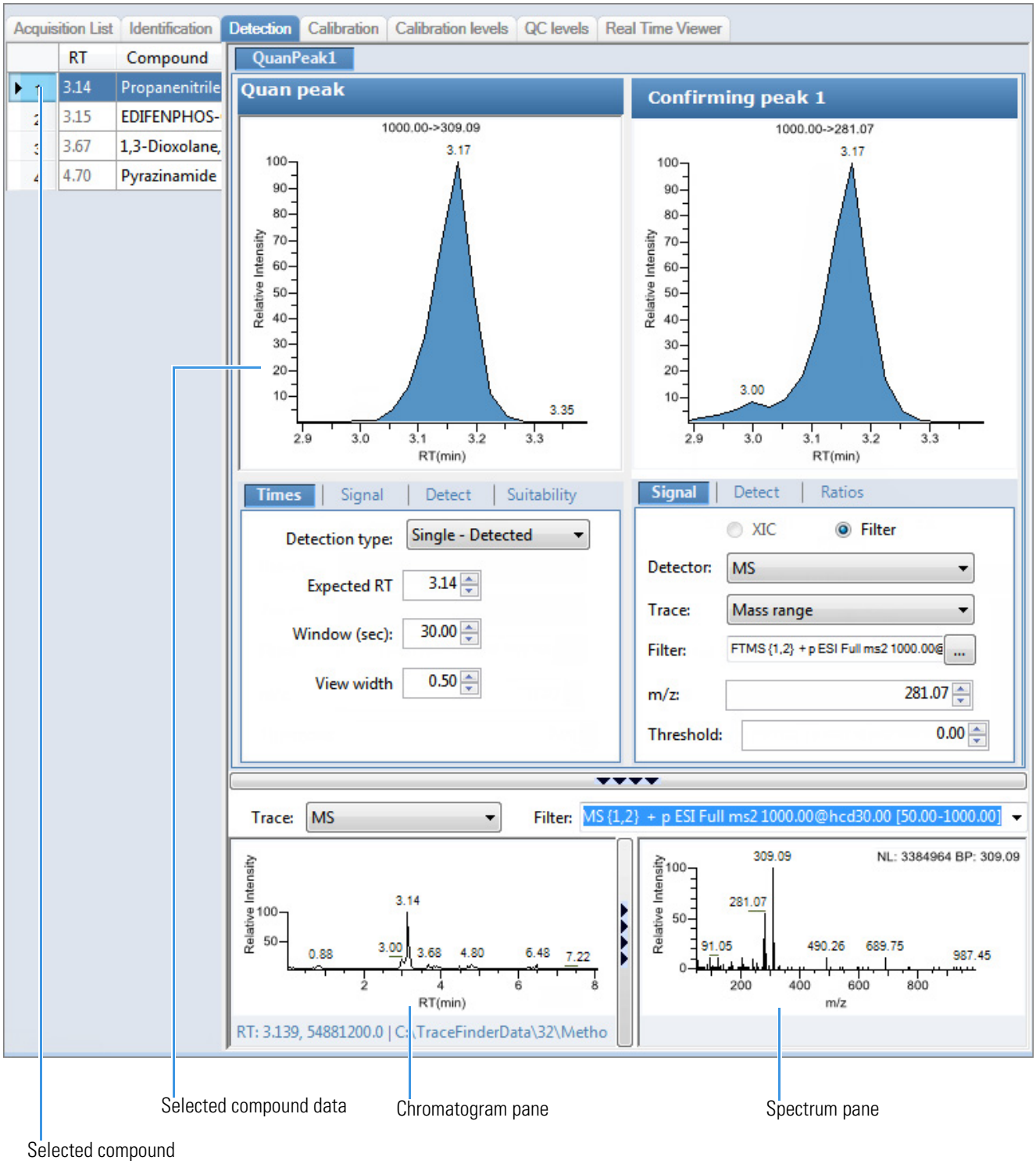


Table 22. Detection page panes

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 225.
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	Displays a combination of the Detector and Trace values used for the raw data file. 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 181. **Note** When you select a detector option other than MS or PDA, the spectrum pane reports "Not Available."
Filter	Displays the filter used for the raw data file. Available only when you set the Trace parameter to MS.
Reference Chromatogram and Spectra	Displays a reference chromatogram and spectra for the raw data file. 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 .
Additional pages	
Times	Defines the retention time and window for a quantitative peak. See "Times" on page 174.
Signal	Defines the detector and detection parameters used to display each chromatogram trace. See "Signal" on page 176.
Detect	Defines the peak detection algorithm and its options. See "Detect" on page 185.
Spectrum	Defines a reference mass spectrum for a quantitative peak or compound. See "Spectrum" on page 199.
Ratios	Defines the criteria for evaluating, confirming, or qualifying ions. See "Ratios" on page 213.

Times

Use the Times page to define the expected retention time or a retention time range for a quantitative peak.

Figure 40. Times page

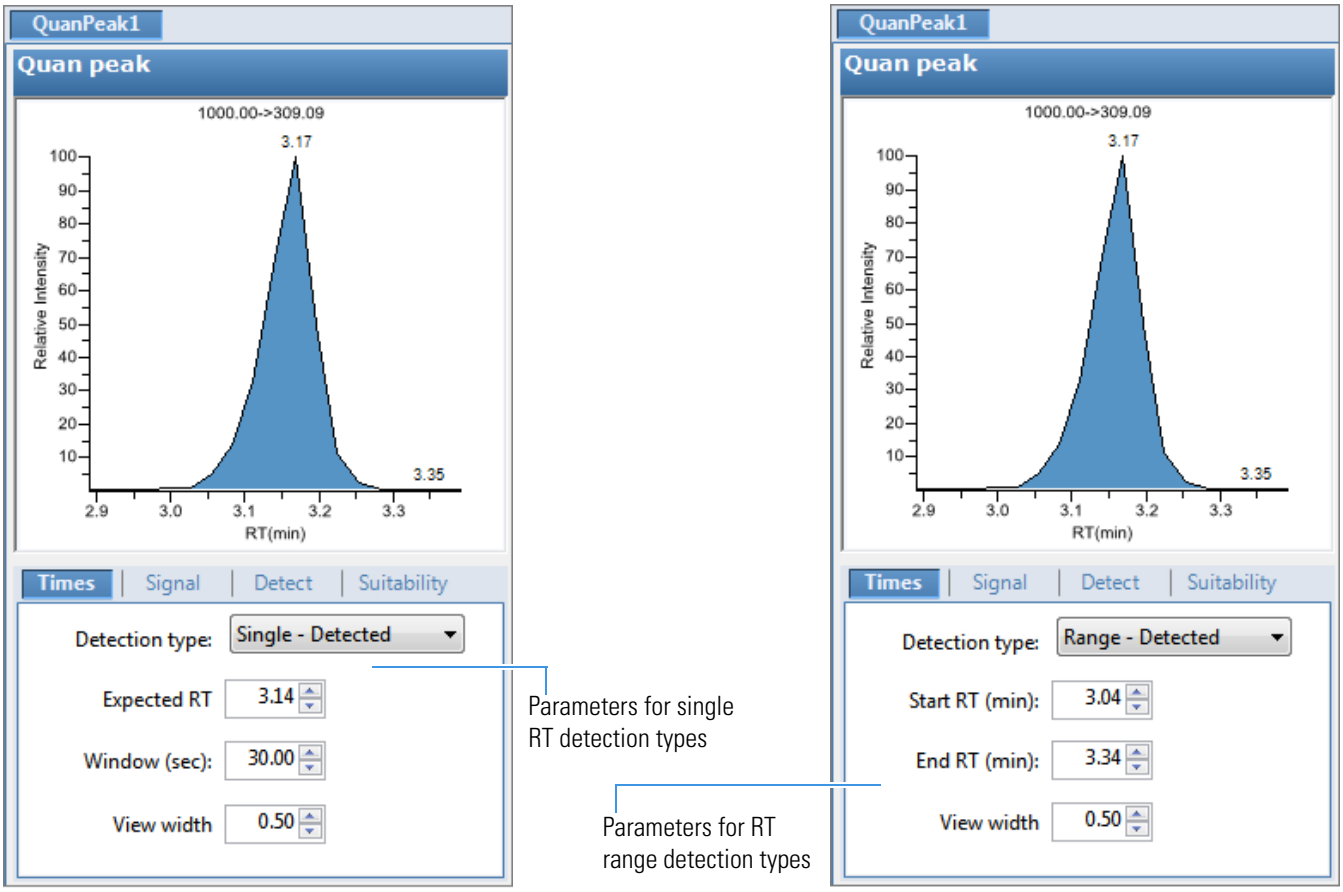


Table 23. Times page parameters (Sheet 1 of 2)

Parameter	Description
Detection Type	**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. **Range - Detected**: Specified as a retention time start/end range. **Range - Integrated**: Specified as a retention time start/end range. The application integrates all peaks within the specified time range.
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 23. 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 TraceFinder 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 (*end time* minus *start time*).
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 181. The TraceFinder application can use both analog detectors and mass spectrometer detectors. See "Signal page for a mass spectrometer detector" on page 181 or "Signal page for an analog detector" on page 182.

Follow these procedures:

- To specify ranges of ions for detection and integration
- To specify an XIC filter
- To specify an MS filter

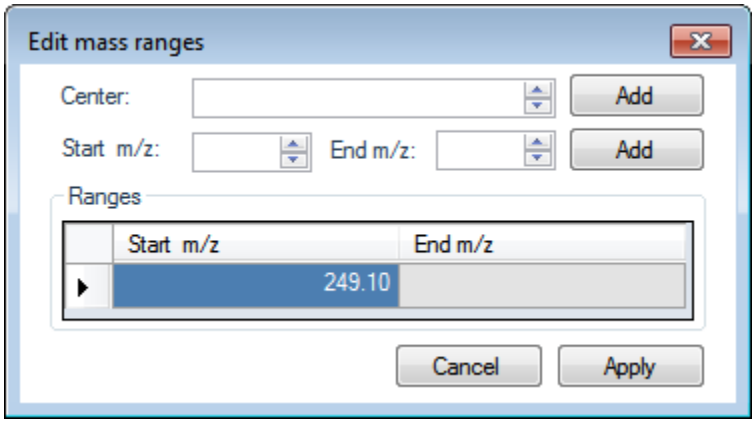
❖ To specify ranges of ions for detection and integration

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 41. 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.

   The Filter box indicates the parameters of the specified XIC filter, as in this example:

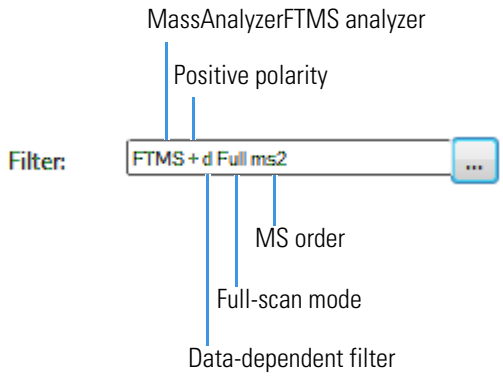


Figure 42. XIC Filter dialog box

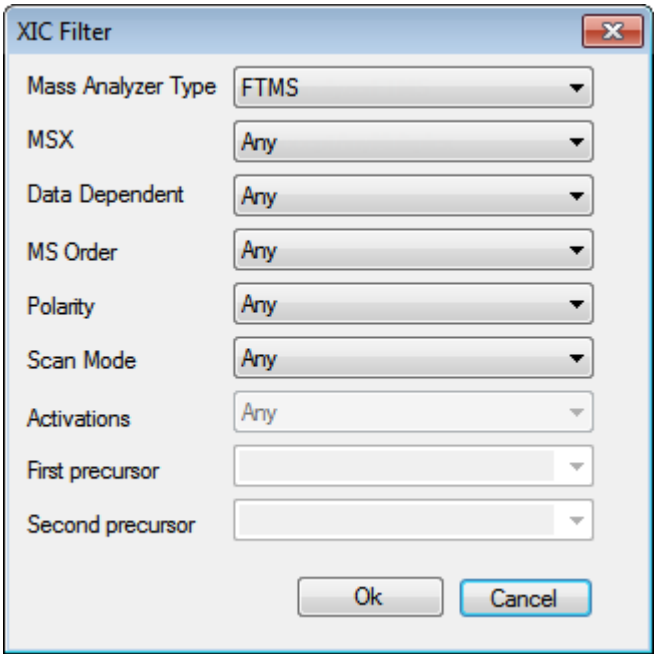


Table 24. XIC Filter dialog box parameters (Sheet 1 of 2)

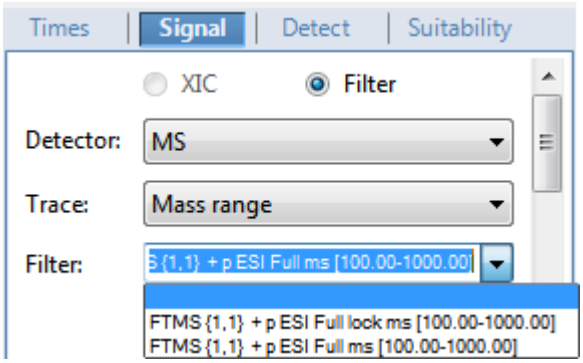
Parameter	Description
Mass Analyzer Type	Any: Allows any mass analyzer. FTMS: Fourier Transform Mass Spectrometer ITMS: Ion Trap Mass Spectrometer Sector: Static electric or magnetic sectors, or a combination of the two SQMS: Single Quad Mass Spectrometer TOFMS: Time-of-Flight Mass Spectrometer TQMS: Triple Quad Mass Spectrometer
MSX	Any: Allows both MSX and non-MSX scans. On: Allows only MSX scans. Off: Allows only non-MSX scans.
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

Table 24. XIC Filter dialog box parameters (Sheet 2 of 2)

Parameter	Description
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 182.

- Signal page for a mass spectrometer detector
- Signal page for an analog detector

Figure 43. Signal page for a mass spectrometer detector

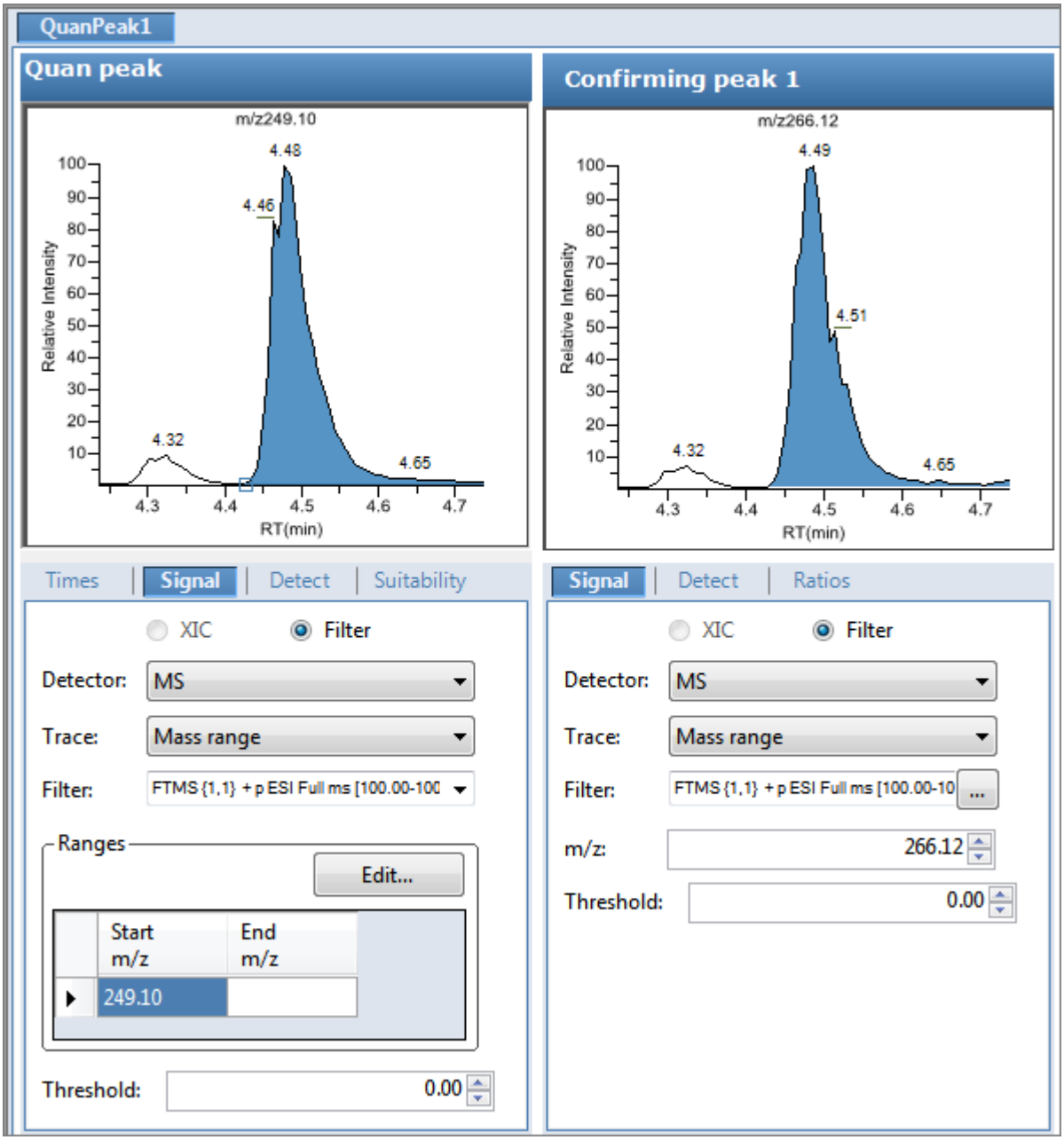


Figure 44. Signal page for an analog detector

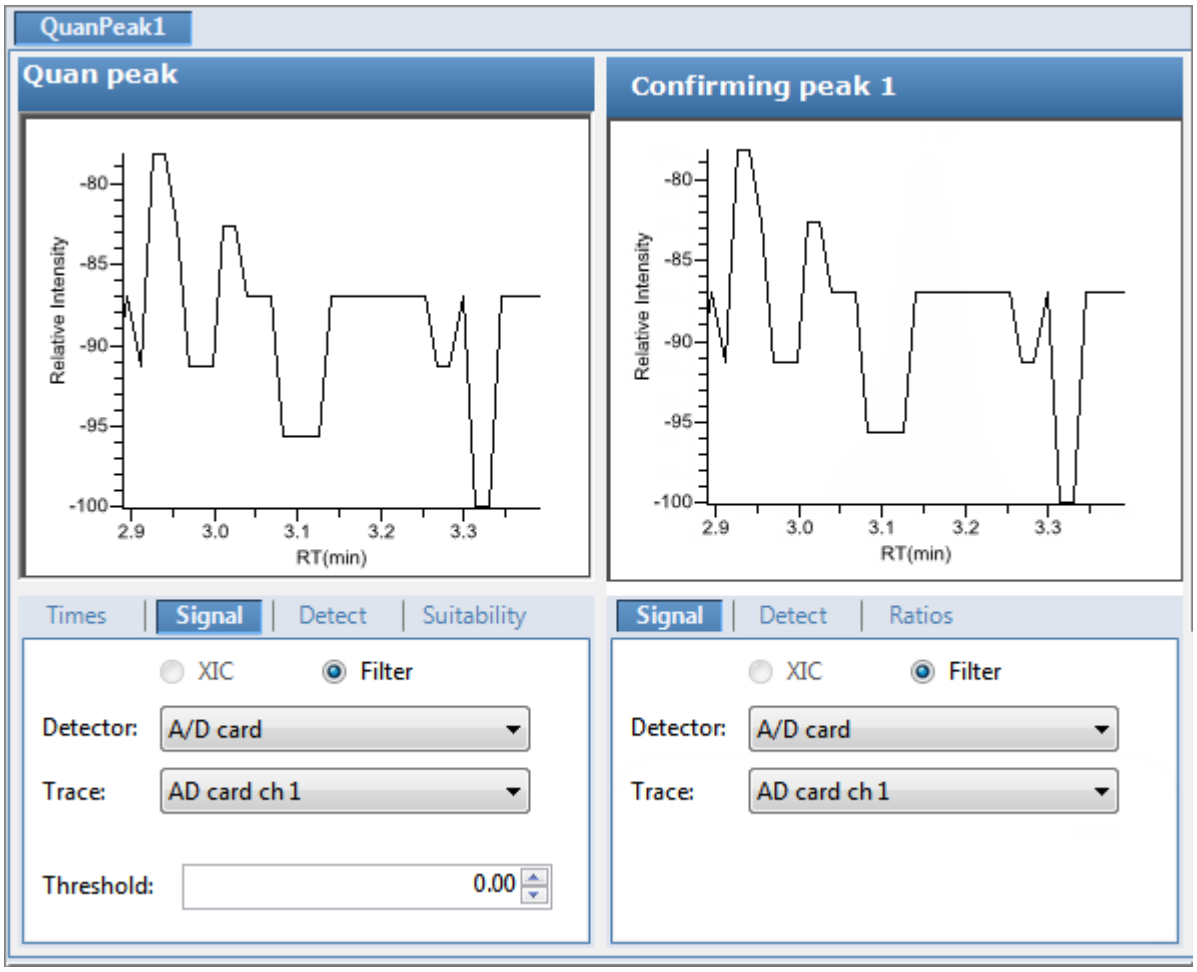


Table 25. Signal page parameters (Sheet 1 of 3)

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 25. Signal page parameters (Sheet 2 of 3)

Parameter	Description
Detector	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 37. MS: Mass spectrometer that ionizes sample molecules and then separates the ions according to their mass-to-charge ratio (*m/z*). 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 a range of wavelengths to be simultaneously detected. 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**. 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. 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.
Trace	Represents a specific range of the data. The TraceFinder application uses the trace to identify the characteristic ions for a compound. 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. PDA detector options: Spectrum Maximum, Wavelength Range, or Total Scan. Analog detector options: Analog 1, Analog 2, Analog 3, or Analog 4. You can configure these channel names in your instrument configuration. 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. UV detector options: Channel A, Channel B, Channel C, or Channel D. You can configure these channel names in your instrument configuration.
Filter	Available only when you select the MS detector. Represents a particular data acquisition channel. For example, the filter option *+ c Full ms [35.00-500.00]* represents a positive ion centroid signal acquired in single-stage, full-scan mode from *m/z* 35 to 500.

Table 25. 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 176.
Start *m/z* End *m/z*	Specifies ranges of ions for detection and integration. The application sums the multiple ions specified by these ranges. Ranges specified by a center mass value are listed as a single value in the Start *m/z* column. The application uses a range of one amu centered on this value.

Detect

Use the Detect page to define the peak detection algorithm (sensitivity) and its options and to determine the area under a curve. There are three sensitivity modes: Genesis, ICIS, and Avalon. 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 187.
- For ICIS sensitivity, see "Detect page parameters for ICIS" on page 191.
- For Avalon sensitivity, see "Detect page parameters for Avalon" on page 193.

Figure 45. Detect page for Genesis

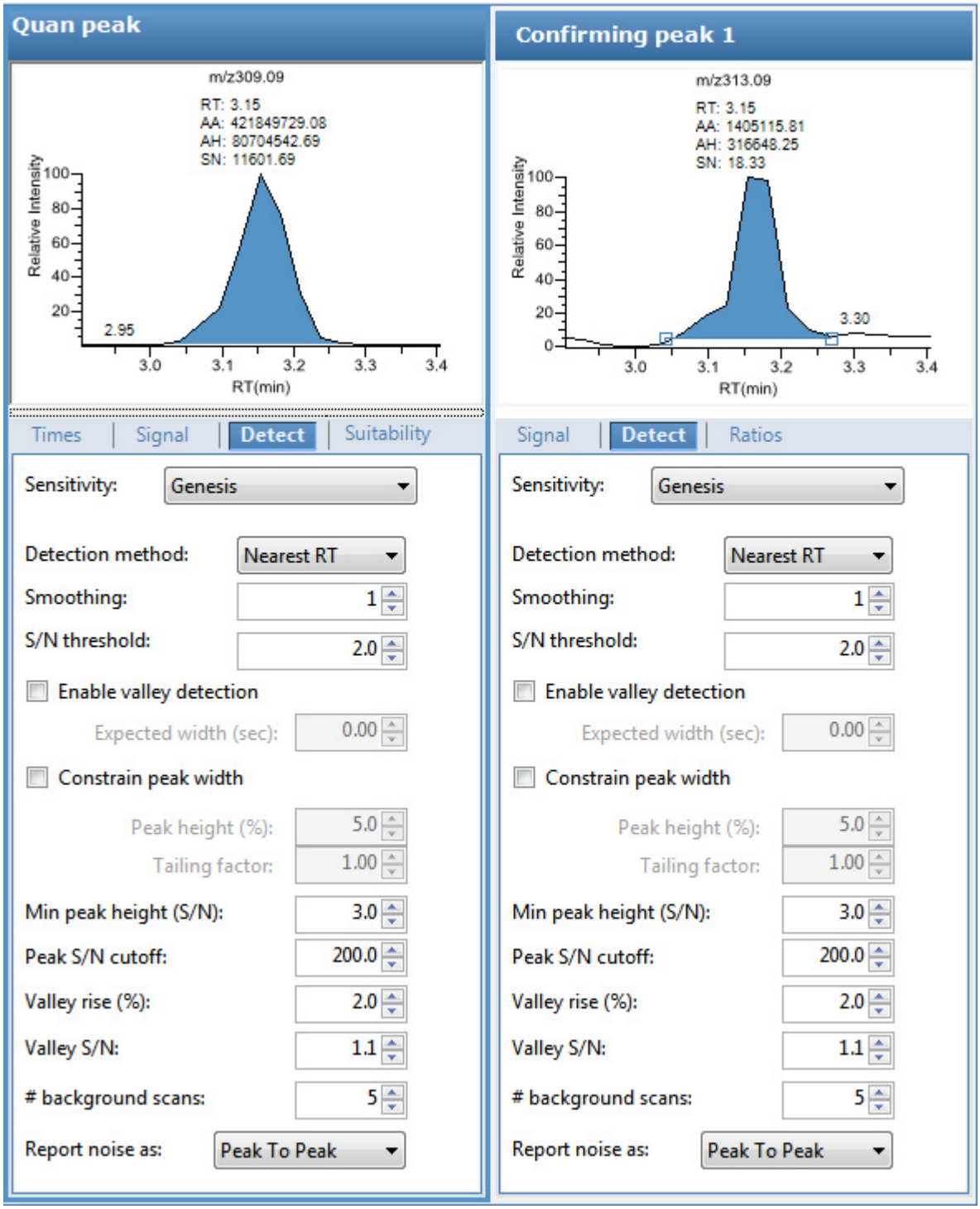


Table 26. Detect page parameters for Genesis (Sheet 1 of 3)

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.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Default: 1 Range: Any odd integer from 1 through 15 points
S/N Threshold	Current signal-to-noise threshold for peak integration. Peaks with signal-to-noise values less than this value are not integrated. Peaks with signal-to-noise values greater than this value are integrated. Range: 0.0 to 999.0
Enable Valley Detection	Uses the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Expected Width (sec)	The expected peak width parameter (in seconds). This parameter controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the *expected width*/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the TraceFinder application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. Range: 0.0 to 999.0
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box 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. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

Table 26. Detect page parameters for Genesis (Sheet 2 of 3)

Parameter	Description
Min Peak Height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0
Peak S/N Cutoff	The peak edge is set to values below this signal-to-noise ratio. This test identifies an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio. When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the TraceFinder application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 10000.0
Valley Rise (%)	The peak trace can rise above the baseline by this percentage after passing through a minimum (before or after the peak). This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. When the trace exceeds rise percentage, the TraceFinder application applies valley detection peak integration criteria. The TraceFinder application applies this test to both the left and right edges of the peak. The rise percentage criteria is useful for integrating peaks with long tails. Range: 0.1 to 500.0
Valley S/N	Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher. Default: 2.0 Range: 1.0 to 100.0
# Background Scans	Number of background scans performed by the TraceFinder application.
Report Noise As	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or a peak-to-peak resolution threshold. Options are RMS or Peak to Peak.
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.

Table 26. Detect page parameters for Genesis (Sheet 3 of 3)

Parameter	Description
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.

Figure 46. Detect page for ICIS

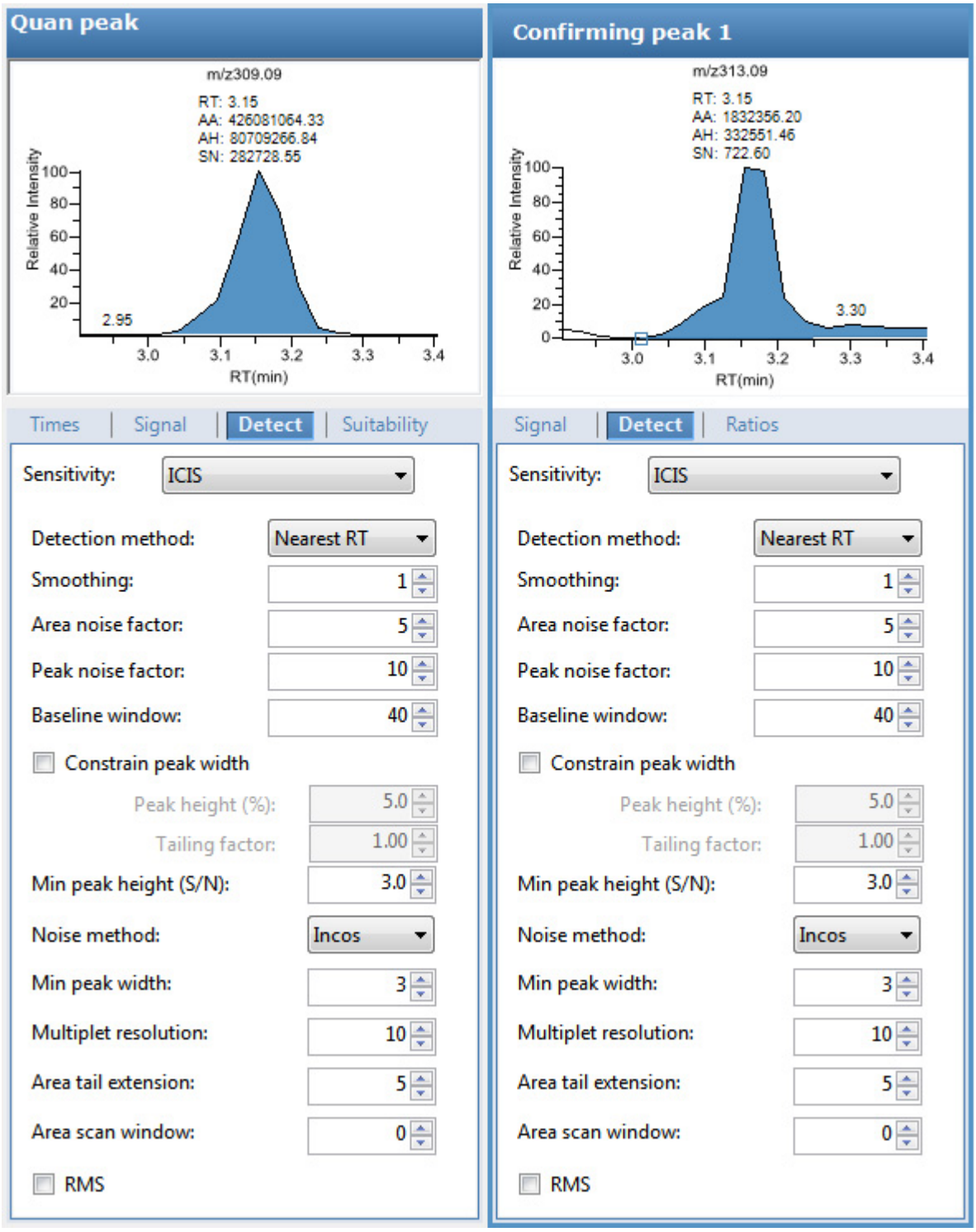


Table 27. Detect page parameters for ICIS (Sheet 1 of 2)

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.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Default: 1 Range: Any odd integer from 1 through 15 points
Area Noise Factor	The noise level multiplier used to determine the peak edge after the location of the possible peak. Default: 5 Range: 1 through 500
Peak Noise Factor	The noise level multiplier used to determine the potential peak signal threshold. Default: 10 Range: 1 through 1000
Baseline Window	The TraceFinder application looks for a local minima over this number of scans. Default: 40 Range: 1 through 500
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. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0
Min Peak Height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0

Table 27. Detect page parameters for ICIS (Sheet 2 of 2)

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. Default: 3 Range: 0 to 100 scans
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. Default: 10 Range: 1 to 500 scans
Area Tail Extension	The number of scans past the peak endpoint to use in averaging the intensity. Default: 5 Range: 0 to 100 scans
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. Default: 0 Range: 0 to 100 scans
RMS	Specifies that the TraceFinder application calculate noise as RMS. By default, the application uses Peak To Peak for the noise calculation. RMS is automatically selected if you manually determine the noise region.
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 47. Detect page for Avalon

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

Parameter	Description
Sensitivity	Specifies the Avalon peak detection algorithm.
Detection Method	Highest Peak: Uses the highest peak in the chromatogram for component identification. Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.

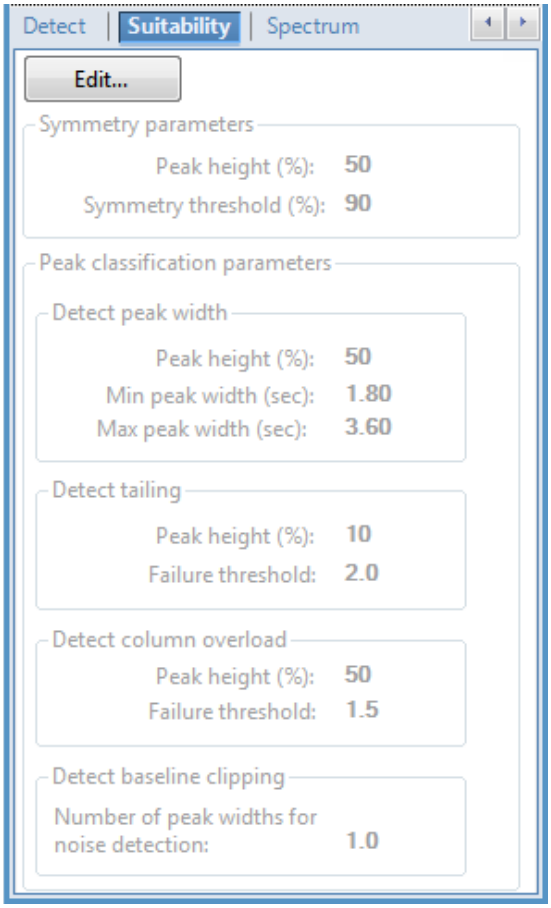
Table 28. Detect page parameters for Avalon (Sheet 2 of 2)

Parameter	Description
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Default: 1 Range: Any odd integer from 1 through 15 points
Autocalc Initial Events	Automatically calculates the events in the Event list.
Edit	Opens the Avalon Event List dialog box. See "Avalon Event List" on page 49.
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.

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.



❖ To set system suitability parameters

1. Click **Edit**.

   The System Suitability dialog box opens. See "System Suitability dialog box" on page 197.

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 48. System Suitability dialog box

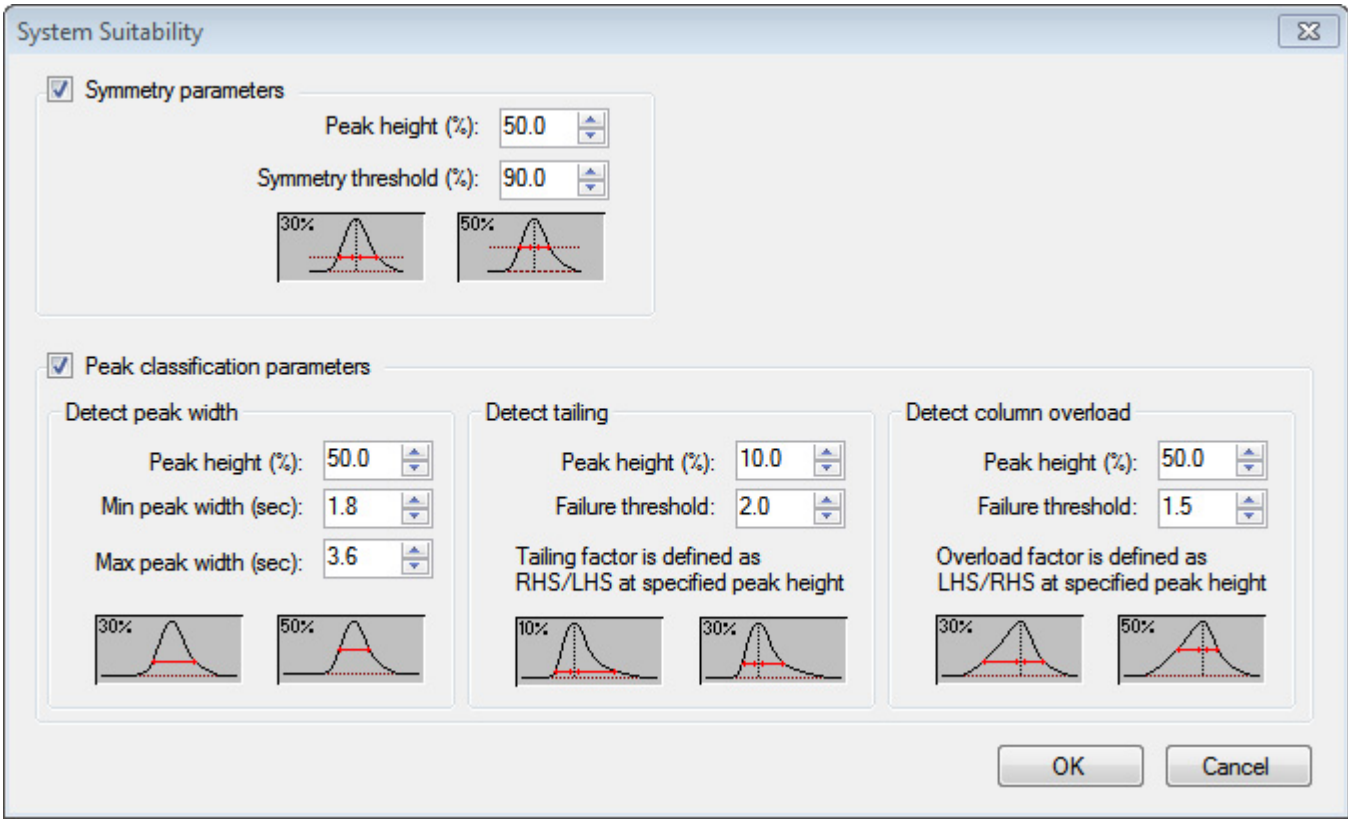


Table 29. System Suitability dialog box parameters (Sheet 1 of 2)

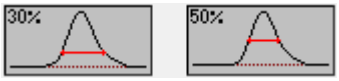
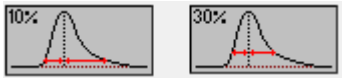
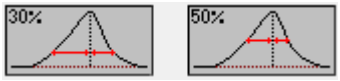
Parameter	Description
Symmetry Parameters	Determines the symmetry of the left and right sides of the detected peak.
Peak Height	The percentage of the peak height at which to compare the symmetry of the left and right peak widths. Left and right widths measured at 30% and 50% of the peak height
Symmetry 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.  Full width measured at 30% and 50% of the peak height
Min Peak Width	Minimum peak width (measured at the specified percentage of the peak height) required to pass the suitability test.

Table 29. 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.  Left and right widths measured at 10% and 30% of the peak height
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.  Left and right widths measured at 30% and 50% of the peak height
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 204.

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 146.

❖ 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.

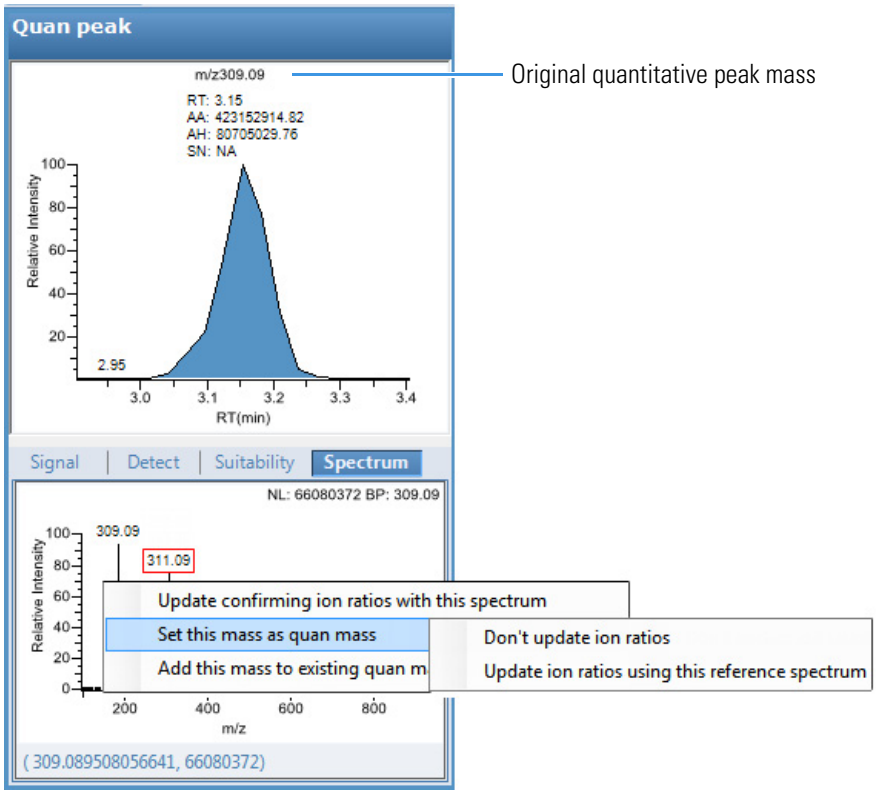
   A red box around the ion's *m/z* value indicates that the ion is selected.

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**

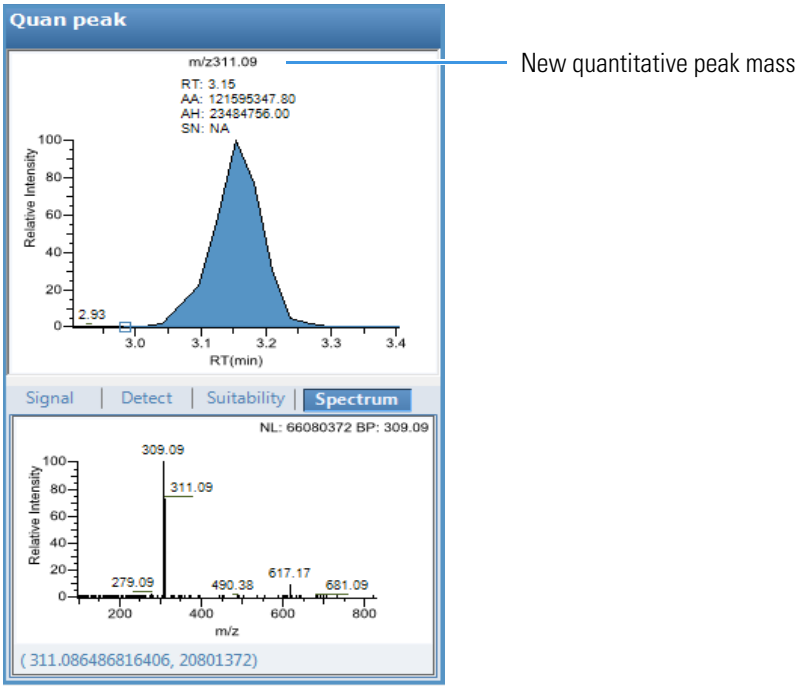
The following examples show an original quantitative peak and a quantitative peak with an updated quantitation mass.

Figure 49. Original quantitative peak mass example



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

Figure 50. 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.

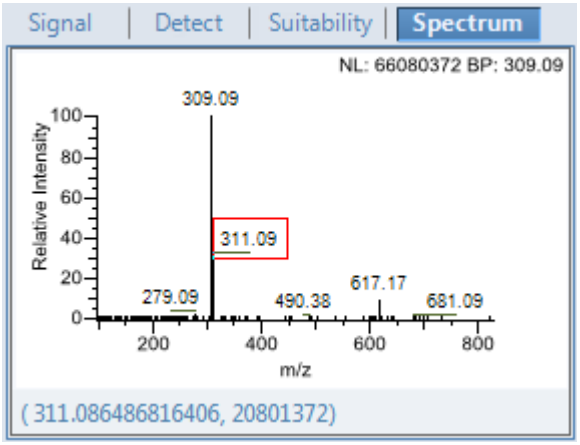
❖ To add a quantitative peak to an existing compound

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

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

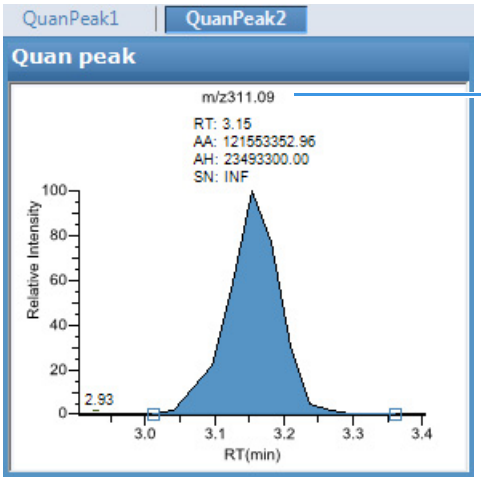
2. In the Spectrum pane, hold the cursor over the *m/z* value for an ion.

   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 TraceFinder application adds this ion as a new quantitative peak.



New quantitative peak mass

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

1. Click the quantitative peak in the chromatogram pane.

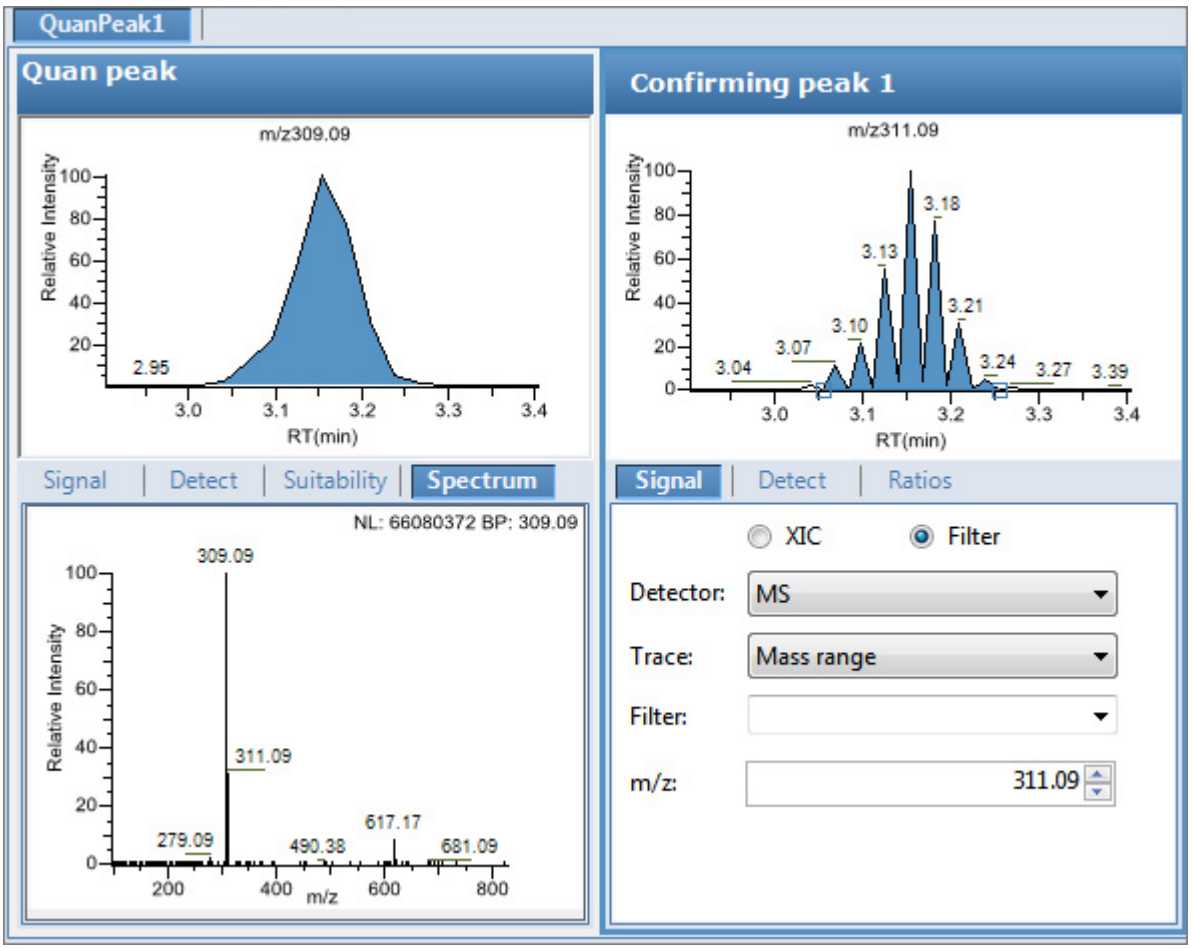
   The mass spectrum for the peak is displayed in the Spectrum pane.

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 TraceFinder 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 51. Spectrum page

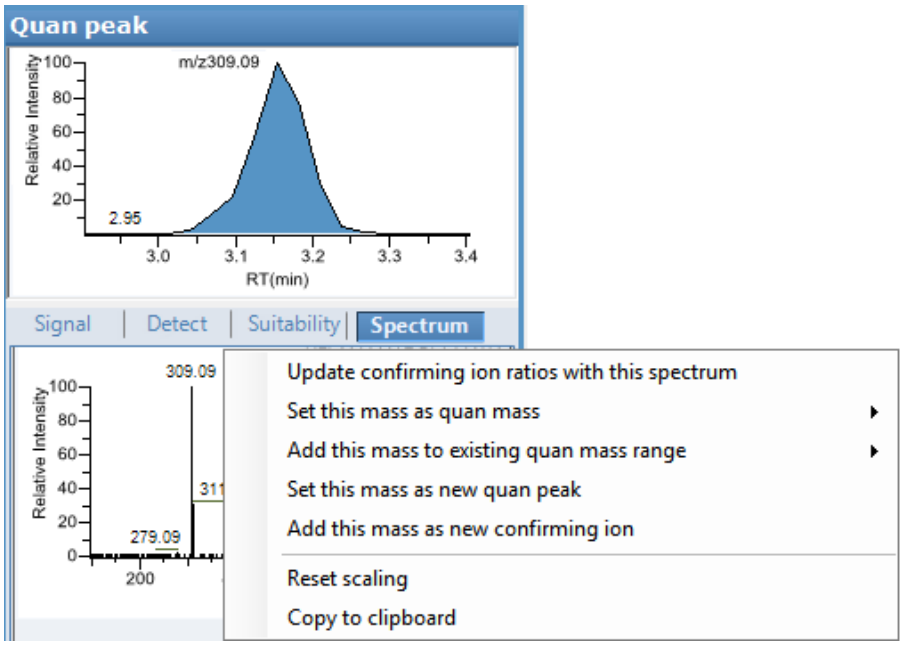


Table 30. Spectrum page shortcut menu commands

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 12.

     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.

   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).
3. Type a threshold value in the Score Threshold box.

   To match a compound, the resulting score percentage from a library search match must be higher than your entered threshold value.
4. (Optional) Select the **Use Reverse Library Searching Only** check box.

   A reverse search compares a library entry to an unknown compound (a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).

Figure 52. Library page

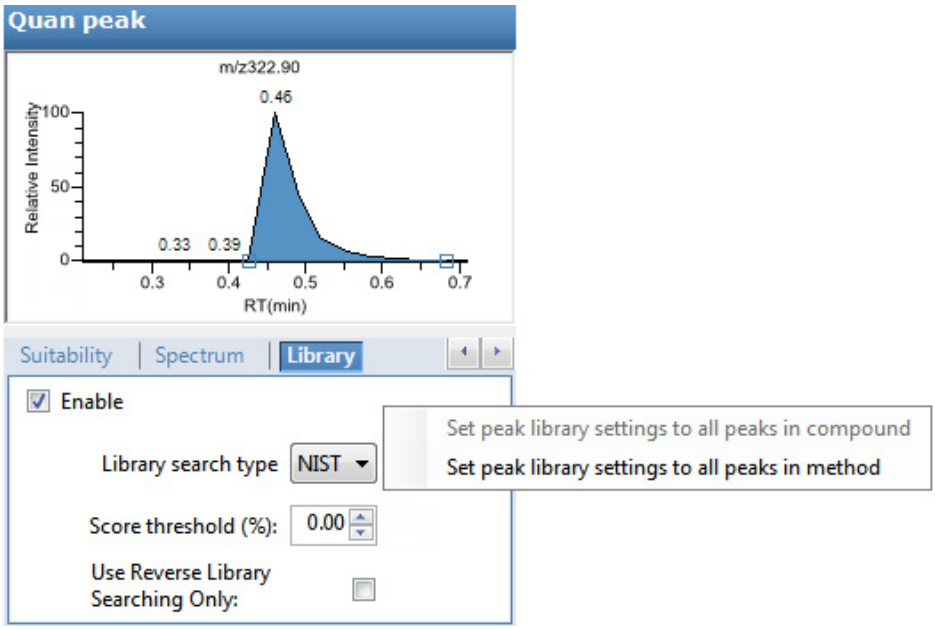


Table 31. Library page parameters

Command	Description
Library Search Type	Specifies the type of library to use for matching. • **NIST**: Uses the NIST library that you installed with the TraceFinder application. • **Library Manager**: Uses the library that you specified in the Configuration console.
Score Threshold (%)	Specifies the minimum score for library matching. To match a compound, the resulting score percentage from a library search match must be higher than this threshold value.
Use Reverse Library Searching Only	A reverse search compares a library entry to an unknown compound (a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
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 53. Isotopes page

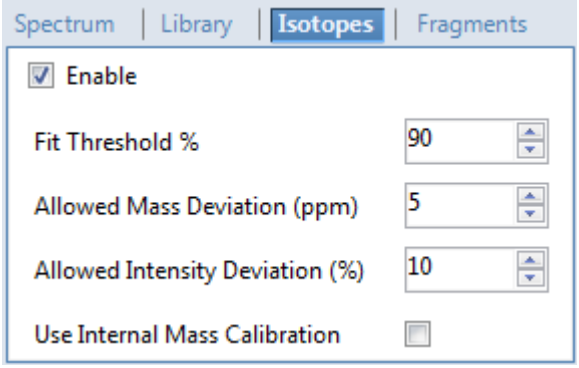


Table 32. Isotopes page parameters (Sheet 1 of 2)

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. Range: 3 to 100 ppm Default: 3 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. 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. Default: 10%
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.

Table 32. Isotopes page parameters (Sheet 2 of 2)

Parameter	Description
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* ± 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 54. Fragments page

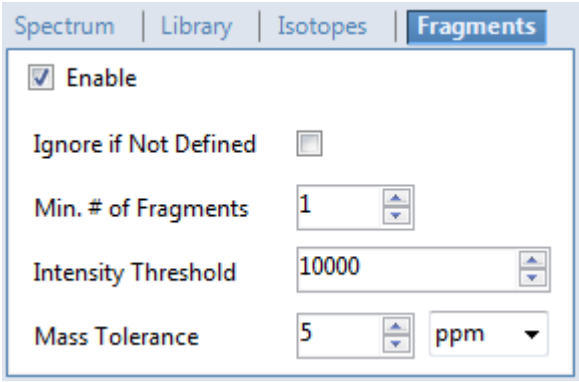


Table 33. Fragments page parameters (Sheet 1 of 2)

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. Range: 1 to 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. Range: 1 to 1e9 Default: 10 000
Mass Tolerance	Specifies the number of millimass units or parts per million to use as the *m/z* ± tolerance value for the fragment ions and is separate from the mass tolerance specified for the parent (see "Editing the Acquisition Page" on page 146). Range: 0 to 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.

Table 33. Fragments page parameters (Sheet 2 of 2)

Parameter	Description
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

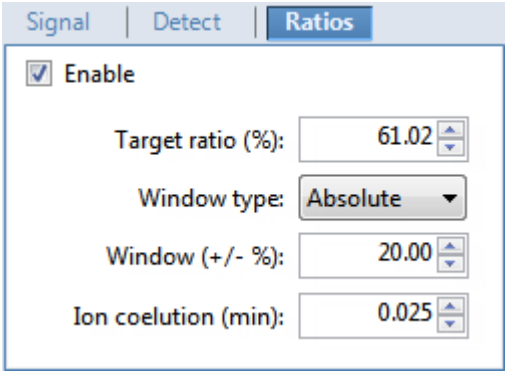
Use the Ratios page to define the criteria for evaluating the confirming or qualifying ions. The TraceFinder application detects compounds that have confirming ion values outside their acceptable window and flags them in the Acquisition mode and in reports.

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%.



   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 55. Ratios page

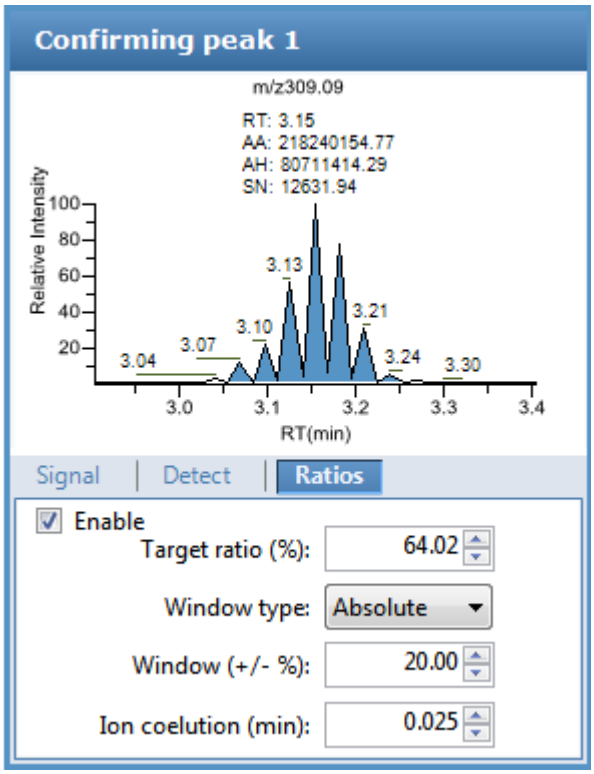


Table 34. Ratios page parameters

Parameter	Description
Enable	Makes the ion ratio criteria available.
Target Ratio (%)	The theoretical ratio of the confirming ion's response to the quantification ion's response.
Window Type	The absolute or relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	The acceptable ion ratio range.
Ion Coelution (min)	The maximum difference in retention time between a confirming ion peak and the quantification ion peak.
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 217.

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 158.
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.

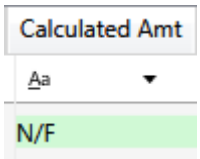
To view the internal standard peak in the Analysis mode, see "Compound Details" on page 468.

❖ 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.



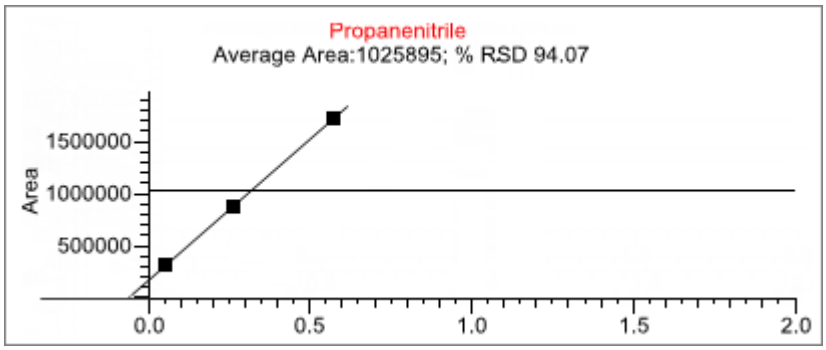
❖ To specify a standard addition standard type for a compound

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 56. 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 35. 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.

Table 35. Calibration page parameters (Sheet 2 of 2)

Parameter	Description
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.
Estimation Method	This column is unavailable for editing when the standard type is set to Estimated. • 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 225.

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 226.

❖ 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-

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.

Manage Calibration levels

	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.
   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.

Acquisition List | Identification | Detection | Calibration | Calibration levels | QC Check levels | Real Time V

	RT	Compound	Cal1	Cal2	Cal3
1	3.15	Pyrazinamide	5.000	10.000	15.000
2	3.67	1,3-Dioxolane, 2-heptyl-			

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 57. Calibration Levels page

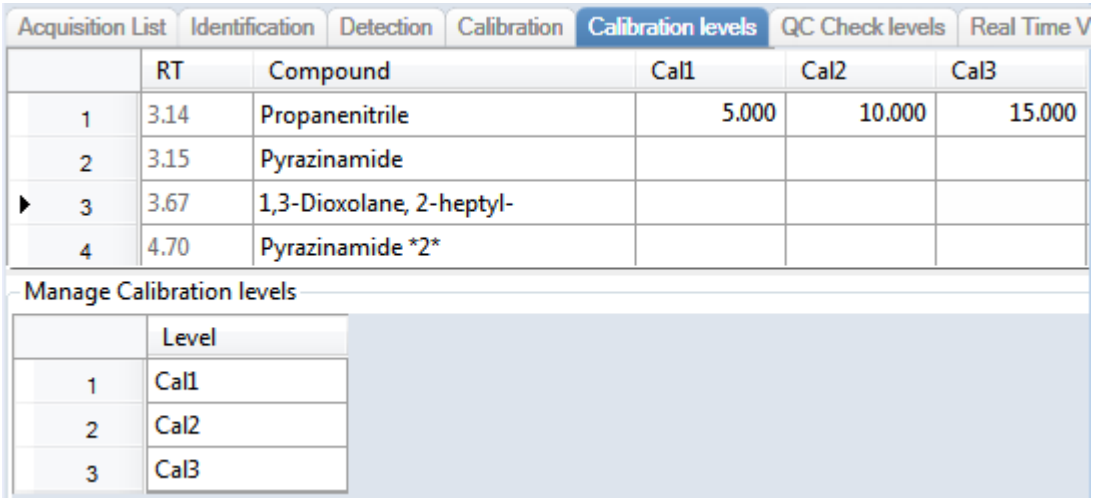


Table 36. Calibration Levels page parameters

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.
CalLevel_1–CalLevel_n	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 225.

QC Check Levels

Use the QC Check Levels page for a master method to define the standards for QC Check levels. You can edit QC Check 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 QC Check Levels page, see "QC Check Levels page" on page 222.

You can use the copy-and-paste functions in the shortcut menu to copy QC Check levels from one column to another or from one master method to another. For detailed instructions, see "Copying and Pasting Column Values" on page 226.

❖ To specify QC Check levels and concentrations

1. Select the compound whose QC Check 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 QC Check Levels area, type a name for the first QC Check level.

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

3. Type a value for the % Test.

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

Manage QC Check levels

	Level	% Test
1	Level1	5.00
* 2		NA

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

Manage QC Check levels

	Level	% Test
1	Level1	5.00
2	Level2	5.00
▶ 3	Level3	5.00

When you finish adding QC Check 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 QC Check level table cell.
   b. Click the cell again to make it editable.
   c. Type a concentration value.
6. Repeat step 5 for all QC Check levels associated with the first compound.

Acquisition List | Identification | Detection | Calibration | Calibration levels | QC Check levels | Real Time V

	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 58. QC Check Levels page

Acquisition List | Identification | Detection | Calibration | Calibration levels | QC Check levels

	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 QC Check levels

	Level	% Test
1	Level1	5.00
2	Level2	5.00
3	Level3	5.00

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 350.

Figure 59. Real Time Viewer page

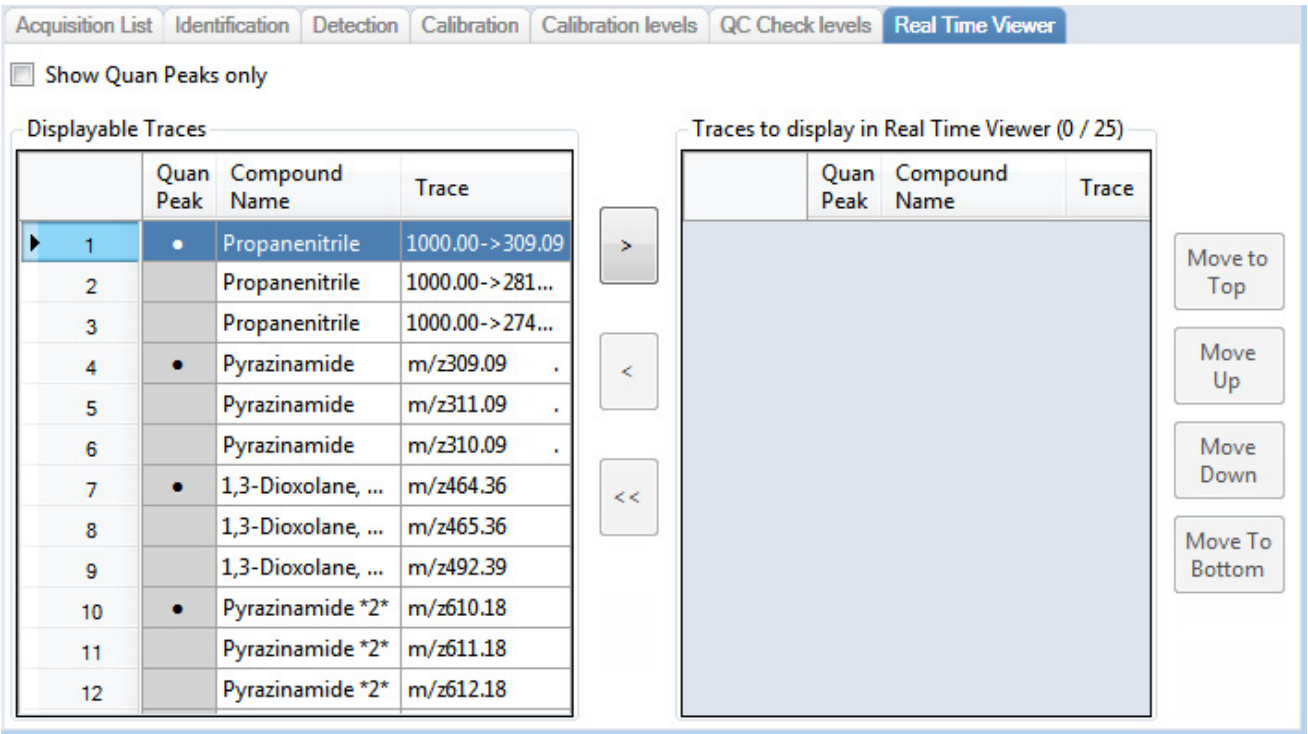


Table 37. Real Time Viewer page parameters (Sheet 1 of 2)

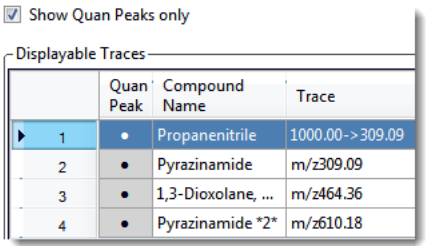
Parameter	Description
Show Quan Peaks Only	Displays only quantitative peaks in the compounds list. Quantitative peaks are indicated with a black dot in the Quan Peak column. 
Displayable Traces	
Quan Peak	Dots indicate quantitative peak traces. Unmarked traces indicate confirming ion peaks.
Compound 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.

Table 37. Real Time Viewer page parameters (Sheet 2 of 2)

Parameter	Description
>	Moves the selected trace to the Traces to Display in Real Time Viewer pane.
<	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 365. 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.

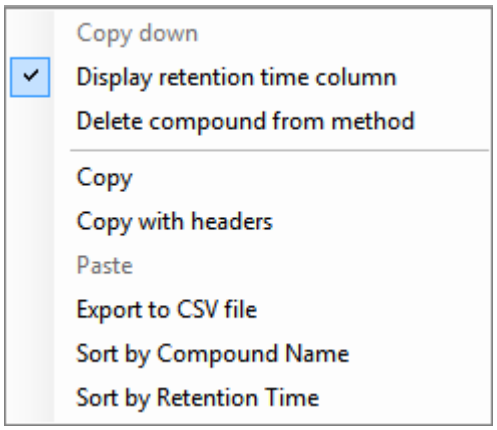


Table 38. Compounds page shortcut menu commands (Sheet 1 of 2)

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.
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.

Table 38. Compounds page shortcut menu commands (Sheet 2 of 2)

Command	Description
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.

Table 39. QC Check 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.
Level_1–Level_n	User-defined quality control levels for the compound.
Manage QC Check Levels	
Level	User-defined quality control level names. The names you enter here become the column headers for the QC Check levels.
% Test	A value for the acceptable difference (as a percentage) between the known amount and calculated (measured) amount of each QC Check level.
Shortcut menu	The QC Check Levels page uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 225.

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.

Following these procedures:

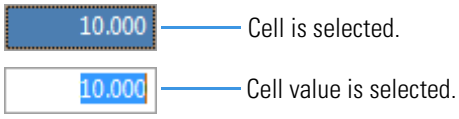
- To copy a value from one cell to another cell

- 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.

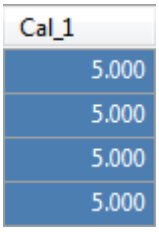
3. In this or another master method, select the cell value or table cell that you want to overwrite.
   - If you copied a cell value, you can select the cell value or simply click in the cell.
   - If you copied an entire cell, you must select a table cell to overwrite.

4. Right-click and choose **Paste** from the shortcut menu.

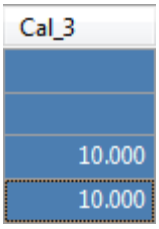
   The application replaces the selected value with the value copied to the Clipboard.

❖ To copy all values in a column to another column

1. Use the SHIFT key to select the column to copy.

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.

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.
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.

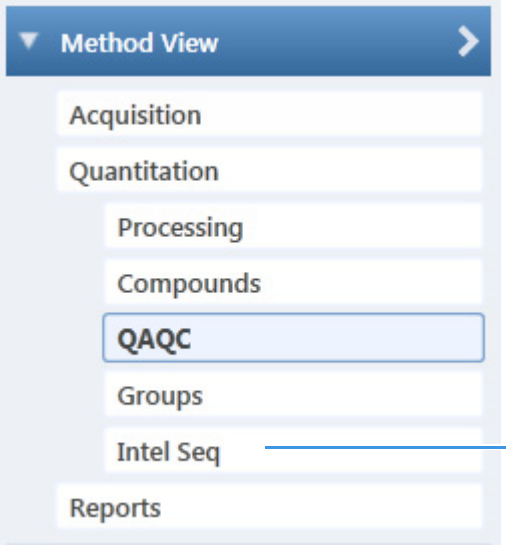
Editing the QAQC Page

Use the QAQC page to set limits and ranges so that the TraceFinder 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 226.

❖ 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
- QC Check
- Negative
- ISTD
- Solvent Blank
- Hydrolysis
- 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 60. Limits page

Limits | Calibration | QC Check | Negative | ISTD | Solvent Blank | Hydrolysis | 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 40. 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.
Cutoff	Also called limit of reporting (LOR) in some industries. This is the lowest amount that can be reported, as determined by each laboratory's standard operating practices.
ULOL (Linearity Limit)	Upper limit of linearity. This is usually the highest calibrator amount.
Carryover Limit	The highest amount of a substance that does not leave a residual amount in the instrument. If a substance has a carryover limit of 5, amounts higher than 5 usually dirty the instrument and leave residue behind, tainting the following sample. A carryover limit of less than 5 does not leave any residual amounts of the substance.

Calibration

Use the Calibration page to define acceptable criteria for initial calibration. The TraceFinder application 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 61. Calibration page

Limits | Calibration | QC Check | Negative | ISTD | Solvent Blank | Hydrolysis | 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 41. 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 217.
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.

QC Check

Use the QC Check page to review the calibration on an ongoing basis. The TraceFinder 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 Quality Control report, the TraceFinder application flags the calculated values for internal standard compounds that exceed these limits.

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

Figure 62. QC Check page

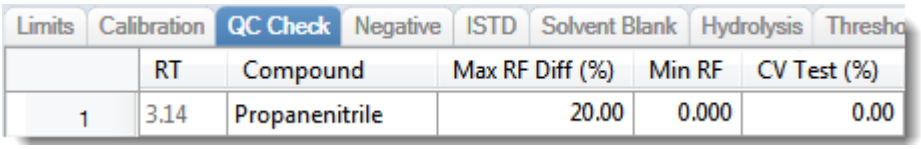


Table 42. QC Check page parameters

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 sample and the average response factor from the calibration (when in average RF mode).
Min RF	The minimum response factor for the QC 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.

Negative

Use the Negative page to define acceptable levels of target compounds in blank samples. The TraceFinder 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 Negative page, see Negative page parameters.

In the Negative report, the application flags the calculated values for target compounds that exceed these limits.

❖ To specify the maximum concentration as a percentage

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

❖ To specify the maximum concentration

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

Figure 63. Negative page

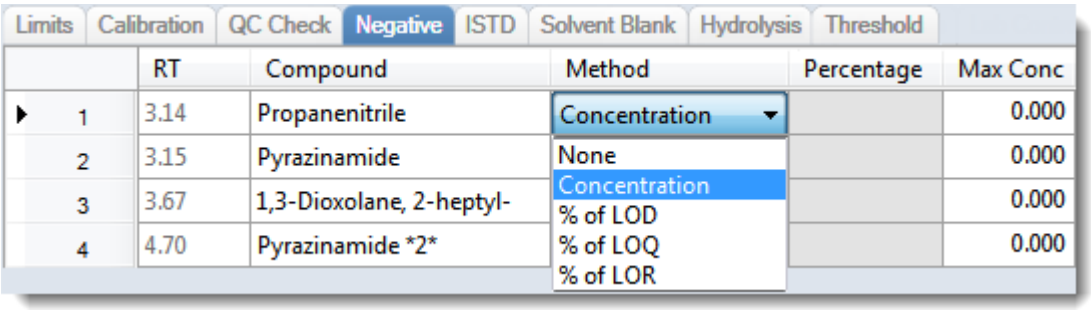


Table 43. Negative page parameters

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 TraceFinder 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 64. ISTD page

Limits | Calibration | QC Check | Negative | ISTD | Solvent Blank | Hydrolysis | 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 44. 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 (%) Max Recovery (%)	The minimum and maximum percent recoveries for the internal standards to define an acceptable range. For check standards, the TraceFinder application compares the response of each internal standard in each sample to a range around the average of the responses of that compound in all of the calibration standards. For all other samples, the application calculates the comparison range around the check standard responses if a check standard is available in the batch. If no check standard is available, the application tests against the initial calibration.
Min RT (–min) Max RT (+min)	The minimum and maximum drift (in minutes) for the internal standards to define an acceptable range. For check standards, the TraceFinder application compares the retention time of each internal standard in each sample to a range around the average of the retention times of that compound in all of the calibration standards. For all other samples, the application calculates the comparison range around the check standard retention times if a check standard is available in the batch. If no check standard is available, the application tests against the initial calibration.
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 TraceFinder application flags the calculated values for target compounds that exceed these limits.

Figure 65. Solvent Blank page

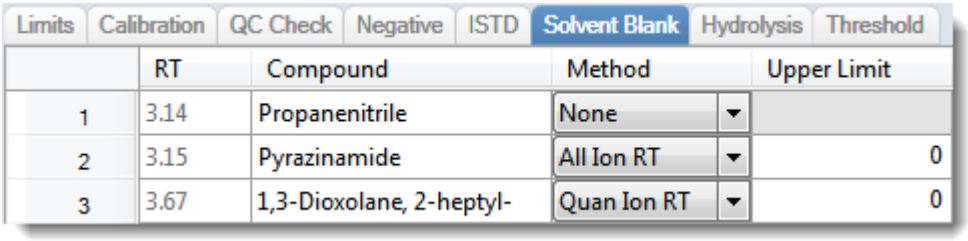


Table 45. Solvent Blank page parameters

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 238) 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 436.

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 412.

In the following figures, the threshold for the dibutyl phthalate compound is 50 percent of the peak height in the threshold sample, the samples Benzo26473, Benzo25557, and Benzo26154 are members of groupB, and the threshold sample for the group is Benzo26473. In the Comparative Data view, 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 66. QAQC page in Method View

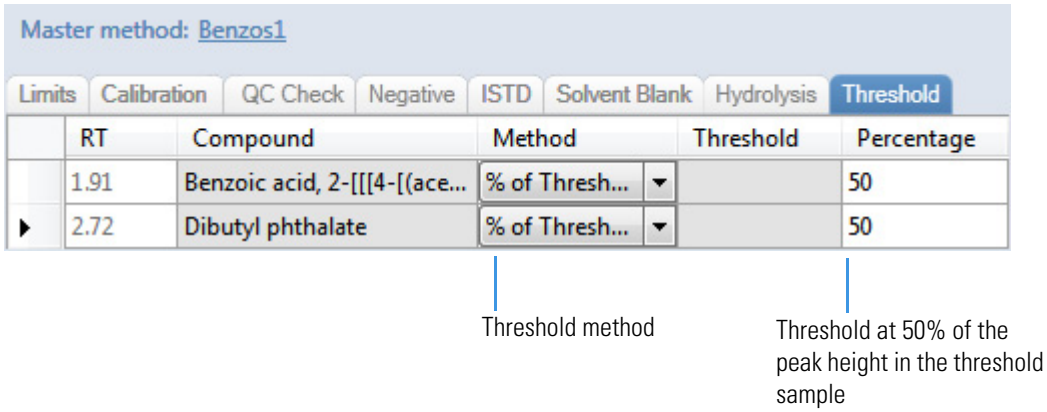


Figure 67. Samples page in Batch View

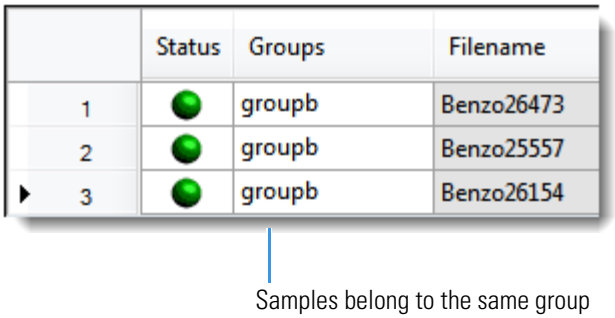


Figure 68. Threshold Samples page in Batch View

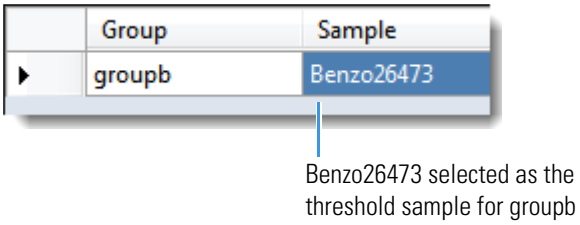


Figure 69. Comparative View in Data Review

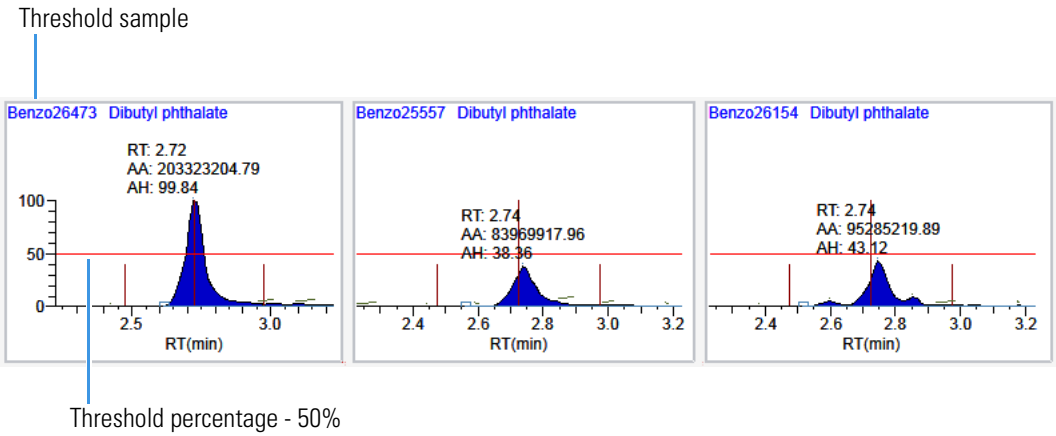


Figure 70. Threshold page

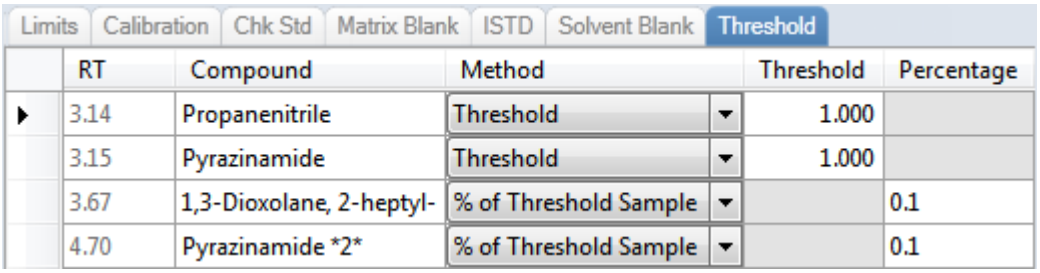


Table 46. Threshold page parameters (Sheet 1 of 2)

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.
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).

Table 46. Threshold page parameters (Sheet 2 of 2)

Parameter	Description
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 412. Default: 0.1 Range: 0.1 to 100.1

Hydrolysis

Use the Hydrolysis page to specify the hydrolysis checks for compounds.

Figure 71. Hydrolysis page

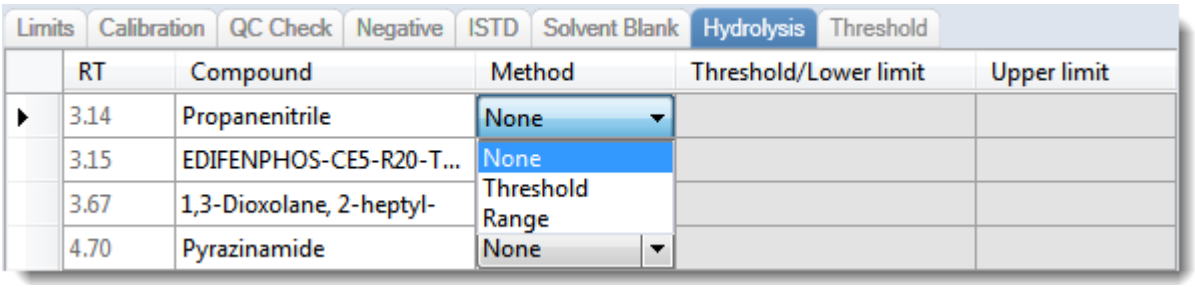


Table 47. Hydrolysis page parameters

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Method	The evaluation process to use, specified as either a lower threshold or a range. To deactivate the hydrolysis test for a specific compound, select **None**.
Threshold/Lower Limit	For compounds using the Threshold method, this specifies the threshold value for the hydrolysis test. Values below this threshold are flagged in the Hydrolysis report. For compounds using the Range method, this specifies the lower limit of the range.
Upper Limit	For compounds using the Range method, this parameter specifies the upper limit of the range.
Shortcut menu	
Copy Down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix C, "Using Copy Down and Fill Down."
Display Retention Time Column	Displays or hides the RT column in the compound list.
Delete Compound From Method	Removes the selected compound from the current master method.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy compound information to another application, such as an Excel spreadsheet. You cannot paste this data back into the method development compound list.
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 compound information to another application, such as an Excel spreadsheet.
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column. The pasted data must be valid data for the selected column.
Undo Last Paste	Removes the last pasted item in the method development compound list.
Export to CSV File	Opens the Save As dialog box where you can save the current compound list to a CSV file.

Editing the Groups Page

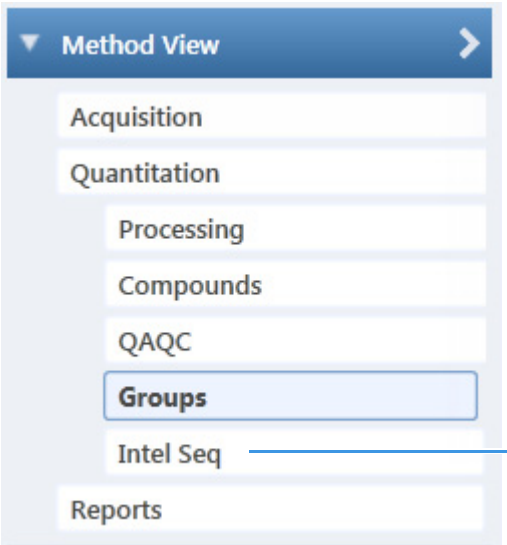
Use the Groups page of the Method View to organize compounds into functional or logical groups. You can use these groups for creating a subset of target compounds. For detailed descriptions of all the features on the Groups page, see "Groups Page."

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

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

❖ To 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**.

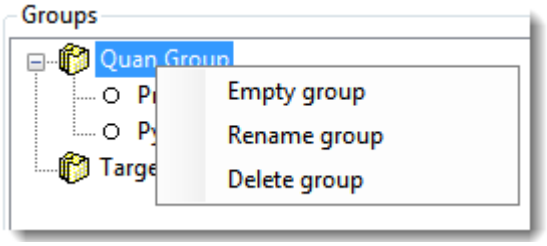
   The Add a New Group dialog box opens.

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

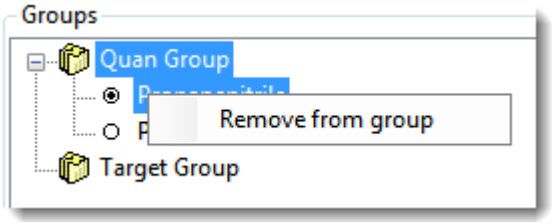
   The new group appears in the Groups area.

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 72. Groups page

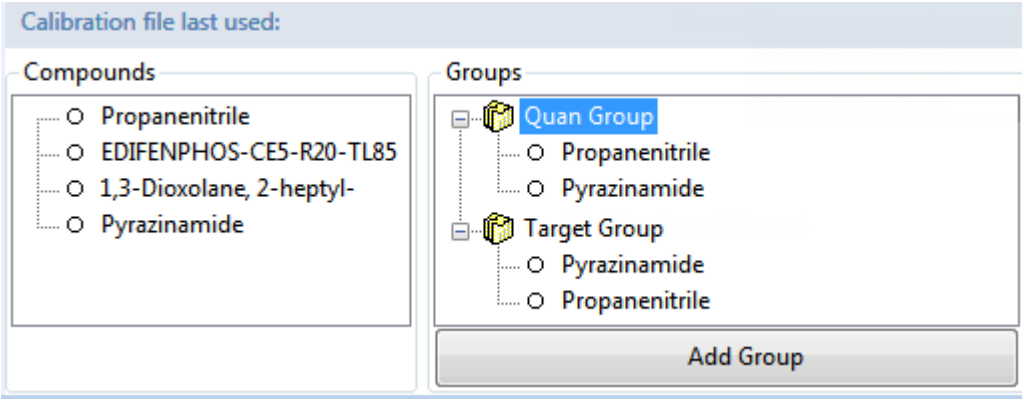


Table 48. Groups page parameters (Sheet 1 of 2)

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.

Table 48. Groups page parameters (Sheet 2 of 2)

Parameter	Description
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.

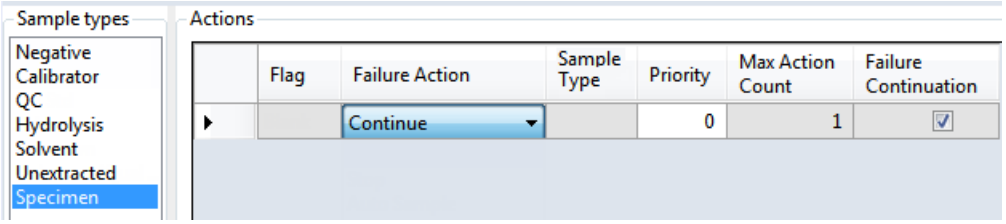
Editing the Intelligent Sequencing Page

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.



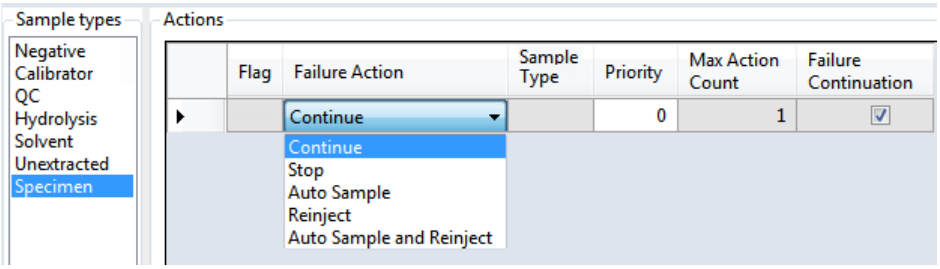
❖ To specify actions for sample acquisition failures

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 248.

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 Negative sample types. The Solvent and Negative sample types do not have Auto Sample or Auto Sample and Reinject failure actions.



   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" on page 247.

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 409.

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 TraceFinder application uses when the acquisition for a sample fails.

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.

Actions

	Flag	Failure Action	Sample Type	Priority	Max Action Count	Failure Continuation
▶	Negative	Continue		0	1	☑

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: • **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.
Sample Type	Specifies either a Solvent or Negative sample type to use for the auto sample injection. Default: Solvent
Priority	The priority value can be any positive or negative integer. 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. The application performs the failure action for the highest priority failure and ignores all others.

Table 49. Actions parameters (Sheet 2 of 2)

Parameter	Description
Max Action Count	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. Default: 1
Failure Continuation	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. Default: Selected 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.

Sample-Specific Failure Flags

Each sample type has a specific set of failure flags.

Sample Type	Flag
Negative	• Negative
Calibrator	• Cal Out of Range • Ion Ratio Failure • Carryover
QC	• Ion Ratio Failure • Out of Range
Hydrolysis	• Ion Ratio Failure • Hydrolysis
Solvent	• Solvent Flag
Unextracted	• Ion Ratio Failure
Specimen	• Ion Ratio Failure • Carryover

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.

This section includes instructions for the following tasks:

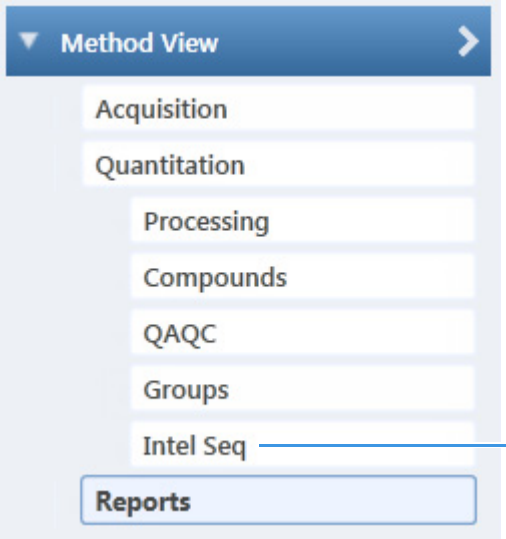
- Specifying Report Formats
- Specifying Quan Report Settings

Specifying Report Formats

For each report type, you can create a hard-copy printout, a PDF file, or an XML file.

❖ To open the Reports page

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



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

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 72.

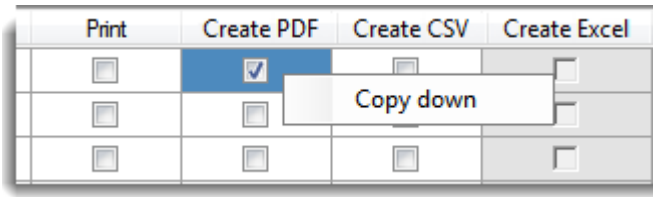
❖ To specify report types and output formats

1. To edit the Report Title, double-click the name and type your new custom title.

   The TraceFinder 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 type, 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. 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 73. Reports page

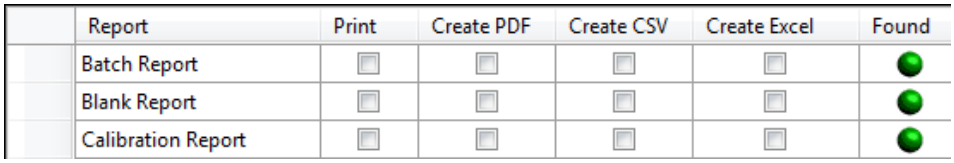


Table 50. Reports page parameters

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.
Found	Indicates that the report template is identified in the C:\TraceFinderData\32\Templates\ReportTemplates folder.

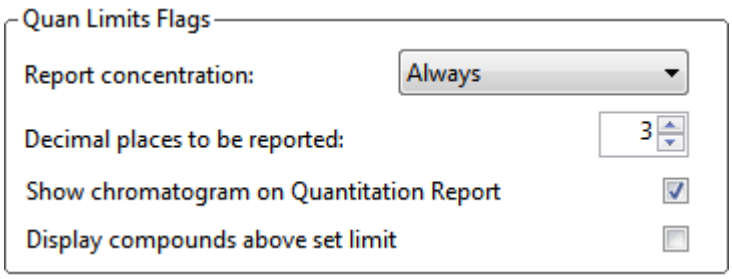
Specifying Quan Report Settings

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 254.

Follow these procedures:

- To specify quantitation limits
- To specify user interface options
- To specify quantitation flag options
- To specify the concentration calculation method
- To track the use of the tune file

❖ To specify quantitation limits



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

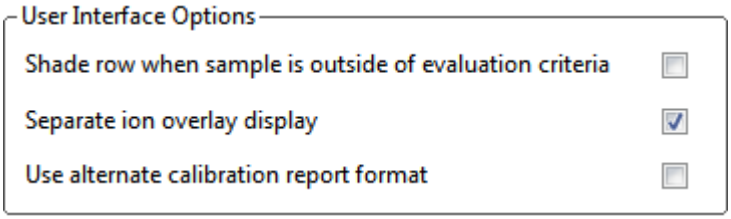
   For a description of concentration limits, see "Editing the QAQC Page" on page 230.

2. To select the number of decimal places to report for calculated concentrations, set the value in the Decimal Places to be Reported box.

3. To include a chromatogram of the sample in the Quantitation Report, select the **Show Chromatogram on Quantitation Report** check box.

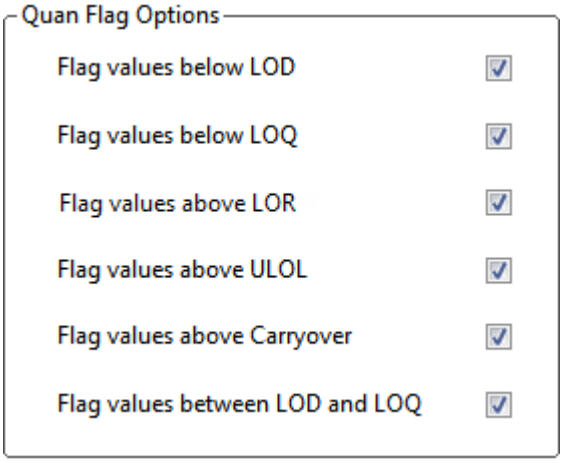
4. To display only valid compounds, select the **Display Compounds Above Set Limit** check box.

❖ To specify user interface options



1. To shade a compound row 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

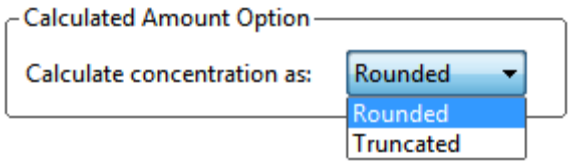


Select the values that you want to display in the report.

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 254.

❖ To specify the concentration calculation method

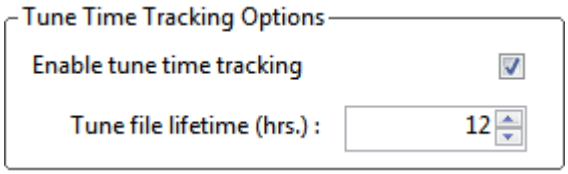


In the Calculate Concentration As box, select **Rounded** or **Truncated**.

- **Rounded**: Rounds the calculated amount to the nearest value using the number of decimal places specified in the Quan Limits Flags area.
- **Truncated**: Truncates the calculated amount at the number of decimal places specified in the Quan Limits Flags area.

See "To specify quantitation limits" on page 251.

❖ To track the use of the tune file



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

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

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

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

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 74. Quan Report Settings page

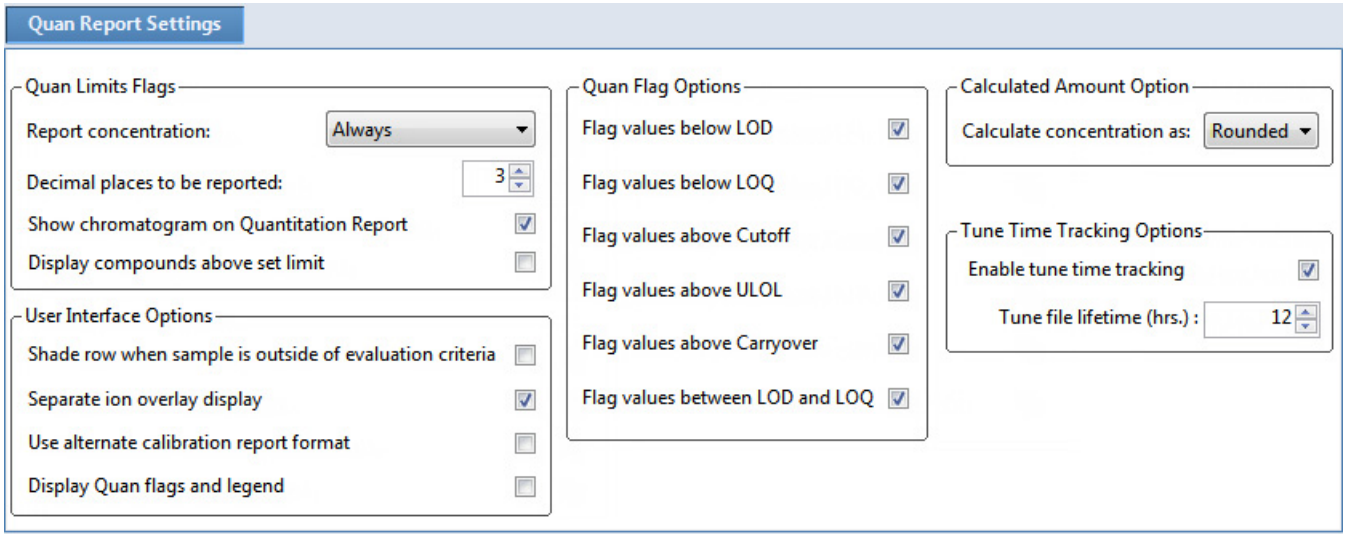


Table 51. Quan Report Settings page parameters (Sheet 1 of 2)

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 TraceFinder 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.
Separate Ion Overlay Display	Separates the ion overlay pane from the confirming ion plots in an analysis.

Table 51. Quan Report Settings page parameters (Sheet 2 of 2)

Parameter	Description
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.
Calculated Amount Option	
Calculate Concentration As	Specifies the Rounded or Truncated method for reporting concentration amounts.
Tune Time Tracking Options	
Enable Tune Time Tracking	Tracks the number of hours between the last instrument tune and each sample acquisition.
Tune File Lifetime	Specifies the maximum number of hours between the last instrument tune and a sample acquisition. Any sample acquired outside this maximum allowable time is flagged in the Batch report.

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.

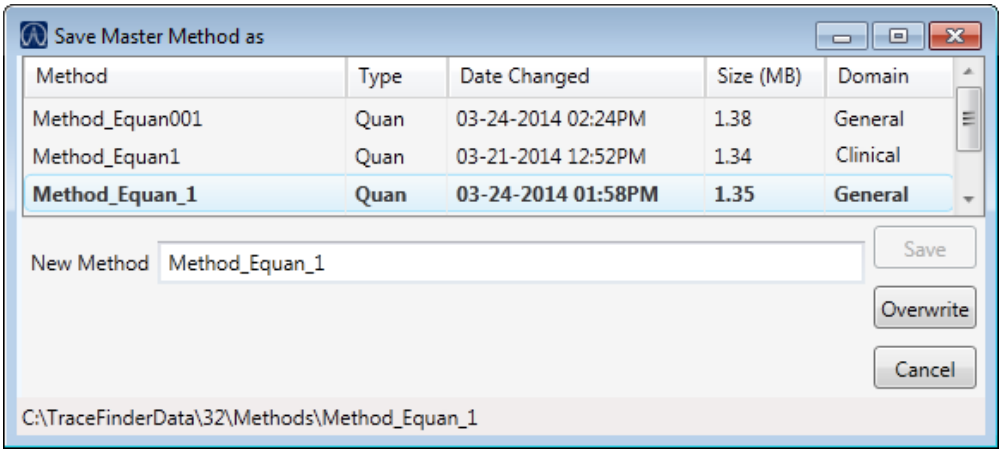


Table 52. Save Master Method As dialog box parameters

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan or Screening.
Date Changed	Date the method was last updated.
Size	Size in megabytes.
Domain	TraceFinder domain for which the method was created.
New Method	Name of the new method to create.
Path	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 263.

The application uses the settings in the method template to identify the data to display in the Qualitative View. See "Qualitative View" on page 444.

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.

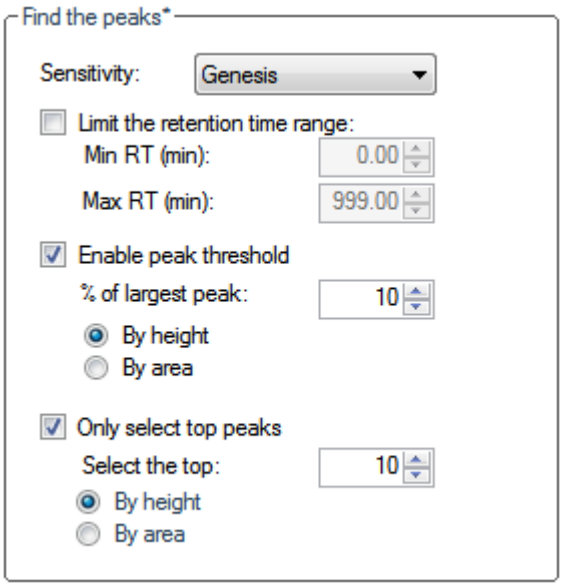
   The Method Development navigation pane opens.

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 263.

❖ To specify peak criteria



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.

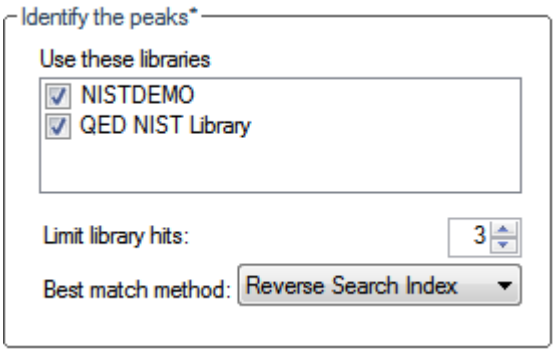
2. To look for peaks only in a certain range of the entire chromatogram, select the **Limit the Retention Time Range** check box and specify a retention time (RT) range.

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 TraceFinder 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



Note Parameters in the Identify the Peaks* area might also be used for qualitative peak processing.

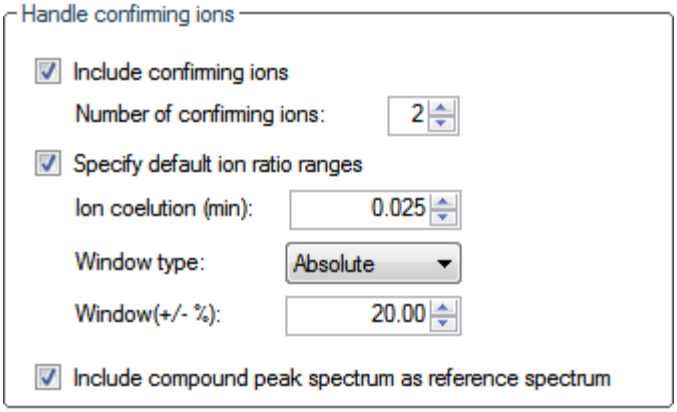
1. In the Use these Libraries box, select the libraries that you want to search.

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

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

3. To specify how to sort the library searches, select a value from the Best Match Method list.

❖ To specify confirming ions



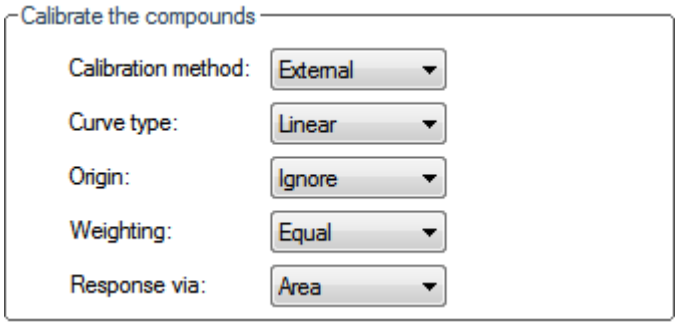
1. To set the number of confirming ions, select the **Include Confirming Ions** check box and enter a value in the Number of Confirming Ions box.

   This value is the number of other ions in the spectrum whose ratio is compared to the quantitation ion. Using this ratio, you can then determine if it is the target compound or something else. You can set this value to integers from 1 to 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.

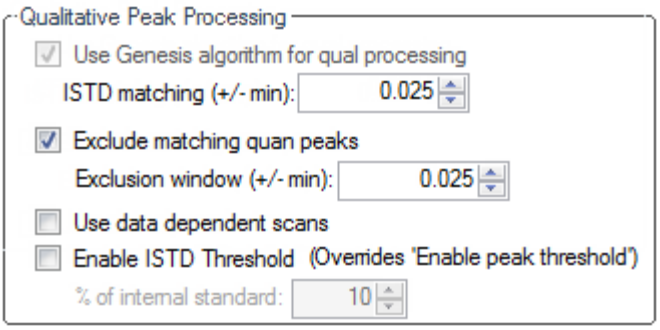
❖ To calibrate the compounds



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/X^2**: Specifies a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity.
   - **1/Y**: Specifies a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio).
   - **1/Y^2**: Specifies a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).
5. From the Response Via list, select **Area** or **Height**.
   - **Area**: Specifies that the TraceFinder application use this area value in response calculations.
   - **Height**: Specifies that the application use this height value in response calculations.

❖ To specify qualitative peak processing



1. Select the **Use Genesis Algorithm for Qual Processing** check box and specify a value for internal standard matching.

   The application uses the Genesis algorithm to match internal standards in a range plus/minus the value that you specify. For additional information about the Genesis algorithm, see "Genesis Detection Method" on page 42.

   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 MS^n scan.

   This option constrains the Data Review to only data-dependent scan spectra. See "Working in the Local Method View" on page 519.

   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 TraceFinder 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 258.

   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 TraceFinder application saves the new method template in the following folder:

   …\TraceFinderData\32\Templates\Methods\Clinical

   Saved method templates are available when you create a method using Method Forge. See "Creating a New Method with Method Forge" on page 125.

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 75. Method Template Editor dialog box

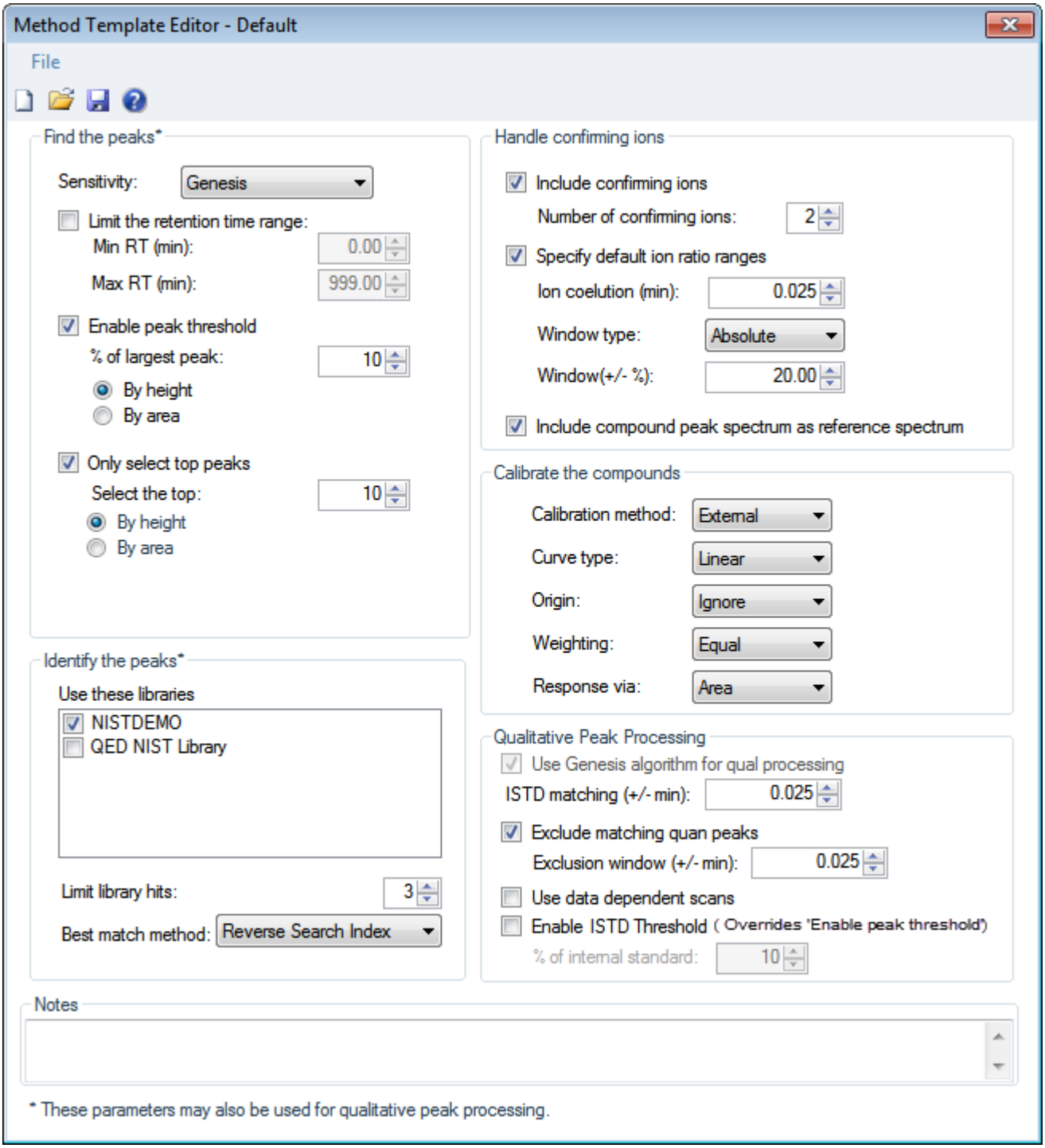


Table 53. Method Template Editor dialog box parameters (Sheet 1 of 3)

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 hits returned when the system searches a spectrum against the selected libraries.
Best Match Method	Specifies how to sort the library searches. Valid values: Search Index, Reverse Search Index, Match Probability
Handle confirming ions	
Include Confirming Ions/ Number of Confirming Ions	Specifies the number of confirming ions, which are other ions in the spectrum whose ratio is compared to the quantitation ion to identify the compound. This value defaults to 2 because you typically perform a 3-ion experiment with one quantitation mass and two confirming ions. Range: Integers from 1 to 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 53. Method Template Editor dialog box parameters (Sheet 2 of 3)

Parameter	Description
Origin	Specifies that the origin is ignored, forced, or included in the generated calibration curve. • Ignore: Specifies that the origin is not included as a valid point in the calibration curve when the curve is generated. When you select Ignore, the calibration curve might or might not pass through the origin. • Force: Specifies that the calibration curve passes through the origin of the data point plot when the calibration curve is generated. • Include: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select Include, the calibration curve might or might not pass through the origin.
Weighting	Specifies the weighting for the calibration data points. • Equal: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select Equal, the calibration curve might or might not pass through the origin. • 1/X: Specifies a weighting of 1/X for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their quantity. • 1/X^2: Specifies a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity. • 1/Y: Specifies a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio). • 1/Y^2: Specifies a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).
Response Via	Specifies if the TraceFinder application uses area or height in response calculations. • Area: Specifies that the application use this peak area value in response calculations. • Height: Specifies that the application use this peak height value in response calculations.
Qualitative Peak Processing	
Use Genesis Algorithm For Qual Processing	The application uses the Genesis algorithm to match internal standards.
ISTD Matching	Excludes all the target compounds found in the method and does not list these compounds in the TIC Report or in the Qual Mode view in the Data Review.
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.

Table 53. 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 519. 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.

Importing Published Master Methods

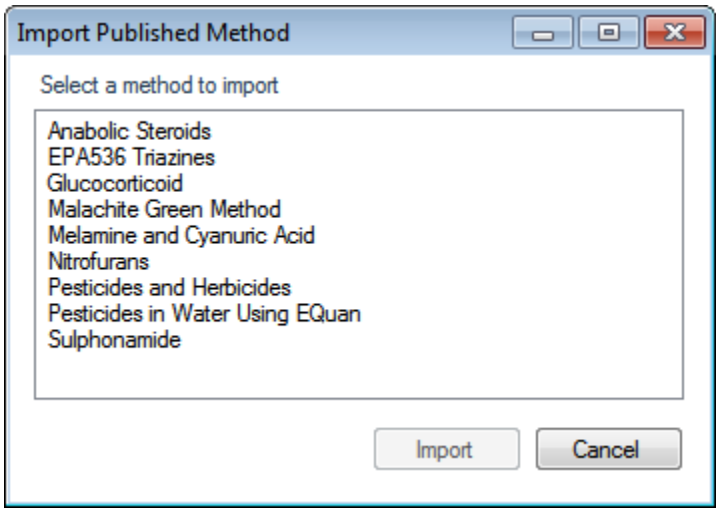
In the TraceFinder application, you can import published methods to use for detecting, processing, and reporting. The TraceFinder installation provides the following folder of published methods:

…\Thermo\TraceFinder\3.2\Clinical\Published Master Methods

❖ To import a published master method

1. Choose **Method View > Import Published Method** from the main menu.

   The Import Published Method dialog box opens.



2. Select a method to import.
3. Click **Import**.

   The application reports that the method successfully imported and saves the method in the following folder:

   …\TraceFinderData\32\Templates\Methods\Clinical

   You can use any of the Open Method commands to open this method just as you would a method that you created.

Exporting Mass Data

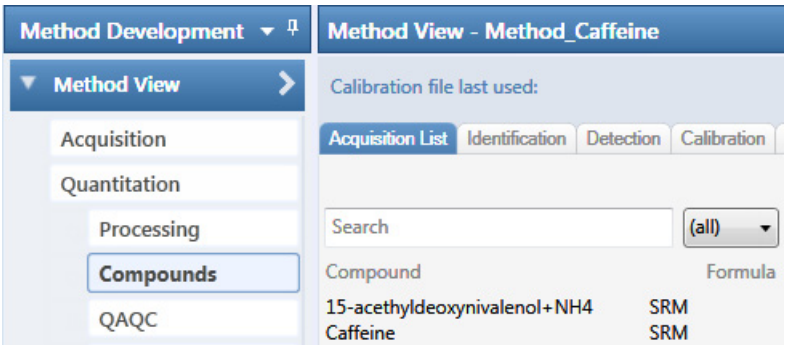
You can export the mass data list from the Compounds page to an XML file that can be read by the TSQ, ISQ, Q Exactive, TSQ Endura, or TSQ Quantiva applications. You can export mass data only from quantitation methods.

❖ 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 156. For information about editing the experiment type for a compound, see "Editing Compounds in the Database" on page 89.

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 mas data in the Acquisition List to the following folder, using a format compatible with your configured instrument:

   …\TraceFinderData\32\Methods*Methodname*

   For examples of exported mass lists, see the following:

   - "Triple Quadrupole Format" on page 81
   - "Q Exactive Format" on page 81
   - "TSQ Quantiva/Endura SIM Format" on page 81
   - "TSQ Quantiva/Endura SRM Format" on page 82

6

Using the Method Development Mode for Screening Methods

This chapter includes method development tasks for creating and editing screening master methods. When user security is activated, you must have Method Development Access permission before accessing these features.

Contents

- Opening a Master Method
- Creating a Master Method
- Editing a Master Method
- Saving a Master Method to a New Name
- Importing Published Master Methods

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

When you create a master method, the TraceFinder application uses the method to determine how the software works with a set of samples to provide a set of meaningful results. The application uses an instrument method to define how raw data is acquired. 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 TraceFinder application applies your master method to a batch, which is a list of one or more samples to be processed and reported. Together, the master method and batch provide a workflow-oriented approach to the data processing and information reporting for batches of samples.

Opening a Master Method

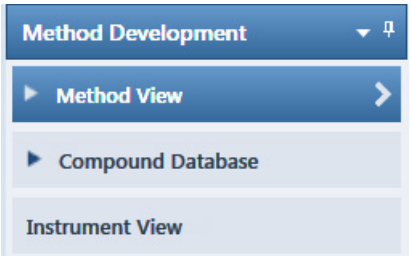
A target screening master method contains compound databases, identification and confirmation criteria used in detecting and processing, and settings for reporting compounds.

When you open a target screening master method, the Method View navigation pane displays the available pages for screening methods. For descriptions of all the features in the Method Development navigation pane, see "Method Development navigation pane" on page 272.

❖ To open a 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.

Figure 76. Open Master Method dialog box

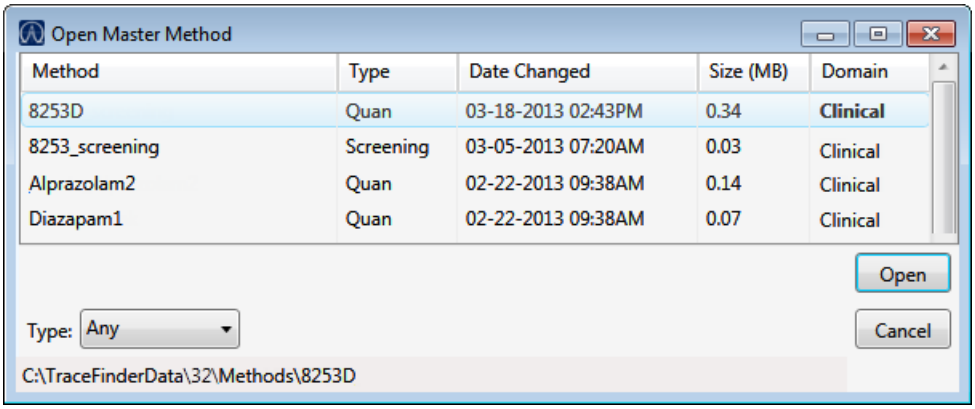


Table 54. Open Master Method dialog box parameters (Sheet 1 of 2)

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan or Screening.
Date Changed	Date the method was last updated.
Size	Size in megabytes.

Table 54. Open Master Method dialog box parameters (Sheet 2 of 2)

Parameter	Description
Domain	TraceFinder domain for which the method was created.
Type	Type of method to display: Quan, Screening, or Any.
Path	Path to the selected method in the TraceFinderData\32\Methods\Clinical folder.

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.

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 275.

The navigation pane displays the available pages for screening methods. For descriptions of all the features in the Method Development navigation pane, see Method Development navigation pane.

Figure 77. Method Development navigation pane

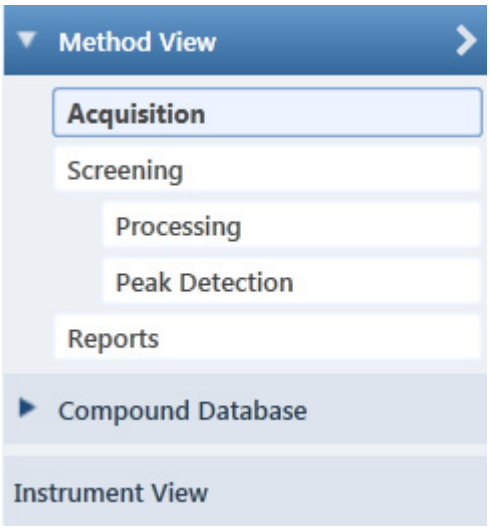


Table 55. Method Development navigation pane commands

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 275.
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 screening method. See "Editing the Processing Page" on page 279.
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 297.
Reports	Displays the Reports page of the Method View. See "Editing the Reports Page" on page 308.
Compound Database	See "Working with the Compound Database" on page 76.
Instrument View	See "Working with Instrument Methods" on page 113.

Creating a Master Method

The following procedure includes the minimum parameters you must define to create and save a master method. For a detailed description of how to modify all parameters in a master method, see "Editing a Master Method" on page 275.

❖ To create a new method

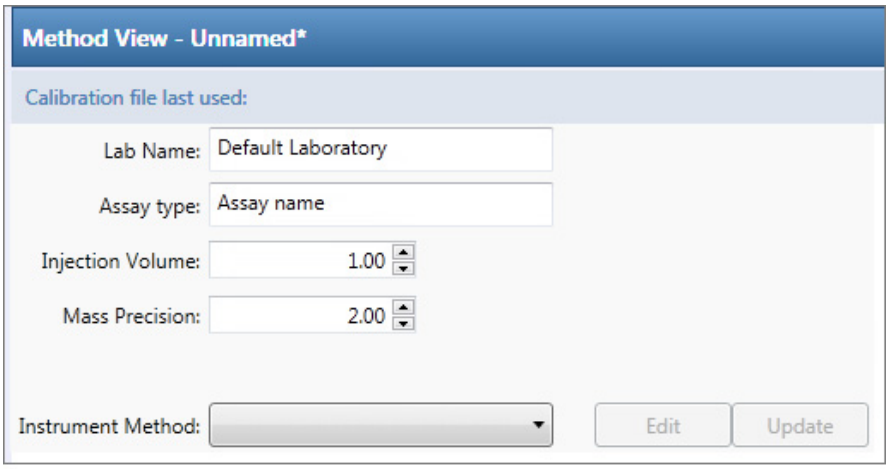
1. Choose **File > New > Master Method** from the main menu.

   The Create Master Method dialog box opens.

2. Select the **Create Screening Method** option and click **OK**.

   The Method View for a target screening method includes the Acquisition, Processing, Peak Detection, and Reports pages.

   The Acquisition page for the method opens.

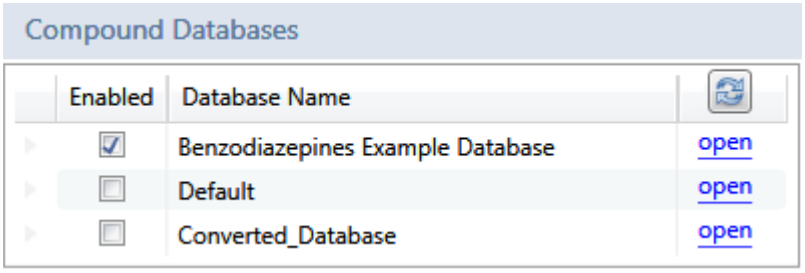
   

3. From the Instrument Method list, select an instrument method.

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\3.2\Clinical\Databases

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.

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.

This section includes 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 277.

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.

   Range: 0.1 to 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 TraceFinder 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.

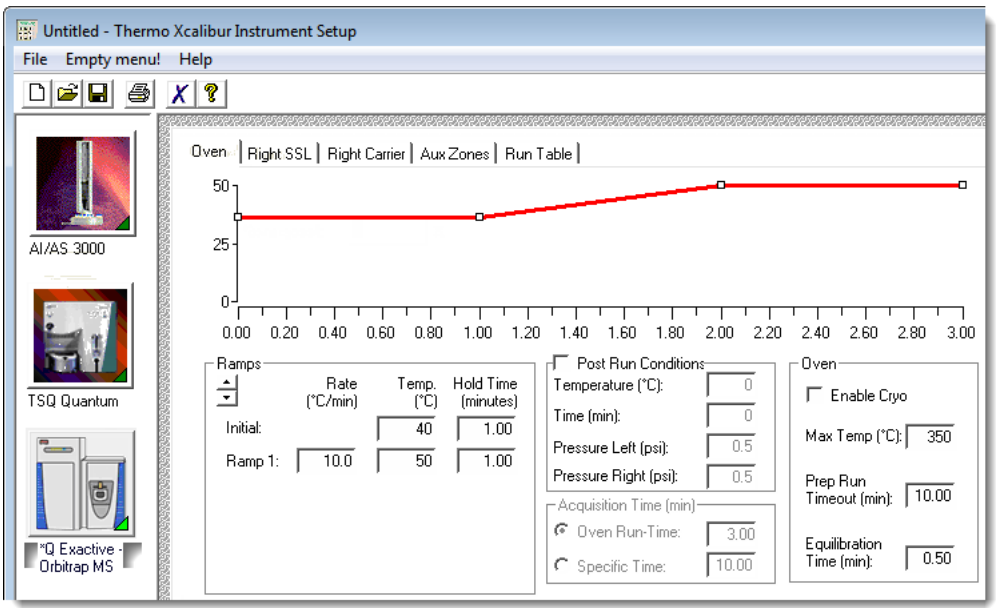
   Valid values: Integers from 2 to 6, inclusive

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

7. To edit the instrument method, click **Edit**.

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

   Figure 78. Thermo Xcalibur Instrument Setup window



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

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

   The TraceFinder 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 79. Acquisition page for a screening method

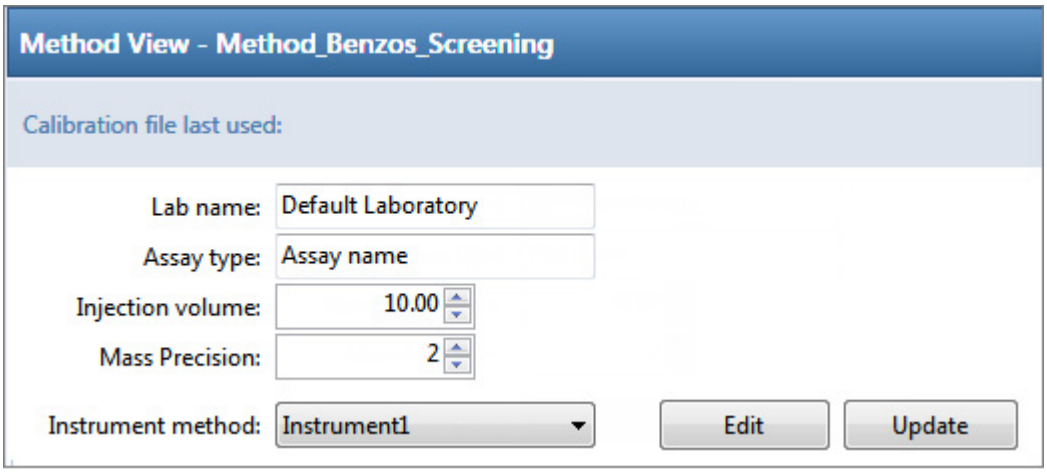


Table 56. Acquisition page parameters (Sheet 1 of 2)

Parameter	Description
Lab Name	The laboratory name to be displayed on the top of each printed, saved, or exported report. Default: Default Laboratory To specify this default laboratory name, see "Specifying Application Defaults" on page 35.
Assay Type	The name for the analysis type to be targeted by the method. The assay type associates the method with the analysis of a compound or specific class of compounds (for example, you might use an assay type of PAH for the analysis of Polynuclear Aromatic Hydrocarbons).
Injection Volume	The system uses the injection volume (in µL) for sample injection. For a more detailed explanation, refer to the documentation for the autosampler. The injection volume in the master method overrides the injection volume in the instrument method. The injection volume in the batch overrides the injection volume in the master method. Range: 0.1 to 2000 µL

Table 56. 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 to 6, inclusive
Instrument Method	Instrument method used for acquiring samples.
Edit	Opens the Thermo Xcalibur Instrument Setup dialog box where you can edit the instrument method.
Update	Choose one of the following: • **Send to System Methods**: Overwrites the instrument method in the C:\TraceFinderData\32\Methods folder with the current instrument method. • **Get From System Methods**: Overwrites the current instrument method with the instrument method in the C:\TraceFinderData\32\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.

This section includes instructions for the following tasks:

- To open the Processing page
- To specify peak filter settings

  The Peak Filter Settings pane displays parameters for limiting the display of unwanted data.

- To specify compound databases

  The Compound Databases pane displays all available compound databases.

- To specify identification and confirmation settings

  The Identification and Confirmation Settings pane displays parameters for how compounds are identified or confirmed. For additional information about the confirmation and identification process, see "Understanding the Identification and Confirmation Process" on page 290.

❖ 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 285.

❖ To specify peak filter settings

1. To set a retention time range that excludes searching for peaks outside the range, do the following:
   a. Select the **Use RT Limits** check box.

      The application activates the Search From and To options.

   b. In the Search From box, enter the lower limit; in the To box, enter the upper limit.
2. To use one or more negative samples for subtraction to filter the resulting peaks, do the following:
   a. Select the **Use Matrix Blank** check box.

      The application activates the Amplifier option.

      During automatic processing, the TraceFinder application subtracts the areas of the peaks in the negative samples from the matching areas in the specimen 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 negative samples, the application subtracts only the one with the highest area.

When a compound peak in one negative sample has the same primary ion as another peak in a different negative 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 negative sample, and this same compound has the M+H and M+NH4 ions in another negative sample, the application uses for subtraction the area that results from all of these ions.

When no negative sample exists in the sequence, or if one or more negative 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 TraceFinder application multiplies a negative 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 negative samples to use for subtraction. See "Blank Subtraction in Target Screening Batches" on page 376.

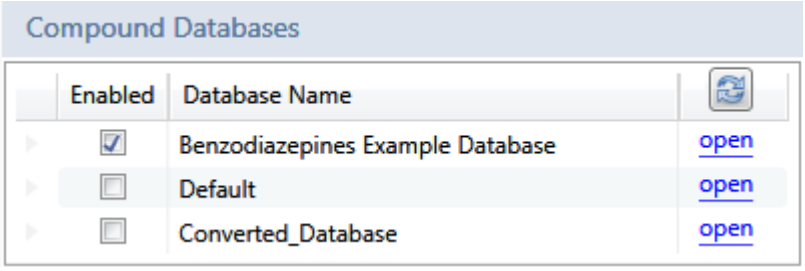
3. In the Chromatogram View Width box, type a value to define the chromatogram viewing range in the Data Review view.

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 TraceFinder 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 specify compound databases



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\3.2\Clinical\Databases folder.

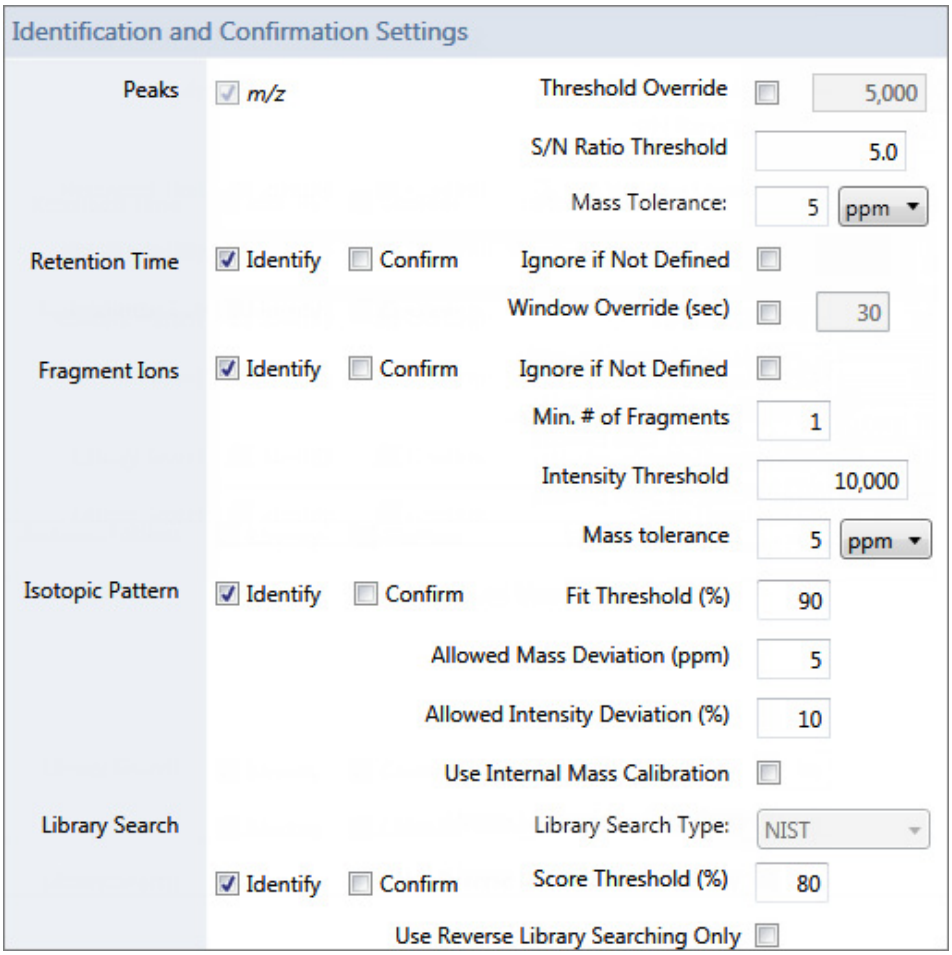
2. (Optional) To edit a database, click **Open** and do the following:

   a. Edit the database.

      See "Editing Compounds in the Database" on page 89.

   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



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 292.

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* ± 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 293.

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 294.

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 294.

Processing Page

Use the features in the Settings pane to specify peak filter settings.

Use the features in the Target Screening Settings pane to specify screening databases and identification and confirmation settings.

Figure 80. Settings pane on the Processing page

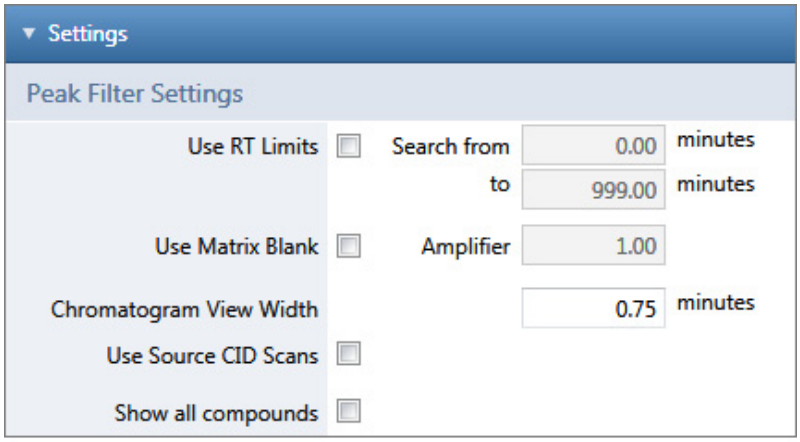


Table 57. Settings pane parameters

Parameter	Description
Peak Filter Settings	
Use RT Limits	Specifies a lower and upper limit for searches. Ranges: 0.00 to 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 TraceFinder application subtracts the areas of the peaks in the selected negative samples from the matching areas in the specimen samples.
Amplifier	The application multiplies a negative area by this value before performing subtraction. The larger the amplifier value, the more peaks the application filters from the final results. Range: .01 to 1000.00 Default: 1.00
Chromatogram View Width	Specifies a a window width to define the chromatogram viewing range in the Data Review view. Range: 0.10 to 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.

Figure 81. Target Screening Settings pane on the Processing page

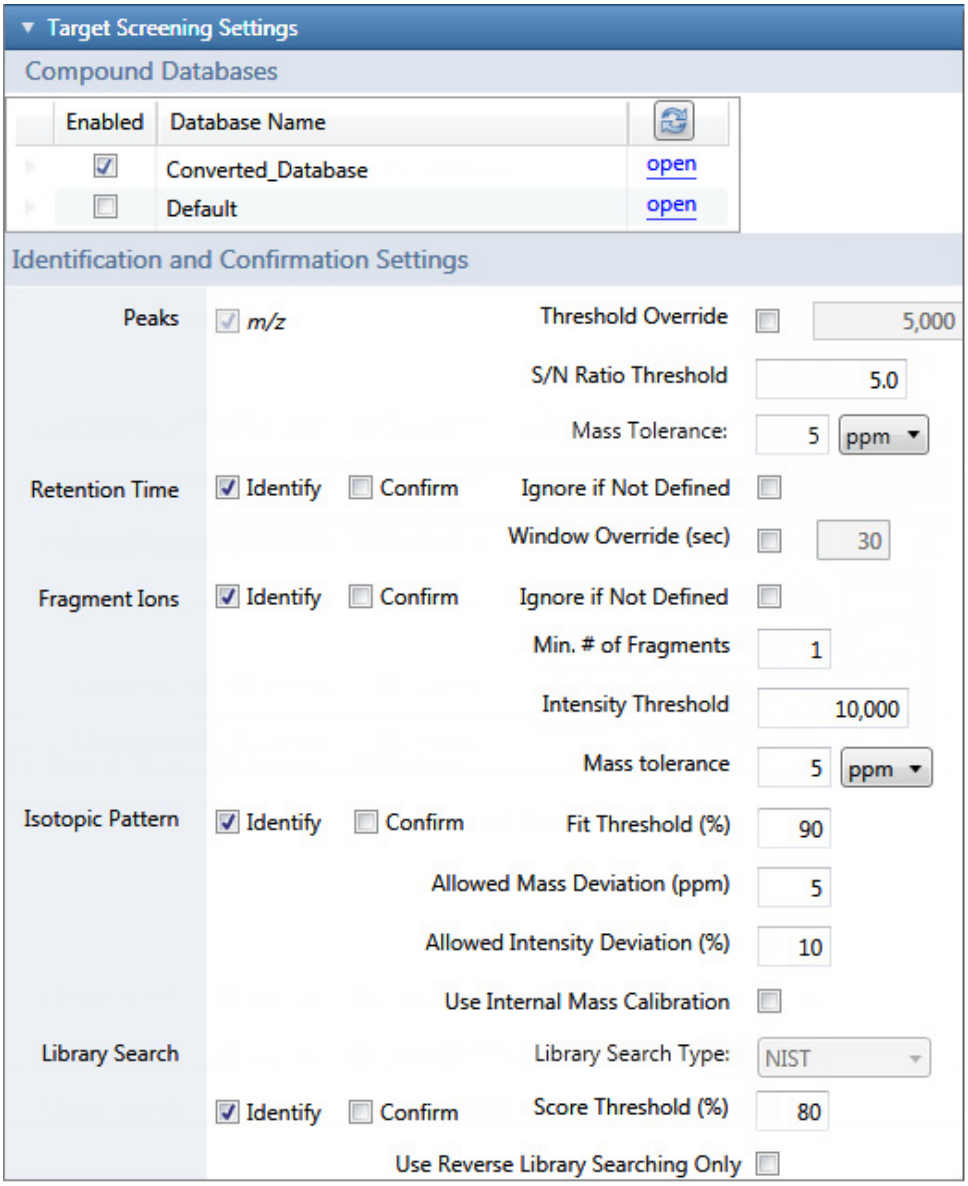


Table 58. Target Screening Settings pane parameters (Sheet 1 of 4)

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 (*m/z*) for filtering compound peaks.

Table 58. Target Screening Settings pane parameters (Sheet 2 of 4)

Parameter	Description
Threshold Override	This threshold overrides the Response Threshold value set in the compound database. The application ignores the peaks with areas below this specified threshold. Range: 1000 to 1 000 000 000 Default: 5000
S/N Ratio Threshold	Includes only peaks with signal-to-noise ratios (S/Ns) above the specified value. Range: 1.0 to 100 000 Default: 5.0
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	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. Range: 0 to 999 seconds Default: 30 seconds
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. Range: 1 to 5 Default: 1

Table 58. Target Screening Settings pane parameters (Sheet 3 of 4)

Parameter	Description
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. Range: 1 to 1e9 Default: 10 000
Mass Tolerance	Specifies the number of millimass units or parts per million to use as the *m/z* ± tolerance value for the fragment ions and is separate from the mass tolerance specified for the parent (see "Editing the Acquisition Page" on page 275). Range: 0 to 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.
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%
Allowed Mass Deviation	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. Range: 3 to 100 ppm Default: 3 ppm

Table 58. Target Screening Settings pane parameters (Sheet 4 of 4)

Parameter	Description
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. 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. Default: 10%
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
Score Threshold	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. Default: 80%
Use Reverse Library Searching Only	Compares a library entry to an unknown compound (a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry). This option is available for both NIST and Library Manager searches.

Understanding the Identification and Confirmation Process

By default, the TraceFinder 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 TraceFinder 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 TraceFinder 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)" on page 291 and "Retention Time" on page 292.

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 294.

4. Fragment Ions

   For additional information about the Fragment Ions parameter, see "Fragment Ions" on page 293.

5. Library Search

   For additional information about the Library Search parameter, see "Library Search" on page 294.

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 275.

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 427.

The Compounds table also displays the *m/z* Expected, *m/z* Measured, and *m/z* Delta values for each compound.

Threshold

The application automatically uses the area and threshold values defined in the selected compound database to identify each sample compound.

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 427.

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 427. 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 TraceFinder 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 TraceFinder 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:
  - The criteria passes when the library score is higher than or equal to the score threshold.
  - The criteria fails when the library score is lower than the score threshold.
- 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):
  - The criteria passes when the library score is higher than or equal to the score threshold.
  - The criteria fails when the library score is lower than the score threshold.
- 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:
  - The criteria passes when the library score is higher than or equal to the score threshold. The Lib Match Name, Library Score, and Library Match Rank columns display their values in green text.
  - The criteria fails when the library score is lower than the score threshold. 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 TraceFinder 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, while 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

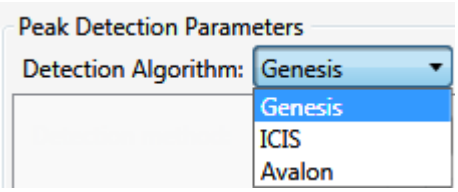
Use the features on the Peak Detection page to specify any of the following peak detection algorithms: Genesis, ICIS, or Avalon.

❖ 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 301.
   - 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 304.

3. Specify the parameters for the selected detection algorithm.

Genesis Detection Method

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

Figure 82. Genesis peak detection

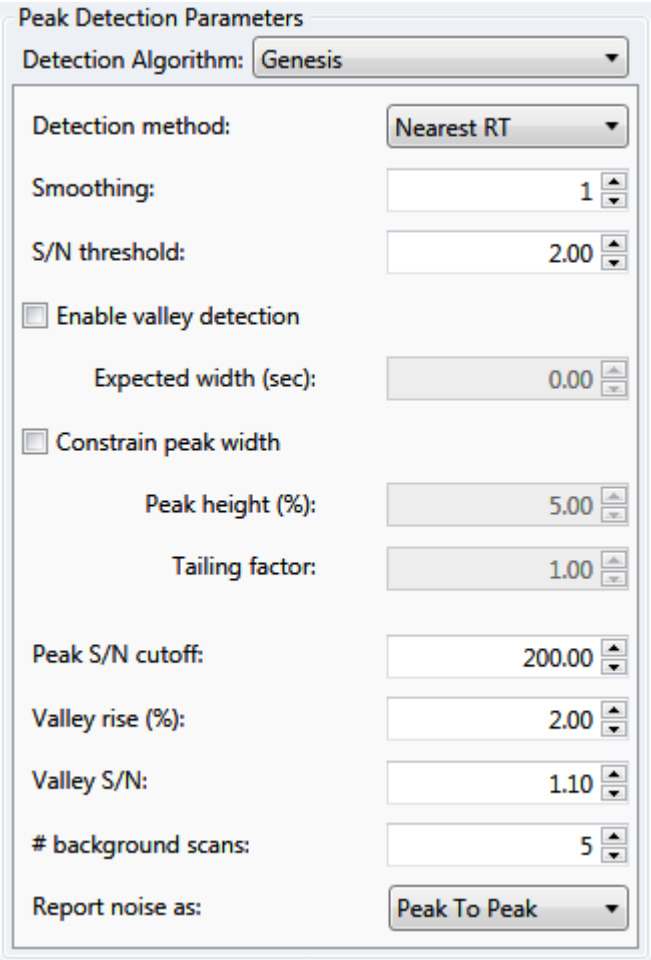


Table 59. Genesis peak detection parameters (Sheet 1 of 3)

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 59. Genesis peak detection parameters (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. The ICIS peak detection algorithm uses this value. Default: 1 Range: Any odd integer from 1 through 15 points
S/N threshold	Current signal-to-noise threshold for peak integration. Peaks with signal-to-noise values less than this value are not integrated. Peaks with signal-to-noise values greater than this value are integrated. Range: 0.0 to 999.0
Enable Valley Detection	Uses the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Expected Width (sec)	The expected peak width parameter (in seconds). This parameter controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the *expected width*/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the TraceFinder application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. Range: 0.0 to 999.0
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a 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. Range: 0.0 to 100.0%

Table 59. Genesis peak detection parameters (Sheet 3 of 3)

Parameter	Description
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0
Peak S/N Cutoff	The peak edge is set to values below this signal-to-noise ratio. This test assumes it has found an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio. When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the TraceFinder application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 10000.0
Valley Rise (%)	The peak trace can rise above the baseline by this percentage after passing through a minimum (before or after the peak). This criteria is useful for integrating peaks with long tails. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. When the trace exceeds rise percentage, the TraceFinder application applies valley detection peak integration criteria. This test is applied to both the left and right edges of the peak. Range: 0.1 to 500.0
Valley S/N	Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher. Default: 2.0 Range: 1.0 to 100.0
# Background Scans	Number of background scans performed by the TraceFinder application.
Report Noise As	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or peak-to-peak resolution threshold. Options are RMS or Peak To Peak.

ICIS Detection Method

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

Figure 83. ICIS peak detection

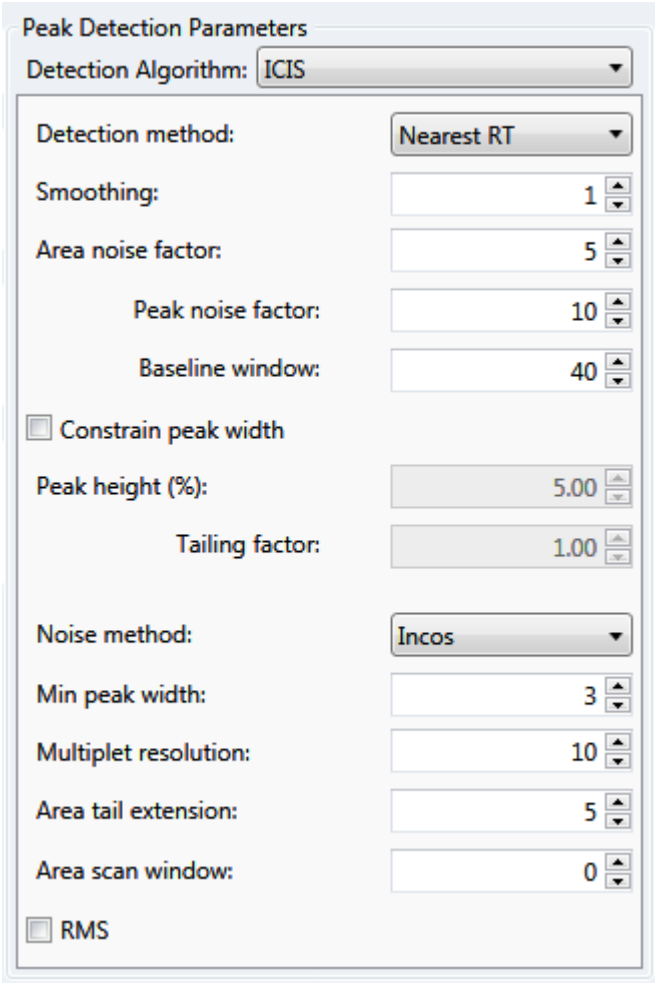


Table 60. ICIS peak detection parameters (Sheet 1 of 3)

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.

Table 60. ICIS peak detection parameters (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. The ICIS peak detection algorithm uses this value. Range: Any odd integer from 1 through 15 points Default: 1
Area Noise Factor	The noise level multiplier used to determine the peak edge after the location of the possible peak. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 5
Peak Noise Factor	The noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value. Range: 1 through 1000 Default: 10
Baseline Window	The TraceFinder application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 40
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box 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. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

Table 60. ICIS peak detection parameters (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. The ICIS peak detection algorithm uses this value. Repetitive: Uses a multiple pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but the analysis takes longer.
Min Peak Width	The minimum number of scans required in a peak. The ICIS peak detection algorithm uses this value. Range: 0 to 100 scans Default: 3
Multiplet Resolution	The minimum separation in scans between the apexes of two potential peaks. This is a criteria to determine if two peaks are resolved. The ICIS peak detection algorithm uses this value. Range: 1 to 500 scans Default: 10
Area Tail Extension	The number of scans past the peak endpoint to use in averaging the intensity. The ICIS peak detection algorithm uses this value. Range: 0 to 100 scans Default: 5
Area Scan Window	The number of allowable scans on each side of the peak apex. A zero value defines all scans (peak-start to peak-end) to be included in the area integration. Range: 0 to 100 scans Default: 0
RMS	Specifies that the TraceFinder application calculate noise as RMS. By default, the application uses Peak To Peak for the noise calculation. RMS is automatically selected if you manually determine the noise region.

Avalon Detection Method

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

Figure 84. Avalon peak detection

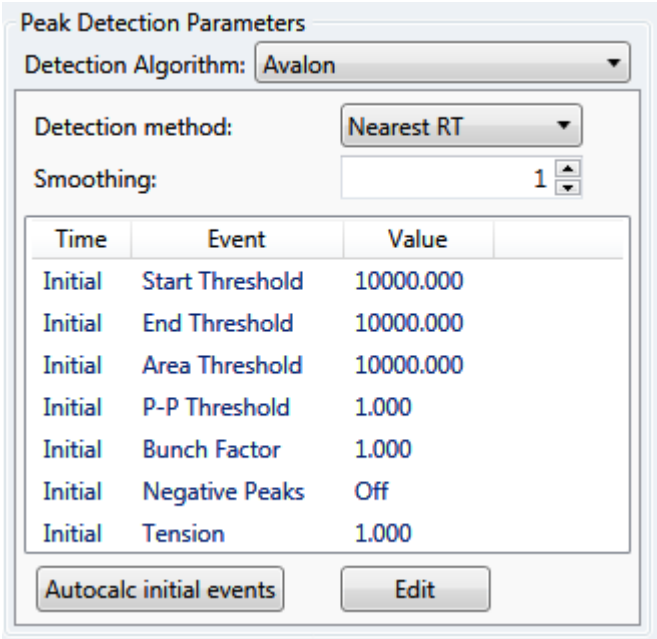


Table 61. Avalon peak detection parameters

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. Default: 1 Range: Any odd integer from 1 through 15 points
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 85. Avalon Event List dialog box

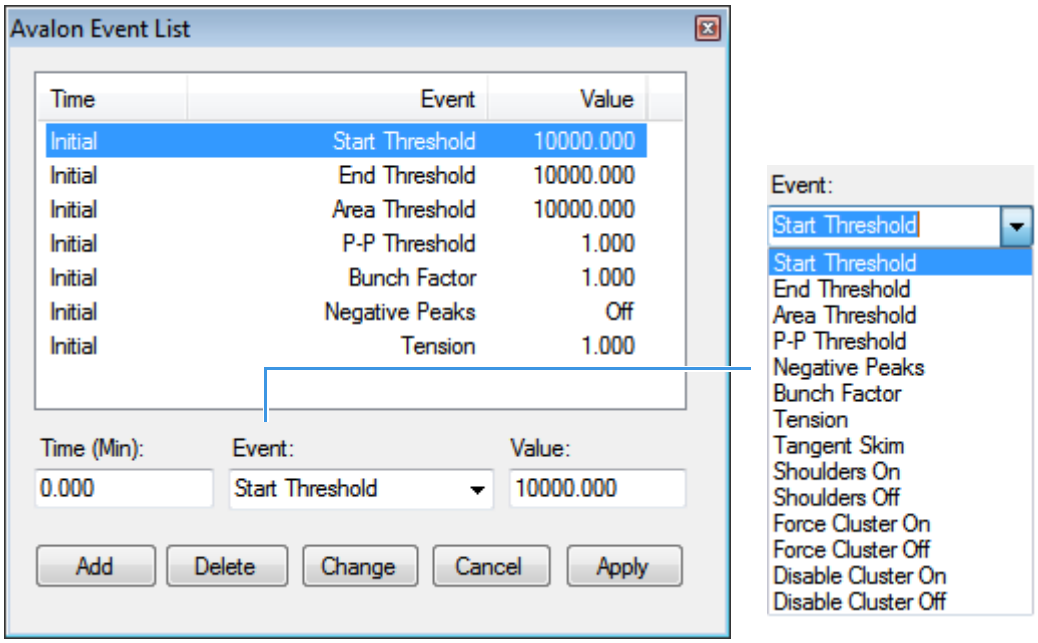


Table 62. Avalon Event List dialog box parameters

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 86. Event types

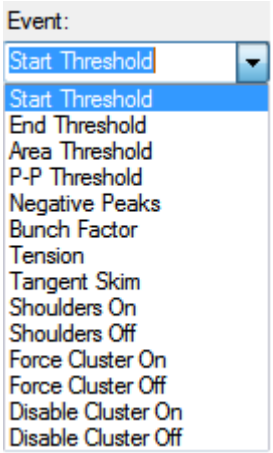


Table 63. Event type descriptions (Sheet 1 of 2)

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

Table 63. Event type descriptions (Sheet 2 of 2)

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

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" on page 309), displaying only the reports that are configured in the Configuration Console. To configure the reports that are available, see "Specifying the Reports" on page 72.

❖ 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 TraceFinder 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 87. Reports page

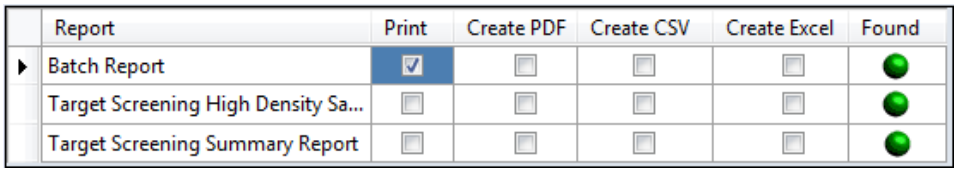


Table 64. Reports page parameters

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.
Found	Indicates that the report template is identified in the C:\TraceFinderData\32\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 quantitative and target screening methods.

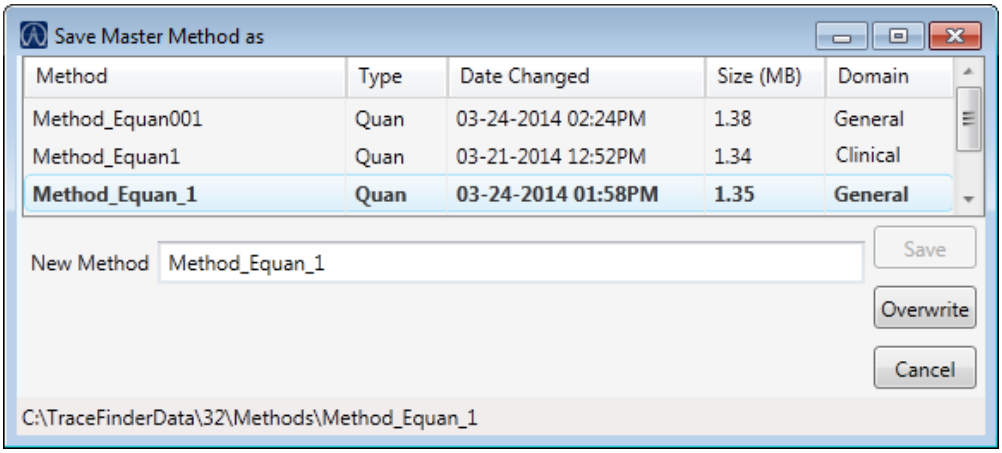


Table 65. Save Master Method As dialog box parameters

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan or Screening.
Date Changed	Date the method was last updated.
Size	Size in megabytes.
Domain	TraceFinder domain for which the method was created.
New Method	Name of the new method to create.
Path	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.

Importing Published Master Methods

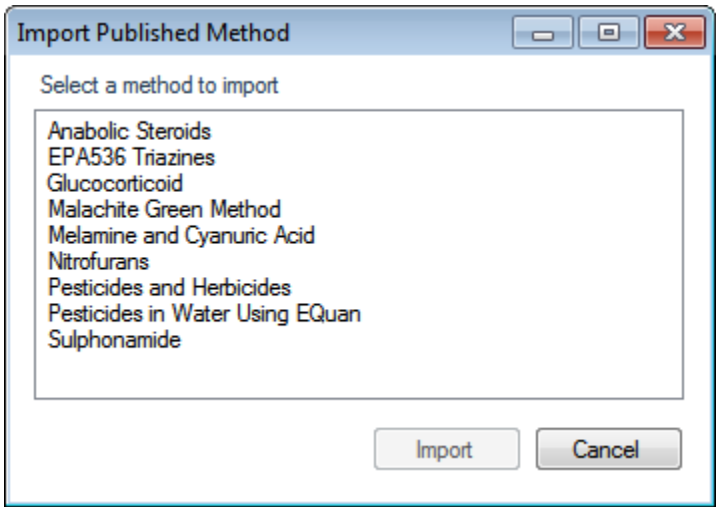
In the TraceFinder application, you can import published methods to use for detecting, processing, and reporting. The TraceFinder installation provides the following folder of published methods:

…\Thermo\TraceFinder\3.2\Clinical\Published Master Methods

❖ To import a published master method

1. Choose **Method View > Import Published Method** from the main menu.

   The Import Published Method dialog box opens.



2. Select a method to import.

3. Click **Import**.

   The application reports that the method successfully imported and saves the method in the following folder:

   …\TraceFinderData\32\Methods\Clinical

   You can use any of the Open Method commands to open this method just as you would a method that you created.

7

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 the Analysis mode 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

This section includes instructions for the following tasks:

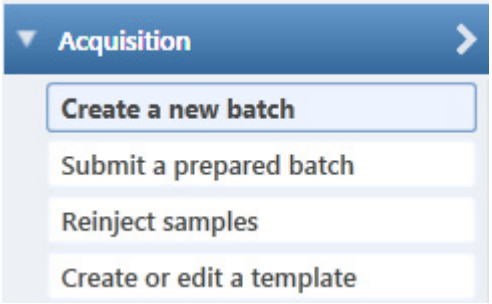
- Opening and Navigating the Acquisition Mode
- Creating and Submitting Batches

Opening and Navigating the Acquisition Mode

❖ **To access the Acquisition mode**

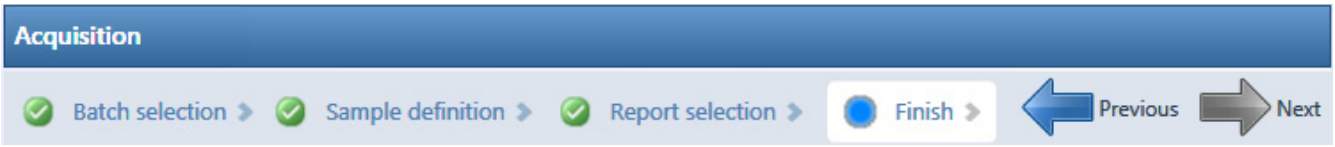
Click **Acquisition** in the navigation pane.

The navigation pane for the Acquisition mode opens.

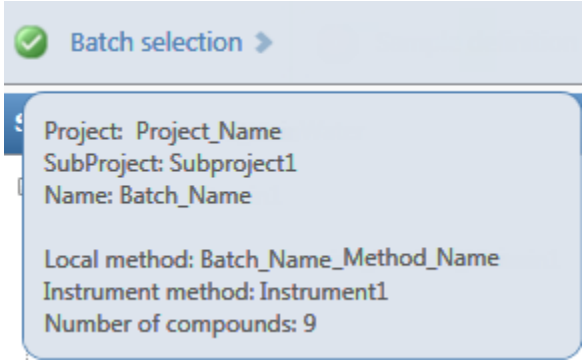


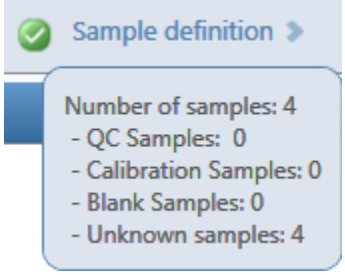
As you progress through the Acquisition mode using any of these methods for creating a batch, the task pane at the top of the view tracks your progress. As you complete each stage, you can hold your cursor over the view name in the task pane to display the parameters that you specified for the batch. See Example task pane when you have completed the Acquisition mode.

Figure 88. 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

Calibration Samples: Calibrator

Blank Samples: Negative

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:

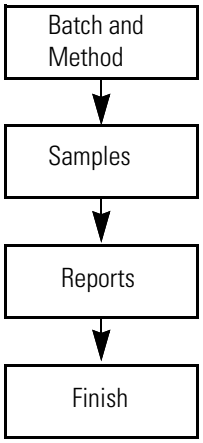
1. Selecting a Batch
2. Defining the Sample List
3. Selecting and Reviewing Reports
4. Submitting the Batch

The Acquisition mode provides multiple techniques for creating either a batch or a batch template.

- To start a new quantitative batch
- To start a new 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 quantitative batch template
- To create a screening batch template

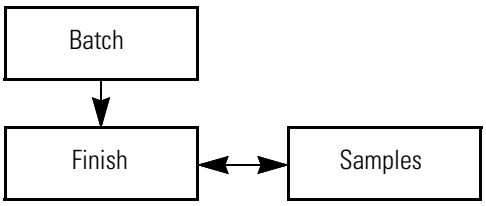
Each batch creation technique has an associated workflow, as shown in the following flowcharts. Each workflow uses a different combination of Acquisition mode pages.

Workflow for Creating an Original Batch



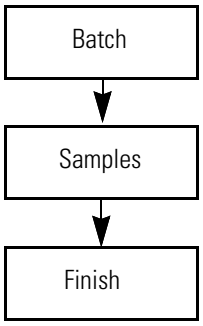
To create an original batch, start with the instructions "To start a new quantitative batch" on page 318 or "To start a new screening batch" on page 320.

Workflow for Acquiring a Prepared Batch



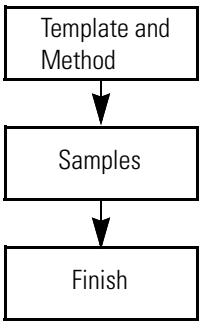
To acquire a prepared batch, start with the instructions "To select a prepared batch" on page 322.

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 323.

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 the instructions "To create a quantitative batch template" on page 323 or "To create a screening batch template" on page 324.

Selecting a Batch

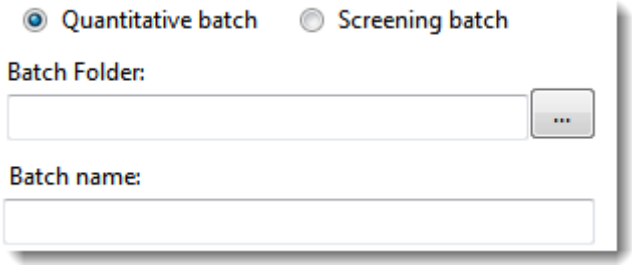
On a Batch Selection page of the Acquisition mode, you can create a new quantitative or screening batch in any of your current projects/subprojects. Or, you can submit a batch that you previously prepared and saved, reinject the samples in a batch that you previously acquired, or create a batch template to use for future batches.

Follow these procedures:

- To start a new quantitative batch
- To start a new 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 quantitative batch template
- To create a screening batch template

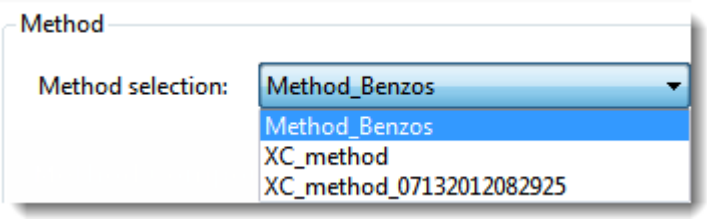
❖ To start a new quantitative batch

1. Click **Create a New Batch** in the navigation pane.
2. Select the **Quantitative Batch** 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.

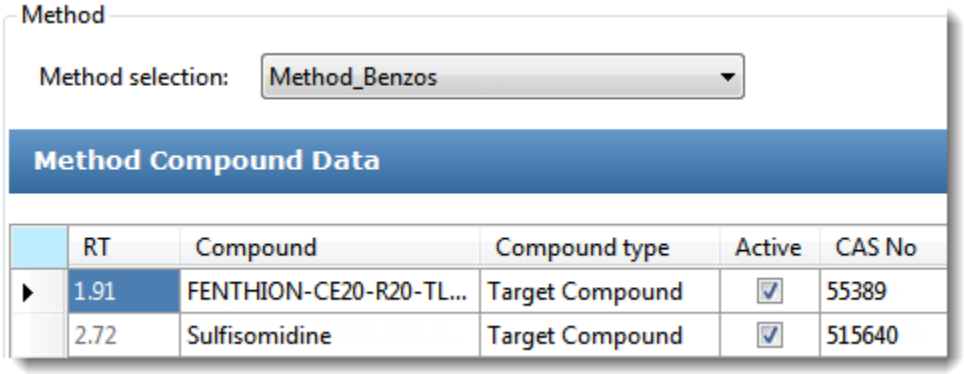


If the name you enter is not unique, a red warning flashes.

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.

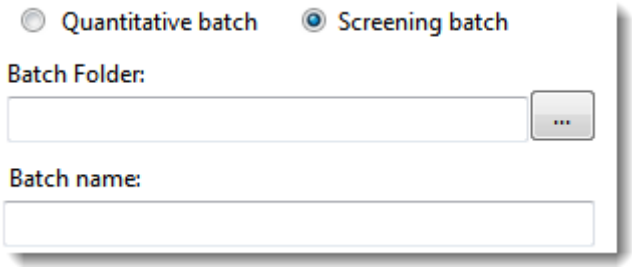


6. To continue to the next page, click **Next**.

   The Sample Definition page opens. See "Defining the Sample List" on page 326.

❖ To start a new screening batch

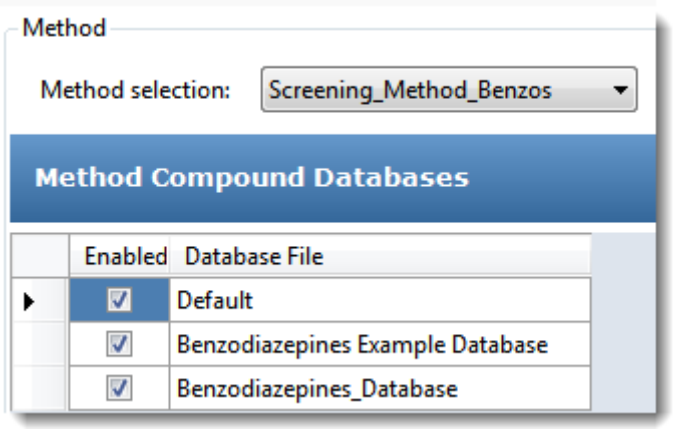
1. Click **Create a New Batch** in the navigation pane.
2. Select the **Screening Batch** option.
3. Select the batch folder where you want to create the new batch.
4. Type a name for the new batch in the Batch Name box.



If the name you enter is not unique, a red warning flashes.

5. 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.



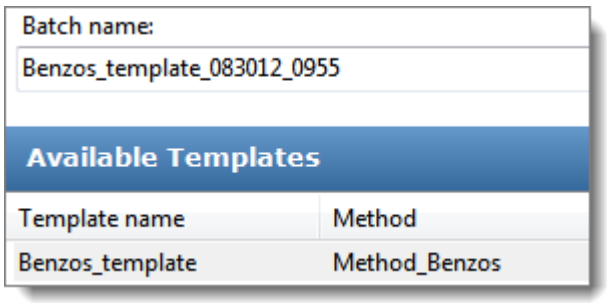
6. To continue to the next page, click **Next**.

The Sample Definition page opens. See "Defining the Sample List" on page 326.

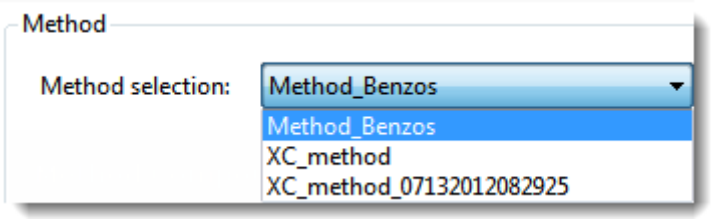
❖ To start a new batch from a template

1. Click **Create a New Batch** in the navigation pane.
2. Select either the **Screening Batch** or the **Quantitative Batch** 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.



   The system creates a batch name with the selected template name and appends the date and time stamp. You can change the default batch folder or 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.



6. To continue to the next page, click **Next**.

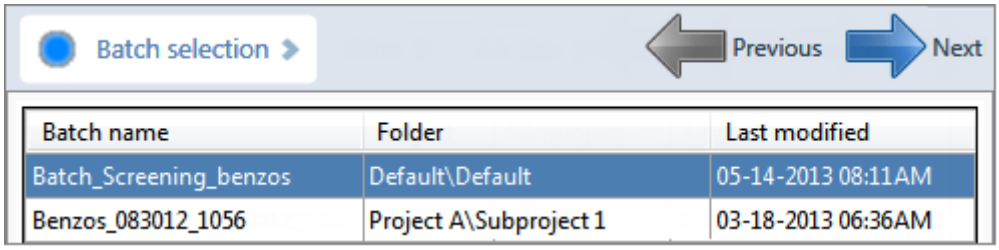
   The Sample Definition page of the Acquisition mode opens. See "Defining the Sample List" on page 326.

❖ To select a prepared batch

1. Click **Submit a Prepared Batch** in the navigation pane.

   The application displays all your unacquired, saved batches. The TraceFinder application stores all unacquired batches in the …\TraceFinderData\32\Projects\… folder.

2. Select the batch that you want to acquire.



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**.

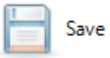
     For detailed instructions, see "Defining the Sample List" on page 326.

   –or–

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

     For detailed instructions, see "Submitting the Batch" on page 342.

   –or–

   - To save the batch to be acquired later, click **Save**,  .

     The TraceFinder application saves your batch in the following folder:

     …\TraceFinderData\32\Projects\...

     The TraceFinder 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 batches, both quantitative and screening.
3. To continue to the next page, click **Next**.

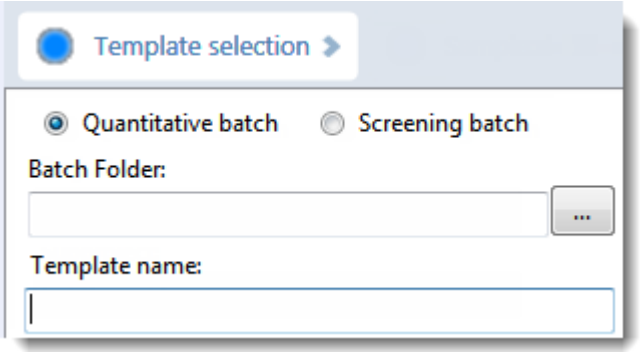
   The Sample Definition page of the Acquisition mode opens. See "Defining the Sample List" on page 326.

   - 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 quantitative batch template

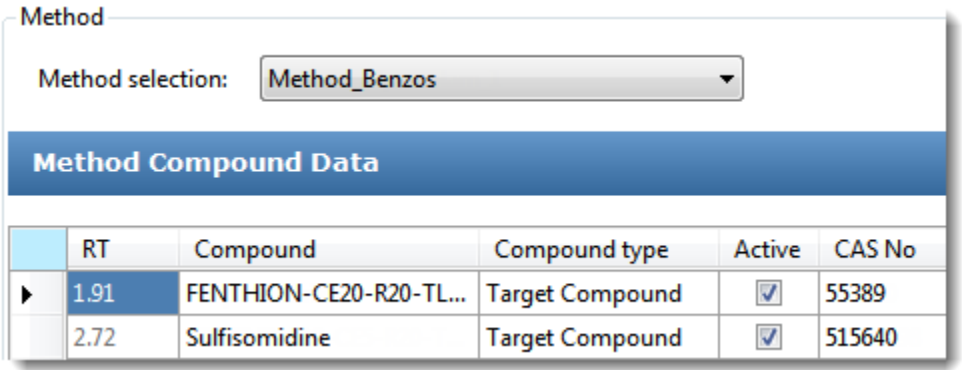
1. Click **Create or Edit a Template** in the navigation pane.

   Note When user security is activated, you must have Acquisition Wizard – Template Editing permission to create a batch template.
2. Select the **Quantitative Batch** 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.



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.



6. To continue to the next page, click **Next**.

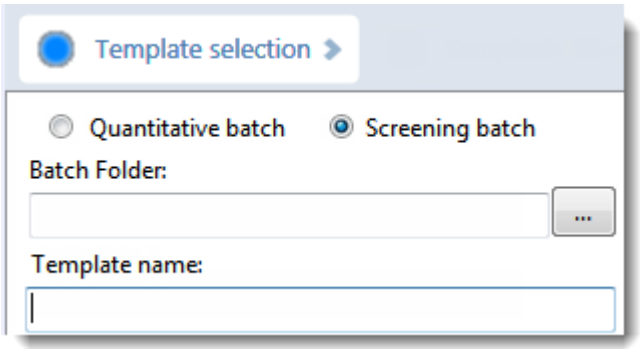
   The Sample Definition page of the Acquisition mode opens. See "Defining the Sample List" on page 326.

❖ To create a screening batch template

1. Click **Create or Edit a Template** in the navigation pane.

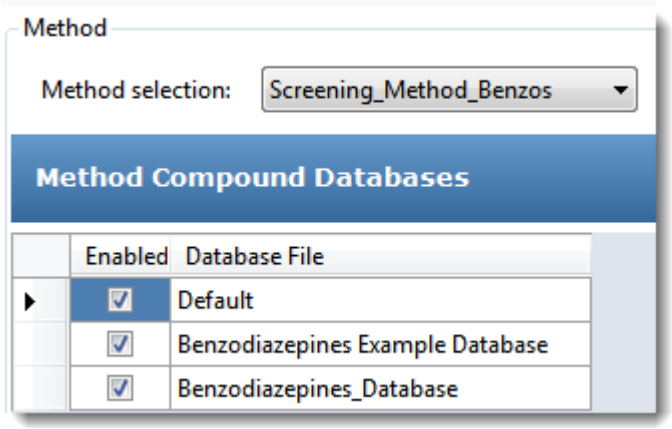
   Note When user security is activated, you must have Acquisition Wizard – Template Editing permission to create a batch template.

2. Select the **Screening Batch** 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.



5. Select a method from the Method Selection list.

   The Method Compound Databases pane displays the screening databases available for the selected method.



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 the Sample List."

Defining the 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 336. 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 339.

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 on the shortcut menu (see the Shortcut Menu section of the "Samples page parameters" on page 336).

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 are creating a batch from scratch, creating a batch from a template, or editing a batch template and you click Next, the Report Selection page opens. See "Selecting and Reviewing Reports" on page 340.
- When you are editing a prepared batch or reinjecting samples and you click Next, the Finish Selection page opens. See "Submitting the Batch" on page 342.

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 1 and then click the **Add** icon, or Add.
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			
Specimen	Hydrolysis	Solvent	QC
Unextracted	Calibrator	Negative	

   For a detailed description of each sample type, see "Sample Types" on page 367.
4. For each Calibrator or QC 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 219.
5. For each sample, type a vial position in the Vial Position column.

   Tip Use the Fill Down command to make entering vial positions easier.
6. 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.
7. (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 Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name columns stay fixed 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 Specimen samples.

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

2. Select the number of samples to insert 1 and then click the **Insert** icon, or Insert.

   The application inserts the Specimen samples above the selected sample.

   Inserted samples

	Status	Filename	Sample type	Groups	Qual Processing	Level
1		cal_std_5	Calibrator			5
2		Unknown2	Specimen			
3		Unknown1	Specimen			
4		cal_std_10	Calibrator			10

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			
Specimen	Hydrolysis	Solvent	QC
Unextracted	Calibrator	Negative	

5. For each Calibrator or QC 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 327.

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. 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.

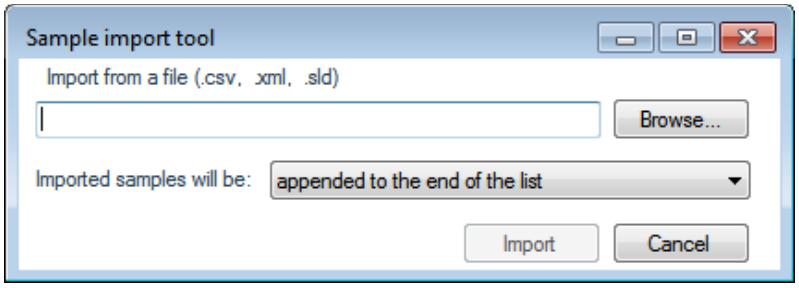
8. (Optional) Type or edit the values for the remaining columns.

   Note When you use the scroll bar at the bottom of the sample list, the Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name columns stay fixed while the other columns scroll right and left.

❖ To import samples into the list

1. Click **Import**, 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 file format must match the TraceFinder file format.

3. From the Imported Samples Will Be list, select either **Appended to the End of the List** or **Inserted at the Selected Row**.

4. Click **Import**.

   The Sample Import Tool dialog box closes, and the application adds the specified samples to the sample list.

   When you import samples from an Xcalibur sequence file (.sld), the TraceFinder 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 TraceFinder application makes the following sample type substitutions.

Xcalibur sample type	TraceFinder sample type
Blank	Negative
Std Bracket	Calibrator

   For each imported sample, the application uses the Instrument Method specified in the local method.

5. For each Calibrator or QC 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 327.

   For detailed instructions about defining calibration levels, see "Calibration Levels" on page 219.

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 Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name columns stay fixed while the other columns scroll right and left.

9. (Optional) When using multiplexing, select a channel for each imported sample.

   Imported samples default to Auto.

❖ To remove samples from the list

1. Select the samples 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 TraceFinder application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth.

   The TraceFinder application copies all parameter values from the original sample.

A green status icon indicates previously acquired samples (acquired and processed) and the sample name is grayed out. A blue status icon indicates samples created for reinjection (not acquired).

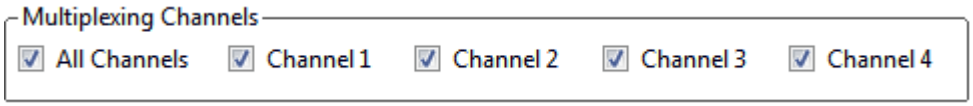
	cal_50_INJ001	Calibrator	10
	cal_50	Calibrator	10
	cal_10_INJ001	Calibrator	10
	cal_10	Calibrator	10

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.

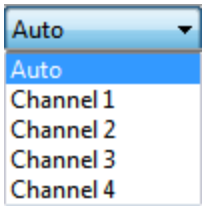
❖ To assign a specific channel to a sample

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.

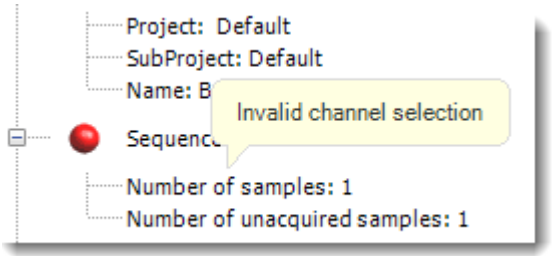
   All samples default to Auto.

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

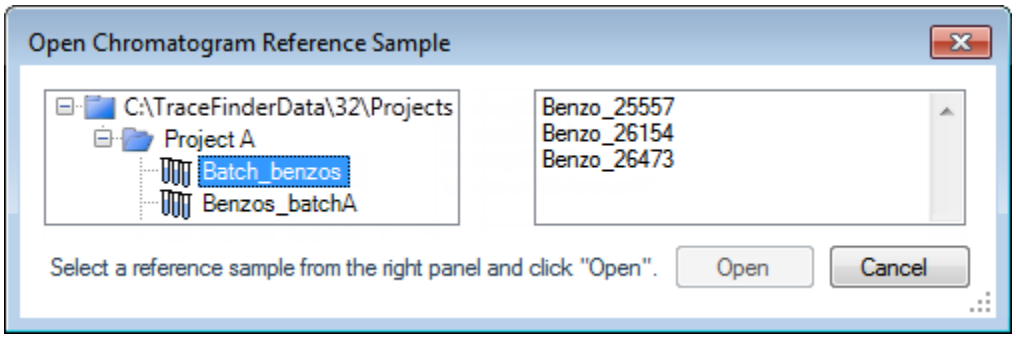
1. Click the **Reference Sample** tab.

   The Reference Sample page in the Sample Definition page opens. See "Reference Sample" on page 339.

   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 Chromatograph 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 TraceFinder 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 TraceFinder 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**.

6. The application adds the reference sample to the Reference Sample page.

7. (Optional) Enter values for Sample ID, Sample Name, Comment, and Barcode Actual.

8. (Optional) Change the Vial Position for the sample.

The application uses the peak in this sample as a reference peak in the Analysis mode. See "Reference Peak" on page 481.

❖ To add an auto sample type

1. Click the **Auto Samples** tab.

   The Auto Samples page opens. See "Auto Samples" on page 338.

2. Right-click and choose **Add Auto Sample** from the shortcut menu, or click the **Add New Auto Sample** icon, 1 .

   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 Negative, click the Sample Type column and select Negative 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 Negative 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 Negative 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**.

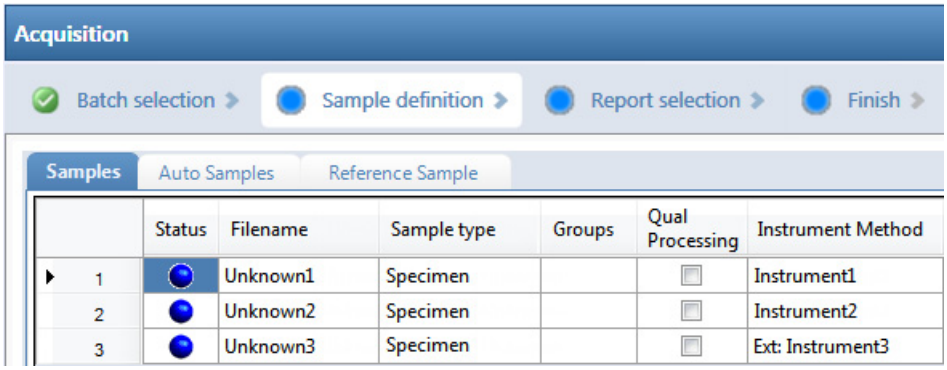
   The application displays the Instrument Method column, defaulting to the instrument method specified in the master method.

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 89. Instrument method column



When you submit the batch, the application saves a copy of the selected instrument methods to the following folders:

External instrument methods:

…\TraceFinderData\32\Projects\…*batch*\Methods*method**ExternalMethods*

Local instrument methods:

…\TraceFinderData\32\Projects\…*batch*\Methods*method*

Samples

Use the features on the Samples page to create a list of samples for the batch.

Figure 90. Samples page on the Sample Definition page

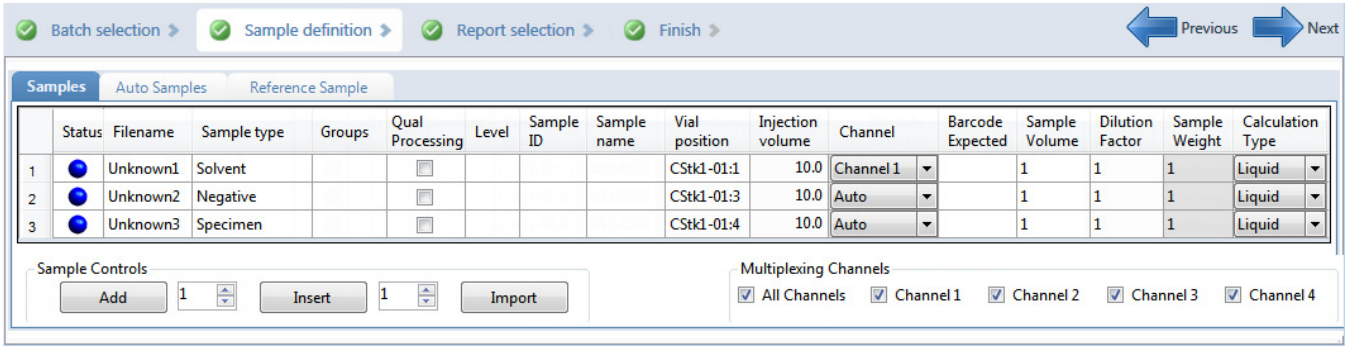


Table 66. Samples page parameters (Sheet 1 of 2)

Parameter	Definition
Previous	Returns you to the previous Acquisition page.
Next	Takes you to the next Acquisition page.
Status color codes	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-*n*	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 66. 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 329.
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" on page 373.
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	Opens the Instrument Setup window where you can edit the parameters of the instrument method. • 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\32\Projects*project**subproject**batch*\Methods*method* folder. For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 113.

Auto Samples

Use the features on the Auto Samples Sample page to identify the Solvent or Negative 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 244.

Each sample type that you specify for a failure action on the Intelligent Sequencing page must be defined on the samples list on the Auto Samples page.

Figure 91. Auto Samples page on the Sample Definition page

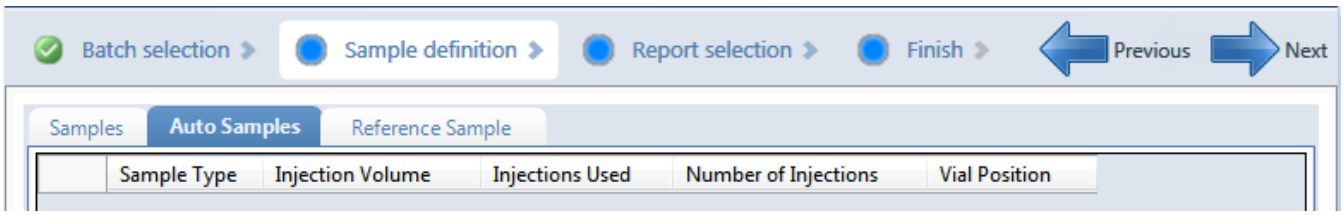


Table 67. Auto Samples page parameters

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 Negative. Default: Solvent
Injection Volume	The injection volume used for the sample acquisition as specified on the Samples page. 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 Negative 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 92. Reference Sample page on the Sample Definition page

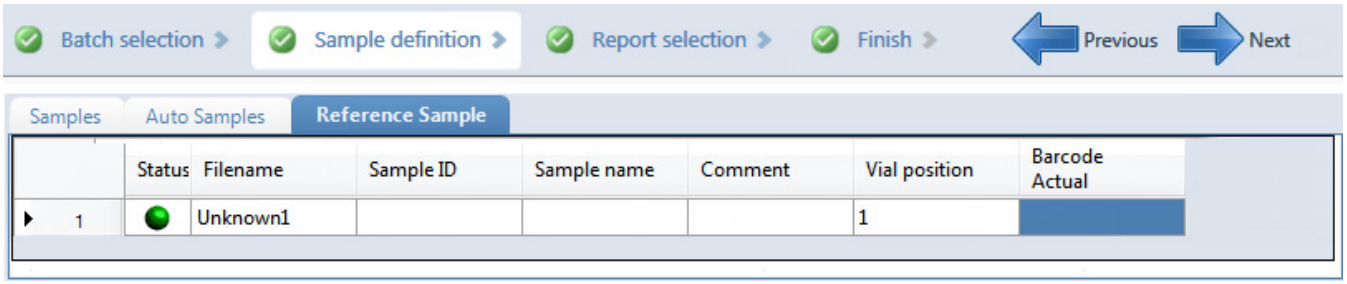


Table 68. Reference Sample page parameters

Parameter	Description
Status	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" on page 341. 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 the Batch" on page 342.

The application writes the resulting output files for your reports to the …\TraceFinderData\32\Projects\…*batch*\Reports folder.

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 93. Report Selection page

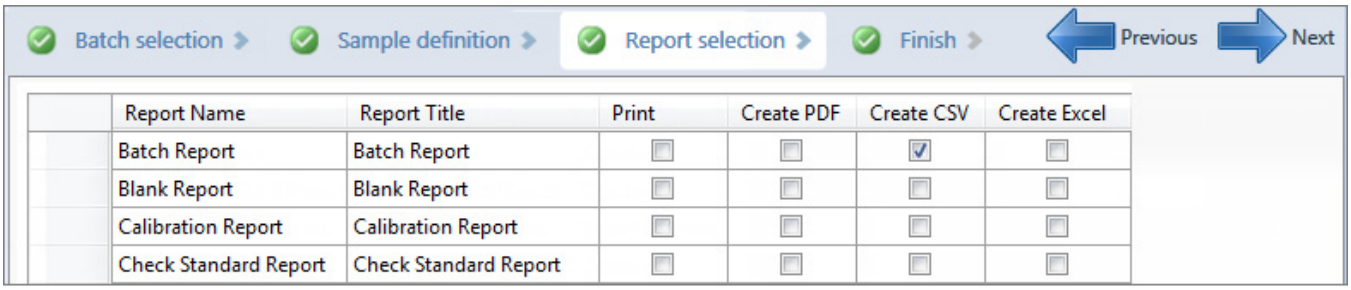


Table 69. Report Selection page parameters

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 the 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 349.

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
- To start an acquisition
- To view the output files

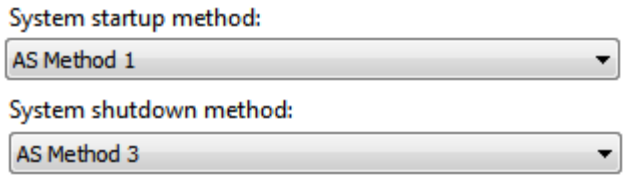
❖ To specify startup or shutdown methods

1. Select a method from the System Startup Method list.

   The TraceFinder application runs this method before running the batch. No autosampler injection takes place. This feature is not available for all instruments.

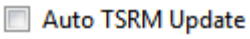
2. Select a method from the System Shutdown Method list.

   The TraceFinder application runs this method after running the batch. This feature is not available for all instruments.



❖ To automatically update the timed SRM information

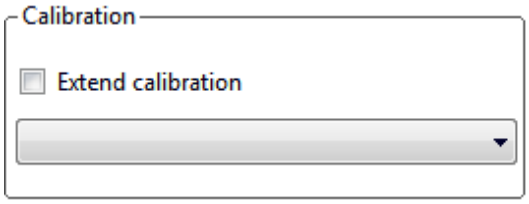
Select the **Auto TSRM Update** check box.



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.

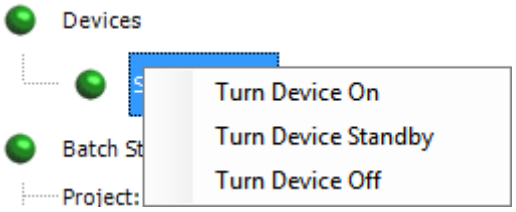


Table 70. Instrument states (Sheet 1 of 2)

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 70. 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 TraceFinder application can control, is turned off. This includes power to all heaters and subassemblies, but in some cases not all subassemblies. Some devices do not have an Off feature. For devices that do have this feature, the device enters a power-saving or consumable-saving mode, and you can switch the device back on. When several runs are queued, the application uses the system power scheme of the last submitted run.
Instrument status indicators	
	Green indicates that the device is turned on or is running.
	Yellow indicates that the device is in standby mode or is waiting for contact closure.
	Red indicates that the device is turned off or that there is an error with the device.

❖ To save a batch for later acquisition

From the Finish page, click **Save**, Save .

The TraceFinder application saves your batch as a prepared file.

❖ To start an acquisition

1. Click **Submit**, Submit .

   The Submit Options dialog box opens. For detailed descriptions of the parameters, see "Submit Options dialog box" on page 346.

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 any of the submitted samples has not been acquired, this option is (by default) selected.

3. To process the submitted samples, select the **Process Data** check box.

   You can process the data with or without performing peak detection. You might, for example, want to turn off peak detection when reprocessing samples.

4. (Optional) Select the **Create Reports** check box.

5. (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.

6. (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.

7. Select the **Use** check box for the device that you want to use for this acquisition.

8. (Optional) Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

   This is usually the autosampler.

9. (Optional) Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

   When this is cleared, individual instruments can start at different times and then have to wait for the last instrument to be ready.

10. Do one of the following:

    To start the selected processes, click **OK**.

    The selected processes begin, and the TraceFinder 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.

    –or–

    Click **Cancel** to exit the Acquisition mode without performing any tasks.

Figure 94. Submit Options dialog box

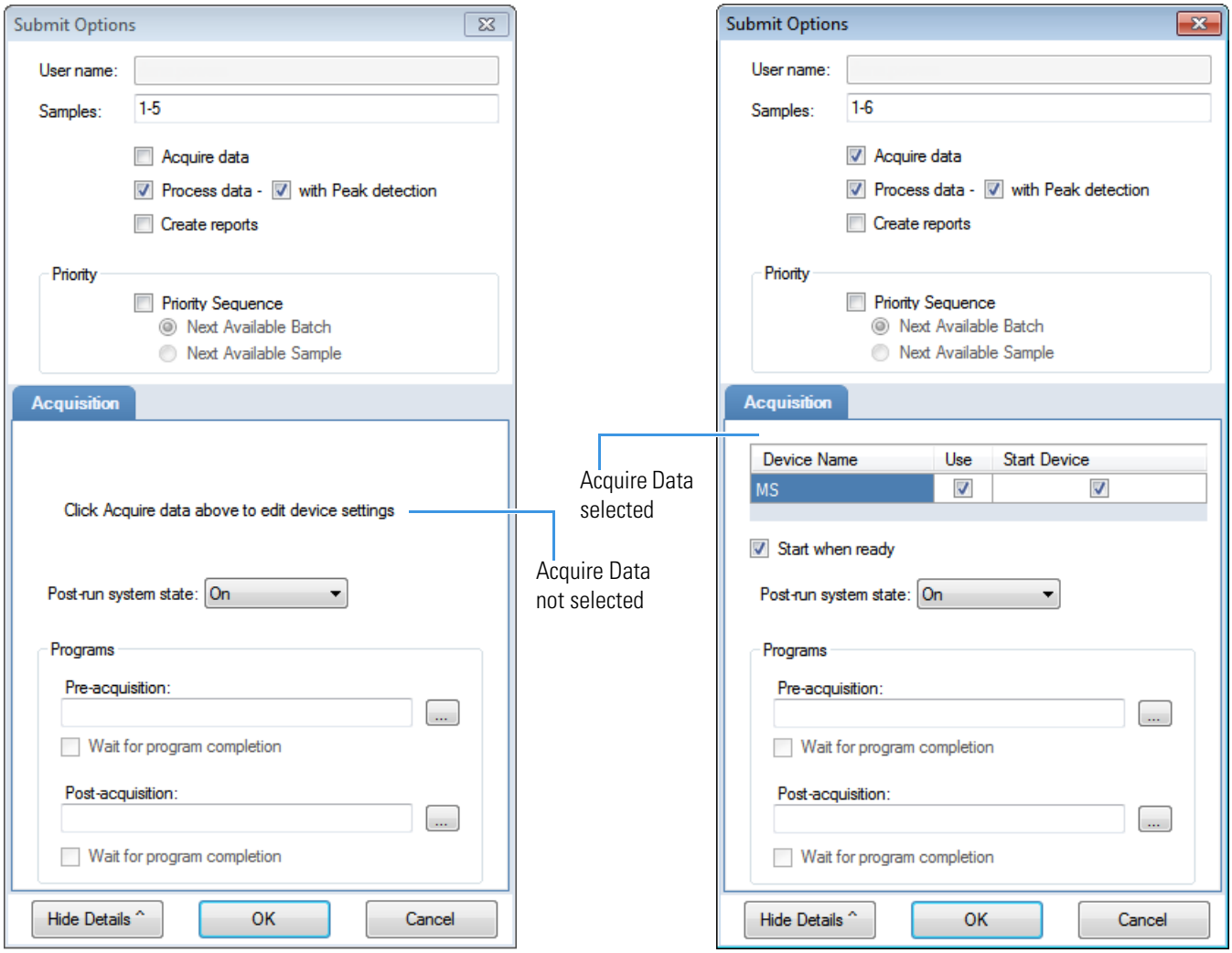


Table 71. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Acquire Data	Submits the current batch to acquisition. • When all submitted samples have been previously acquired, this option is (by default) not selected. • When any of the submitted samples has not been acquired, this option is (by default) selected.
Process Data	(Default) Processes the data for the current batch.

Table 71. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
With Peak Detection	(Default) Processes the data with peak detection. When you clear this option, the application reprocesses samples without performing peak detection.
Create Reports	Creates reports for the current batch.
Priority Sequence	With multiplexing activated, places the batch immediately after the currently acquiring batch. Without multiplexing activated, specifies one of the following priority options to place the batch in the queue: **Next Available Batch**: Places the batch immediately after the currently acquiring batch. **Next Available Sample**: Places the batch immediately after the currently acquiring sample. **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.
Acquisition pane	
Device Name	Lists all configured instruments. If the instrument that you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the TraceFinder application. You cannot configure an instrument while the TraceFinder application is running. Available only when you select the Acquire Data check box.
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.
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 TraceFinder application writes saved batches to the project folder:

…\TraceFinderData\32\Projects\…

For each acquired sample, the application writes an RSX file to the batch Data folder:

…\TraceFinderData\32\Projects\…\Data

The application saves method information to the batch Methods folder:

…\TraceFinderData\32\Projects\…\Methods

The application writes the reports to the batch Reports folder:

…\TraceFinderData\32\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 95. Finish page

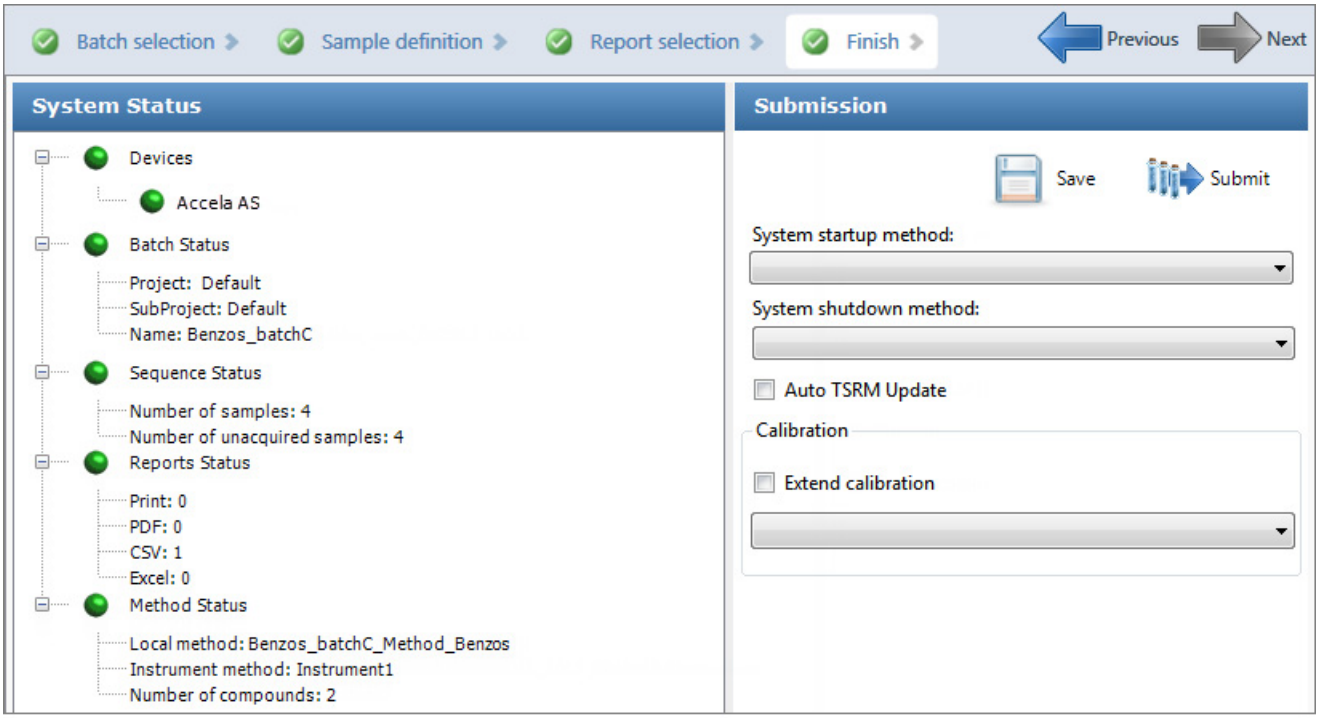


Table 72. Finish page parameters

Parameter	Description
System Status	The System Status pane displays the following: • Devices used for the acquisition • Project, subproject, and name of the batch • Number of 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 System Shutdown Method	The instrument methods that run before and after the batch. No autosampler injection 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	• 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 where you can choose to generate reports.

Real Time Status Pane

You can access the Real Time Status pane from any mode in the TraceFinder application.

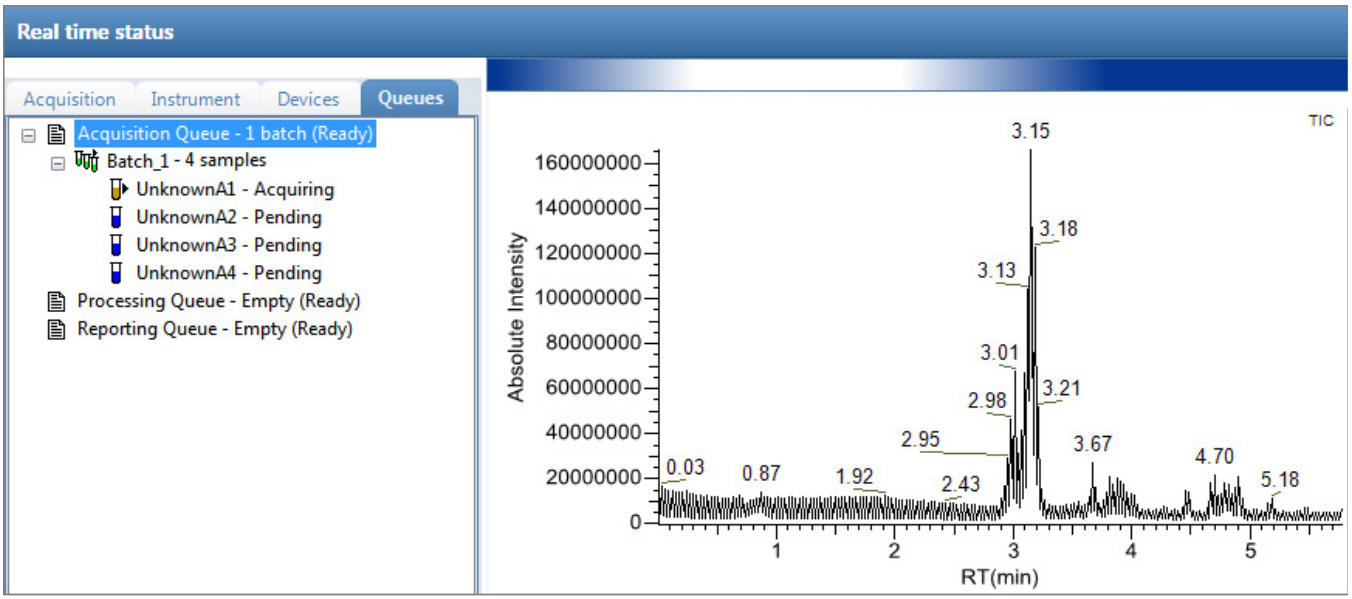
❖ **To access the Real Time Status Pane from any mode**

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 96. Real Time Status pane



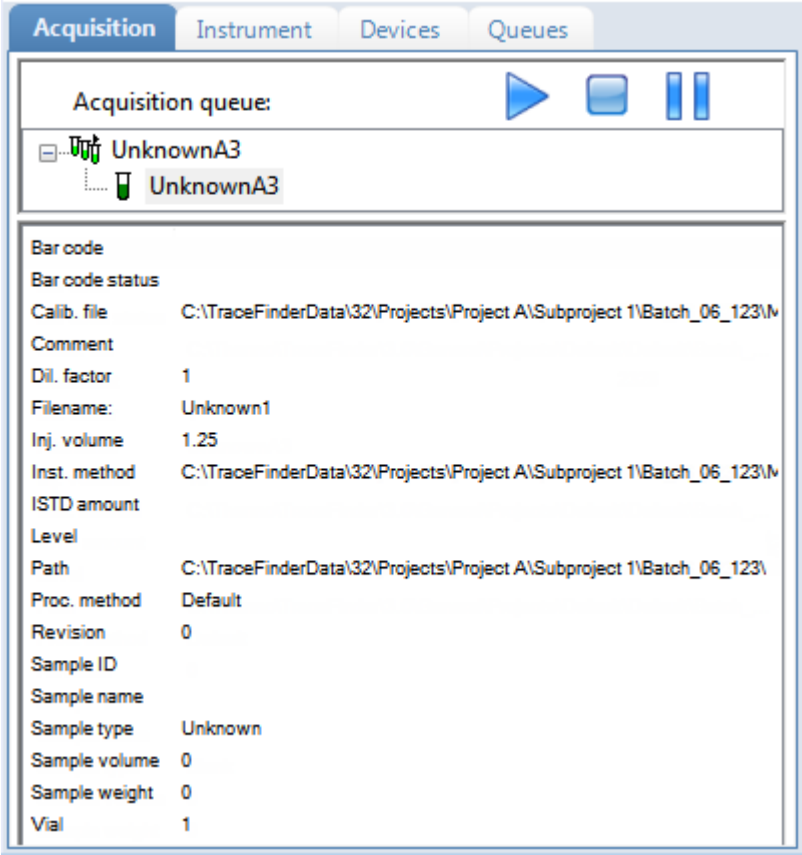
The Real Time Status pane has four pages of information and a real-time trace pane:

- Acquisition Page
- Instrument Page
- Devices Page
- Queues Page
- Real-Time Trace Display

Acquisition Page

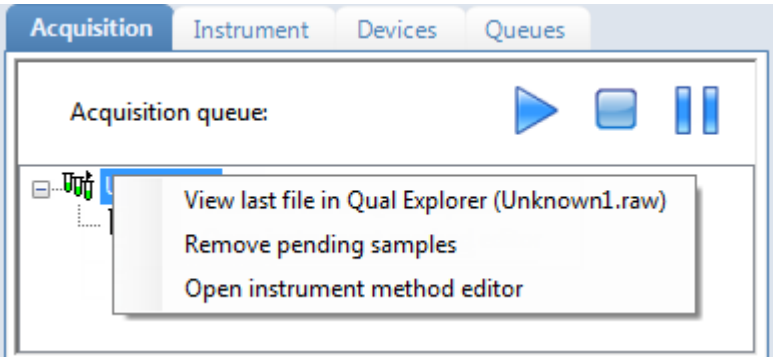
Use the Acquisition page to monitor the progress as the application acquires the samples.

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.

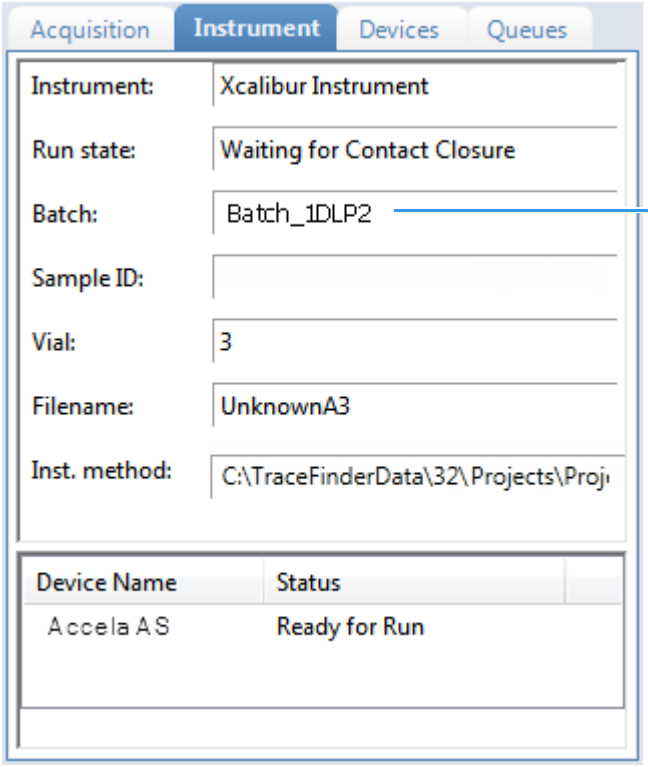
The Thermo Xcalibur Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 113.

> **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.



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 Xcalibur Instrument Setup window opens, displaying the currently running instrument method.

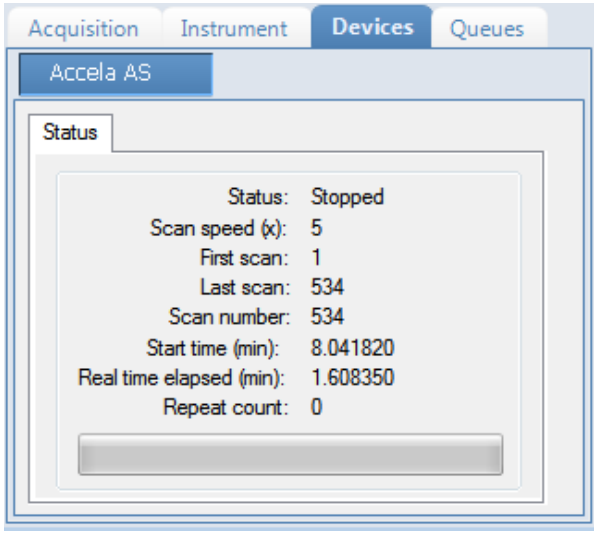
For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 113.

> **Note** Changes you make and save to the instrument method do not affect the currently running batch.

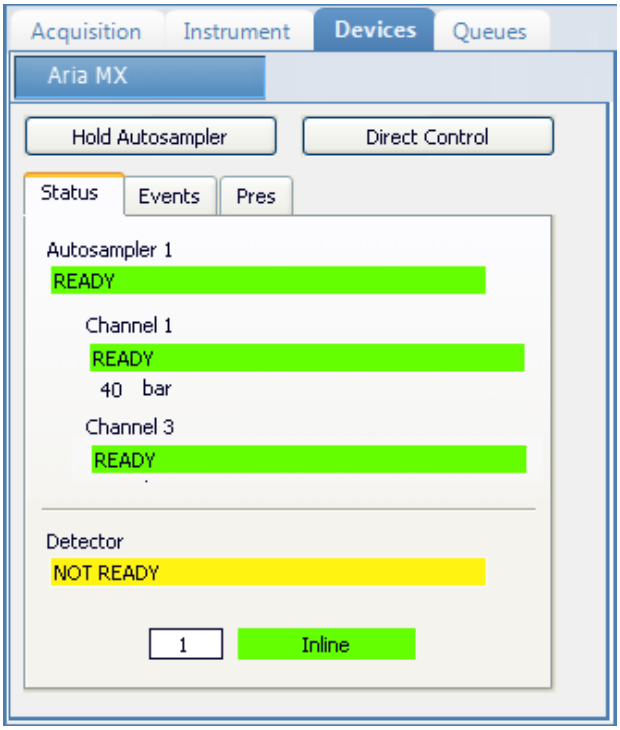
Devices Page

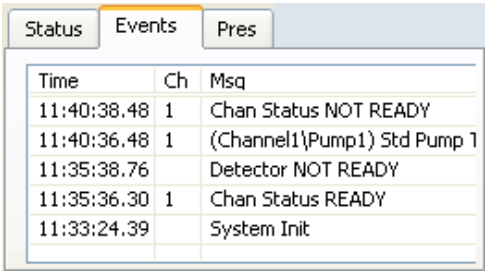
Use the Devices page to monitor the status of the instrument. The feedback you see on the Devices page depends on the instrument you are using. The following examples show an Accela autosampler and an Aria™ multiplexing device.

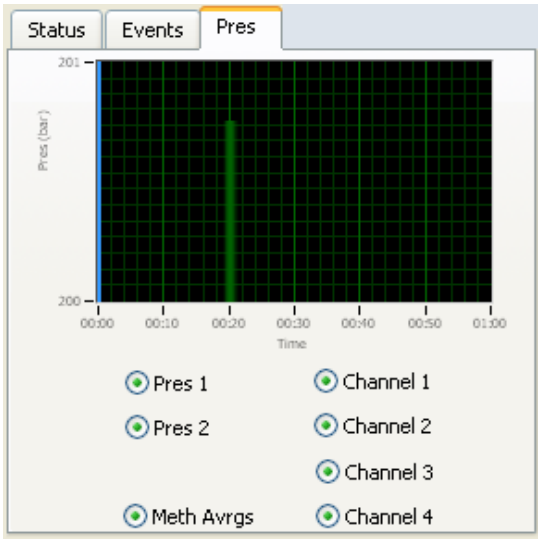
Accela Autosampler Feedback



Aria Multiplexing Feedback







Follow these procedures:

- To pause the autosampler
- To control the channels
- To view the pressure trace
- To access the Aria multiplexing controls
- To view the last acquired file in a qualitative browser
- To open the Instrument Setup window

❖ 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.

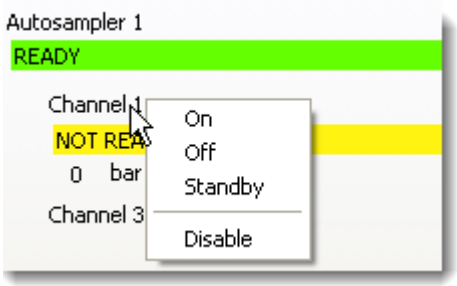


Table 73. Autosampler shortcut menu commands (Sheet 1 of 2)

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.

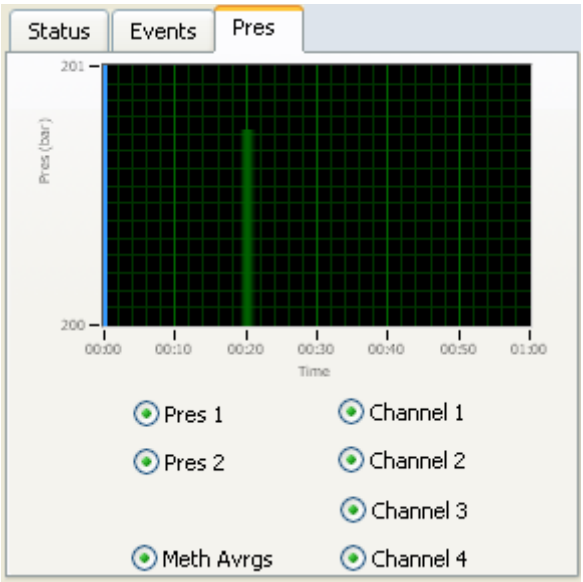
Table 73. Autosampler shortcut menu commands (Sheet 2 of 2)

Command	Description
Standby	After the current sample completes, the application stops acquiring. The pump continues to run.
Disable / Enable	**Disable**: Prevents the channel from receiving samples. When you choose **Disable** during a run, the application finishes the current sample on the channel and then stops. **Enable**: Allows the channel to receive samples. When you disable a channel that is set to **On**, the channel is highlighted in green and the status is READY. You can turn the channel to **Off** or **Standby**.

❖ To view the pressure trace

1. Click the **Pres** tab.

   The Pressure page displays a pump pressure graph for each sample in the batch. A fluctuation or change in the pump pressure could indicate a change in the chromatography conditions.



2. To view the pressure for a specific pump, select the **Pres 1** or **Pres 2** option.

   By default, the pressure for all pumps are displayed.

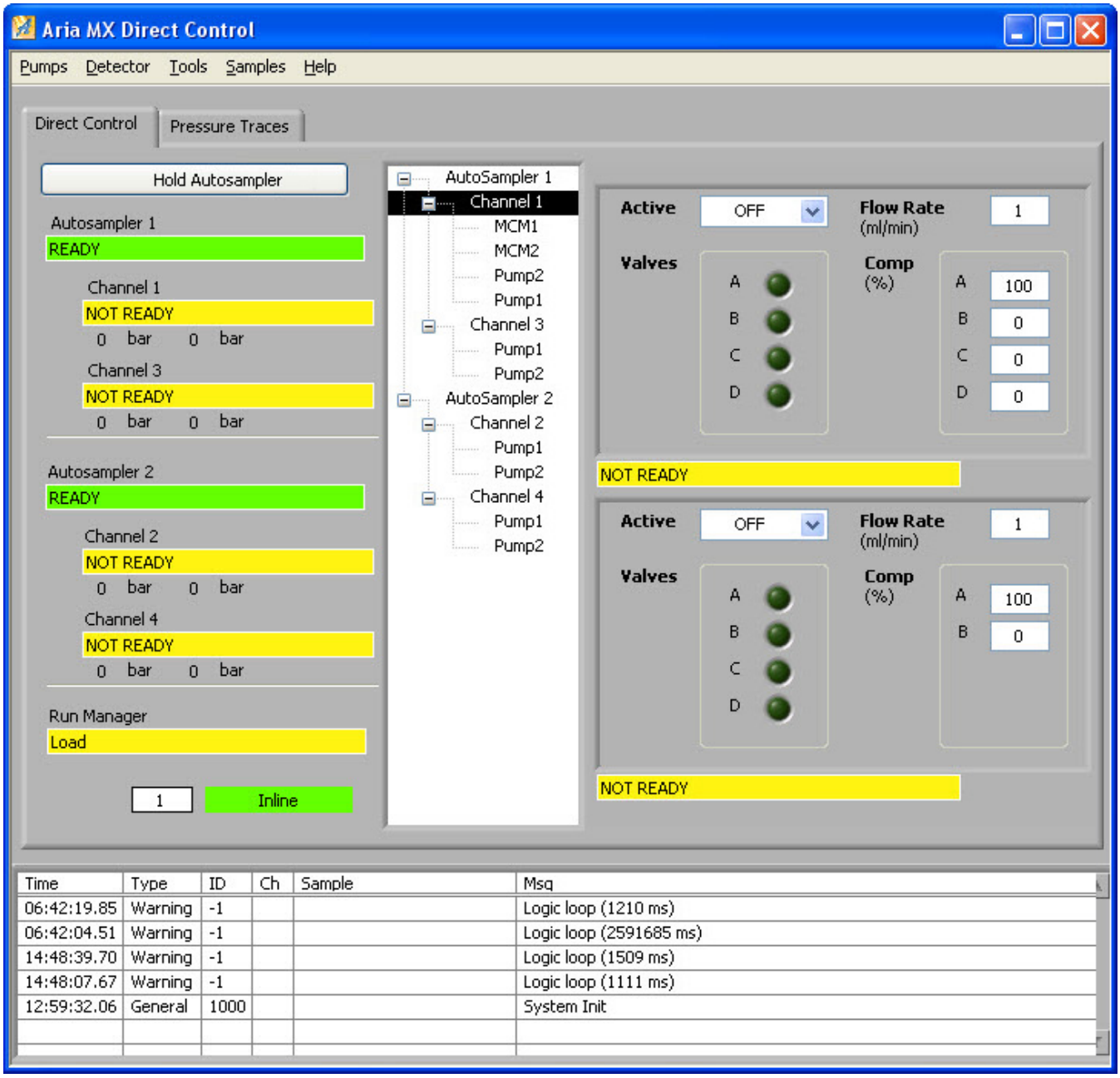
3. To view the pressure for a specific channel, select the corresponding channel number.

   By default, the pressure for all channels is displayed.

❖ **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.

❖ 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.

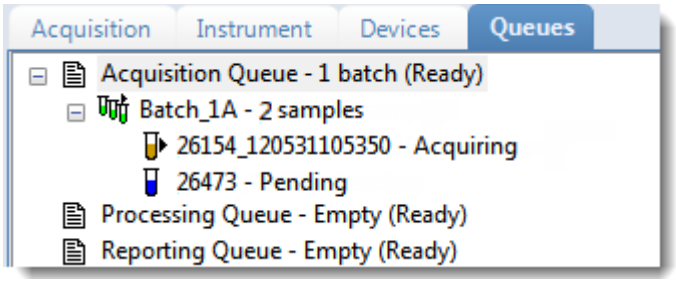
The Thermo Xcalibur Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 113.

> **Note** Changes you make and save to the instrument method do not affect the currently running batch.

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 361.

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

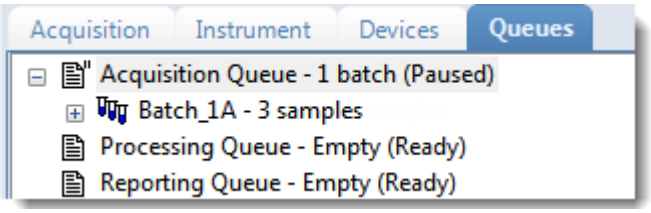
❖ To pause all batches in a queue

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 on the shortcut menu to pause or remove batches in any of the queues on the Queues page.

Figure 97. Queue-level shortcut menu

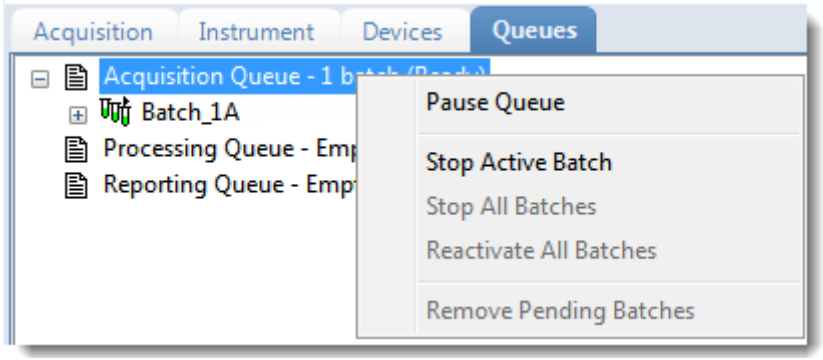


Table 74. Queue-level shortcut menu commands

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

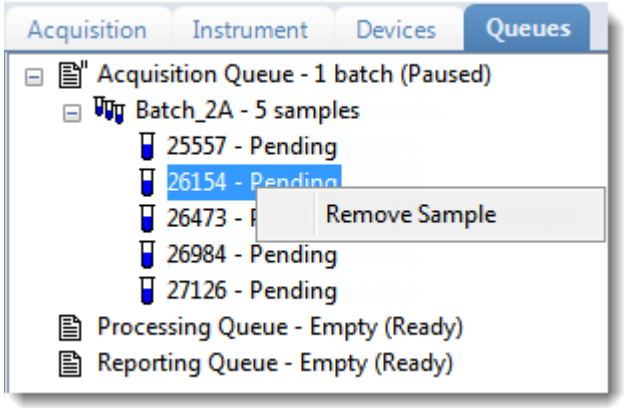
Use the batch-level commands to pause or remove entire batches or samples within batches from any of the queues on the Queues page. See "Batch-level shortcut menu."

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 98. Batch-level shortcut menu

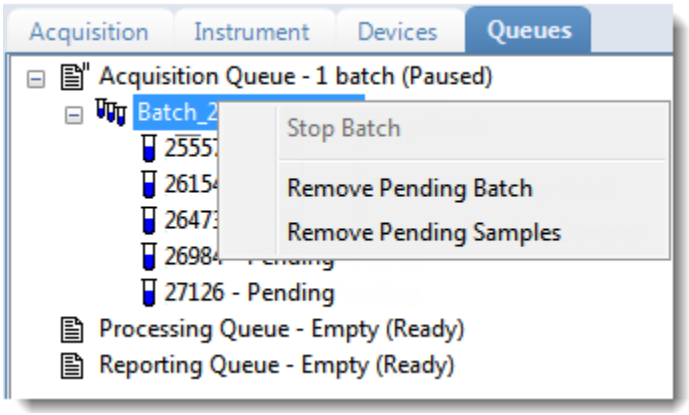


Table 75. Batch-level shortcut menu commands

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

Use the commands on this shortcut menu to open the FreeStyle application or the Instrument Setup window.

❖ 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.

> **Note** You must click in the white space below the list of queues. Clicking on or to the right of the queues displays queue-, batch-, or sample-level shortcut menus.

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.

> **Note** You must click in the white space below the list of queues. Clicking on or to the right of the queues displays queue-, batch-, or sample-level shortcut menus.

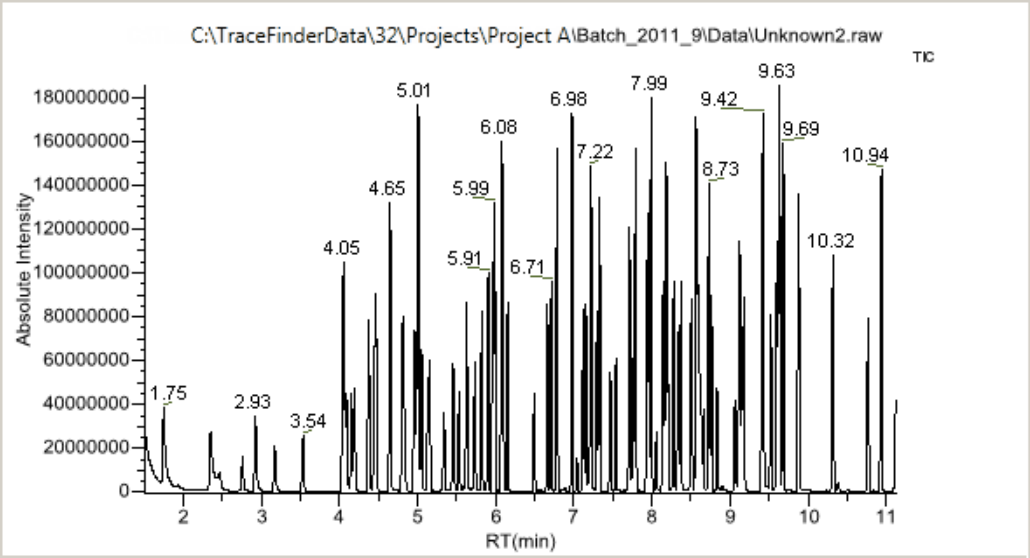
The Thermo Xcalibur Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 113.

> **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.

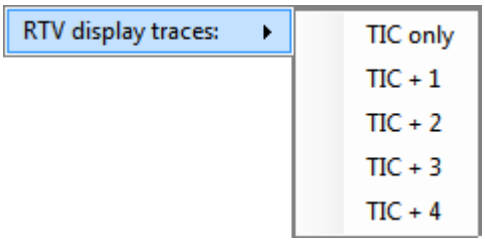


By default, the Real Time Status pane shows only the TIC trace as each sample acquires. To observe specific traces, such as the internal standard, use the RTV Display Traces function to display multiple traces.

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 350.

❖ To display multiple traces

Right-click the chromatogram pane and choose the number of traces to display.

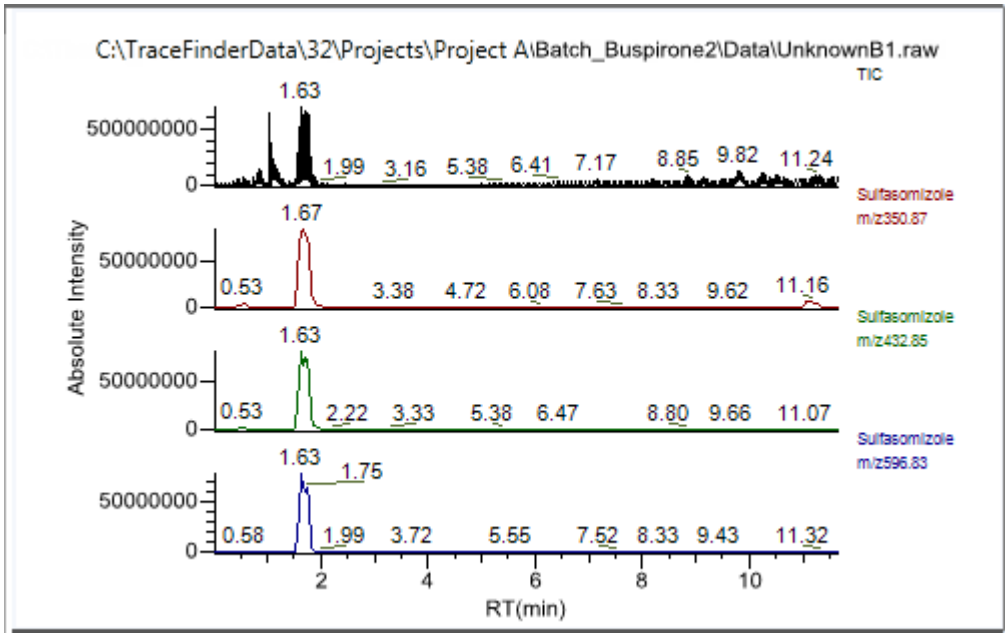


The chromatogram pane displays real-time chromatograms for the selected number of traces.

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.

Figure 99. Real-time trace display with multiple traces



Sample Types

The TraceFinder application uses the following sample types in all sample definitions and reports.

Table 76. Sample type definitions

Sample type	Definition
Negative	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.
Unextracted	Similar to a Negative sample, but contains target compounds. By analyzing a sample, you can confirm that there are no residual compounds in the solvent system that can cause erroneous results.
Calibrator	(Calibration standard) Contains known amounts of all target compounds. The purpose of a standard is to measure the response of the instrument to the target compounds so that the processing software can generate a calibration curve for each compound.
QC	(Quality Check) 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 sample, it compares the measured quantity with the expected value and an acceptability range. The quantitative analysis of a QC sample is classified as *passed* if the difference between the observed and expected quantities is within the user-defined tolerance. A QC sample is classified as *failed* if the difference between the observed and expected quantities is outside the user-defined tolerance.
Solvent	Contains only solvent.
Specimen	Used for quantitative analysis of samples.
Hydrolysis	Checks the degradation of compounds dissolved in water.

8

Using the Analysis Mode

This chapter includes instructions about using the features of the Analysis mode.

Contents

- Working in the Batch View
- Working in Data Review for Quantitation Methods
- Working in Data Review for Target Screening Methods
- Working in the Local Method View
- Working in the Report View
- Working in the Report Designer

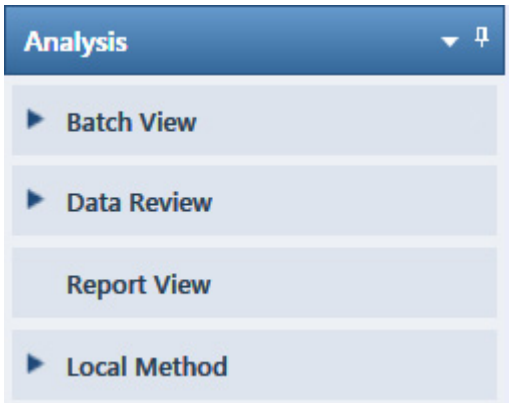
Use the Analysis mode to do the following:

- Submit batches for acquisition, processing, or reports.
- Review batches, batch data, reports, and local methods.

❖ 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 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 on the Batch View shortcut menu to create the sample list and submit samples for acquisition. See "Toolbar" on page 380 or "Batch View Shortcut Menu" on page 384.

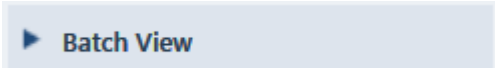
This section includes the following topics:

- Samples Page
- Auto Samples Page
- Reference Samples Page
- Threshold Samples Page

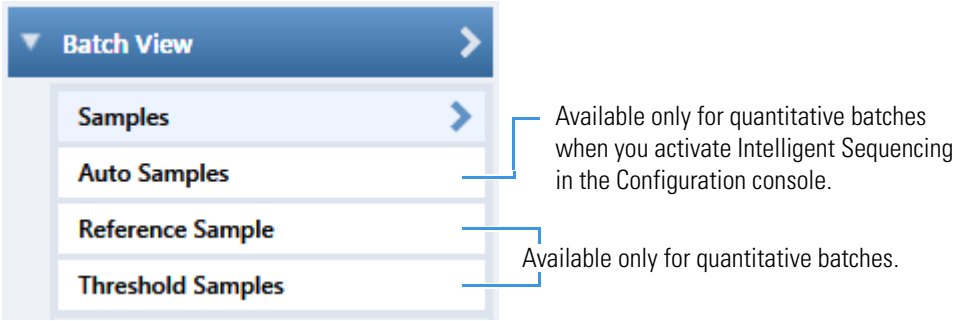
❖ To open the Batch View

1. Click **Analysis** in the navigation pane of the current mode.

2. In the Analysis navigation pane, click **Batch View**.



The Batch View navigation pane opens.



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:

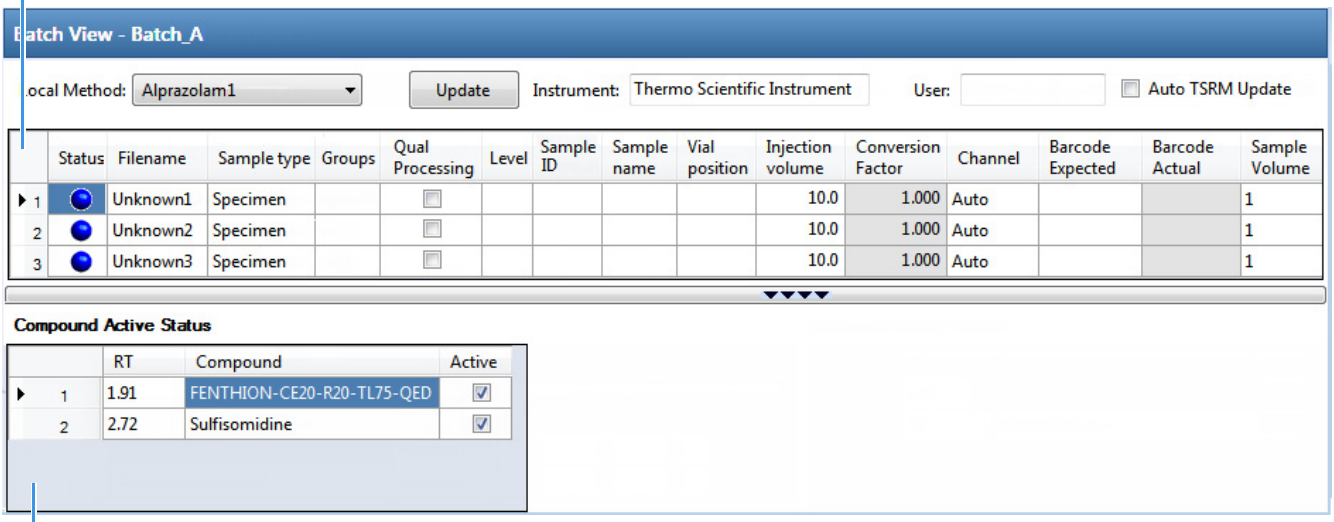
- Samples pane

  Use the samples pane to create a batch. See "Samples Pane" on page 372.

- Compound Active Status pane

  Use the Compound Active Status pane to make specific compounds active or inactive. See "Compound Active Status Pane" on page 386.

Samples pane



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 in Target Screening Batches
- 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 of information, and you can customize which columns to display and their display order.

Follow these procedures:

- To scroll the sample list
- To customize the column display

❖ 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 Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name columns stay fixed 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, 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** You cannot move the Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, or Sample Name columns.

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 100. Modify Columns dialog box

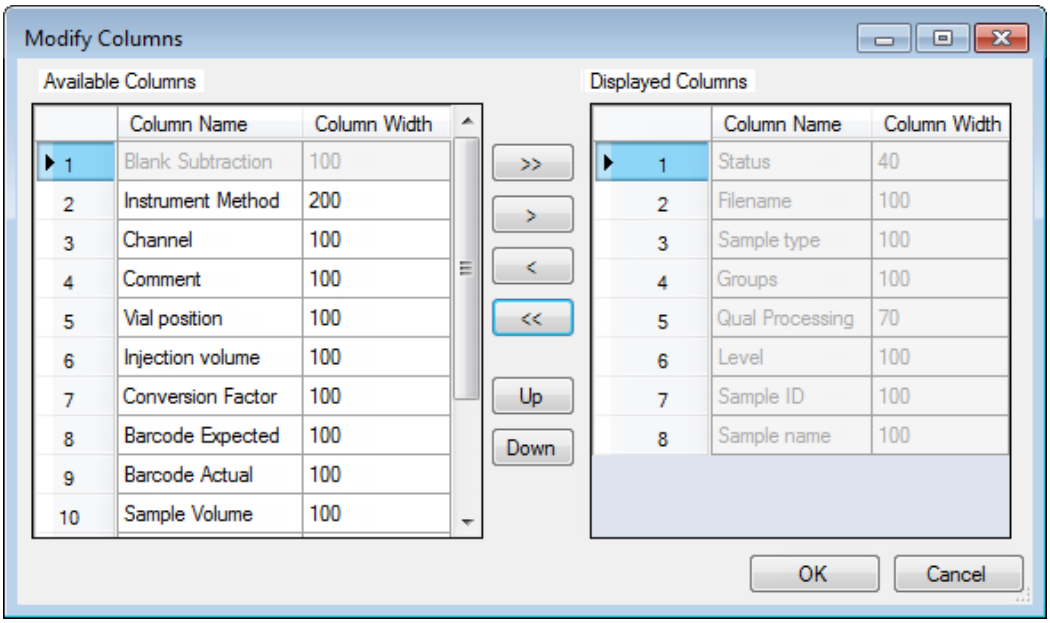


Table 77. Button descriptions for the Modify Columns dialog box

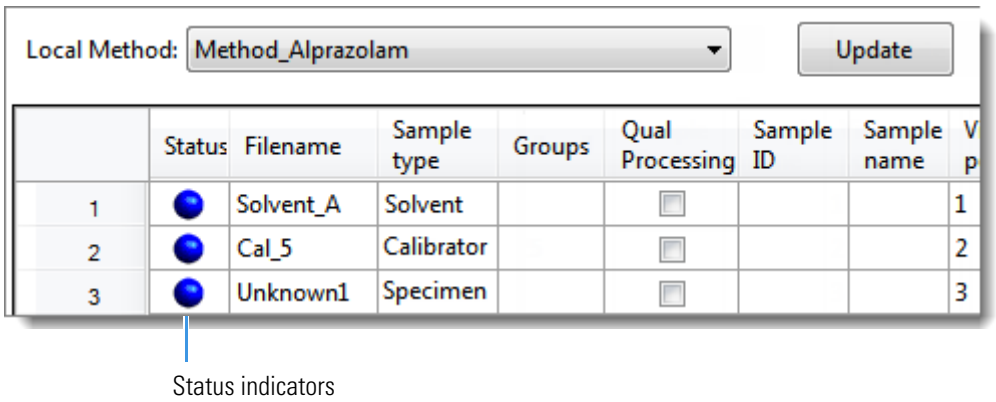
Button	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.	
<	Moves the selected column to the Available Columns pane.
<<	Moves all columns except fixed columns.
Up	Moves the selected column name in the Displayed Columns pane one row up in the column order.
Down	Moves the selected column name in the Displayed Columns pane one row down in the column order.

Note The application adds a Blank Subtraction column to the fixed columns for target screening batches only.

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.



Groups

Use the Groups feature to assign samples to a group. After you create groups, you can choose one of the samples as a threshold sample for the group and then view the samples in the group in the Comparative View in the Analysis mode.

❖ To create a group

1. For each sample, click the Groups column and type the name of a group.

   Note Group names are not case sensitive and are always interpreted as lowercase. For example, if you assign one sample to “GroupA” and another sample to “groupa”, both samples are assigned to “groupa” on the Threshold Samples page.

   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

For information about specifying a threshold sample for a group of samples, see "Threshold Samples Page" on page 412.

For information about viewing grouped samples in Data Review, see "Comparative View" on page 436.

Blank Subtraction in Target Screening Batches

In target screening batches only, use the Blank Subtraction feature to select which negative samples you want to use for peak subtraction. The application subtracts the areas of the peaks in the selected negative samples from the matching areas in the specimen samples.

Status	Filename	Sample type	Blank Subtraction
	Benzo25557	Negative	☑
	Benzo25558	Specimen	☐
	Benzo25559	Negative	☑
	Benzo25560	Specimen	☐

When you process the batch sequence, the application subtracts the peaks in a selected negative sample from all specimen samples that follow it, until it encounters another negative sample.

To activate the Blank Subtraction feature, see "Editing the Processing Page" on page 279.

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* ÷ *DilutionFactor*

Solid: (*SampleVolume* × *DilutionFactor*) ÷ *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* ÷ *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* × *DilutionFactor*) ÷ *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.

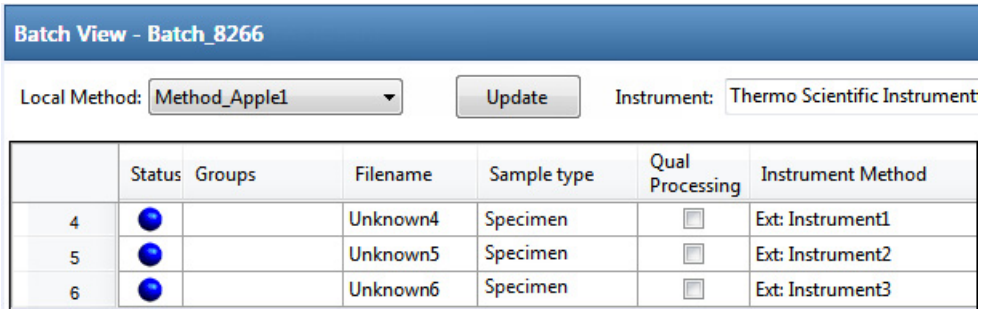
   b. In the Available Columns pane, select **Instrument Method**.
   c. Click [>] to move the Instrument Method column to the Displayed Columns pane.
   d. Click **OK**.

   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\32\Projects\…*batch*\Methods*method**ExternalMethods*

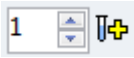
Local instrument methods:

…\TraceFinderData\32\Projects\…*batch*\Methods*method*

Toolbar

The Analysis mode includes this toolbar for creating and submitting a batch.

Table 78. 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 390.
	Inserts a new, empty sample or samples above the selected sample. See the instructions "To insert samples into the list" on page 390.
	Removes the selected samples from the sample list. See the instructions "To remove samples from the list" on page 391.
	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 390.
	Submits only the selected samples for acquisition, processing, or report generation. See the instructions "To submit samples in the batch" on page 401.
	Submits the batch for acquisition, processing, or report generation. See the instructions "To submit samples in the batch" on page 401.
	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 for Quantitation Methods" on page 413.
	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 313.
	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 9, "Using the Audit Viewer."

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 101. Batch View sample list

Local Method: Method_Benzos | Update | Instrument: Thermo Scientific Instrument

	Status	Filename	Sample type	Groups	Qual Processing	Level	Sample ID	Sample name	Vial position	Injection volume
1		UnknownA1	Specimen				1		CStk1-01:7	10.0
2		UnknownA2	Specimen				1		CStk1-01:7	10.0
3		UnknownA3	Specimen				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			

Note

- In target screening batches only, the sample list includes a Blank Subtraction column after the Sample Type column.
- Cells in the sample list that are not editable, such as Barcode Actual, are shaded and empty.

Table 79. Batch View sample list columns (Sheet 1 of 2)

Column	Description
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.
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	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative Default: Specimen
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.
Blank Subtraction	Specifies a negative 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	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. Range: 0.1 through 5000 µL

Table 79. Batch View sample list columns (Sheet 2 of 2)

Column	Description
Calculation Type	**Liquid**: The application calculates the Conversion Factor as *SampleVolume* ÷ *DilutionFactor* **Solid**: The application calculates the Conversion Factor as (*SampleVolume* × *DilutionFactor*) ÷ *SampleWeight* **Manual**: Sample Volume, Dilution Factor, Sample Weight, and Final Units columns are not available, and the Conversion Factor value is editable.
Conversion Factor	Editable only when Calculation Type is Manual. Default: 1
Sample Volume	Default: 1
Dilution Factor	Default: 1
Sample Weight	Available only when Calculation Type is Solid. Default: 1
Final Units	Specifies the calculated amount in the Data Review view or in reports. Default: 1
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 373.
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.

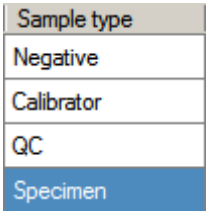
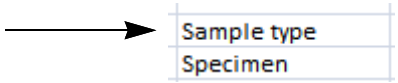
Batch View Shortcut Menu

The Batch View includes a shortcut menu for creating a batch.

Table 80. 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 390.
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 373.
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 80. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
Copy with Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information into another text editor or spreadsheet application. You cannot paste this data back into the sample list. For example  Copy With Headers from TraceFinder  Paste into Excel spreadsheet
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. • 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\32\Projects\…*batch*\Methods*method* folder. For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 113.

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	☑
2	2.72	Sulfisomidine	☑

   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 158.

   - 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.

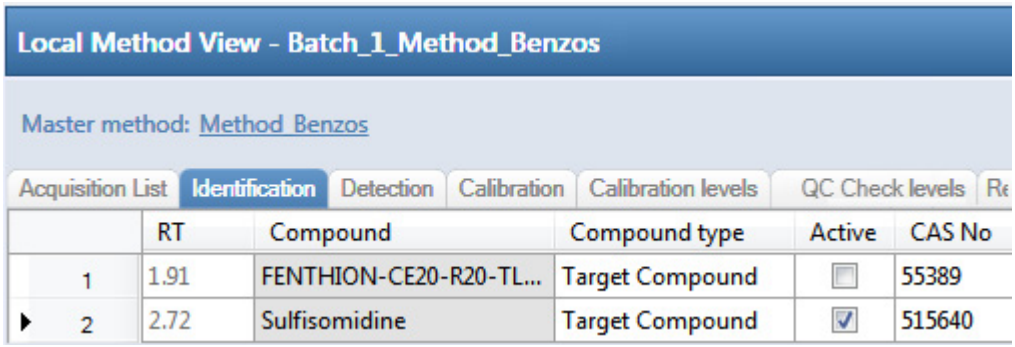
2. Select or clear the **Active** check box for the compound.

   For instructions about changing the active/inactive status in the Data Review view, see "Inactive and Excluded Compounds" on page 466.

Compound Active/Inactive Status

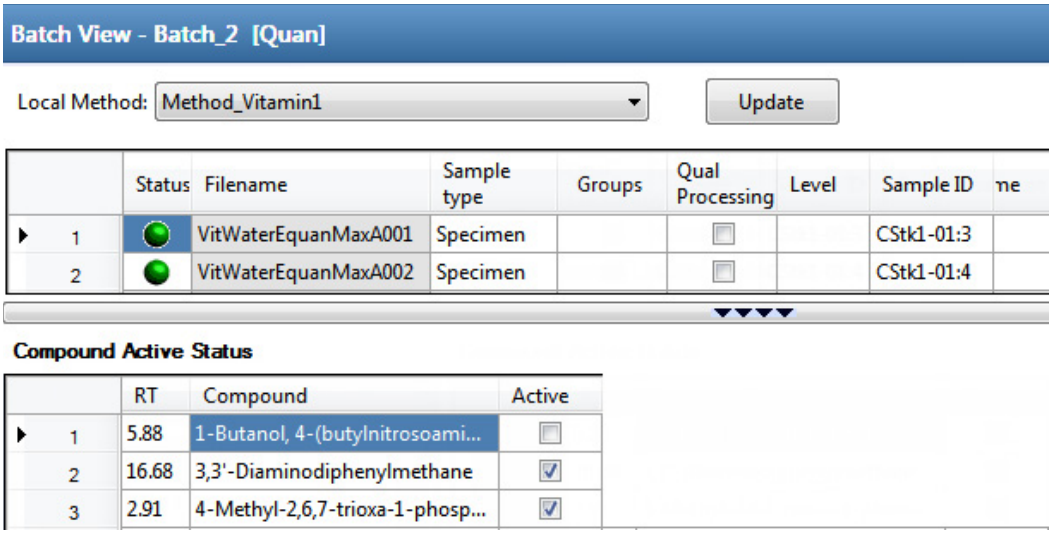
You can specify which compounds are active or inactive in the Local Method View or the Batch View.

Figure 102. Active and inactive compounds in the Local Method View



For details about setting the status on the Identification page, see "Identification" on page 158.

Figure 103. Active and inactive compounds in the Batch View



For details about setting the status in the Batch View, see "Compound Active Status Pane" on page 386.

Creating a New Batch

In the Batch View, you can create a new batch.

Follow these procedures:

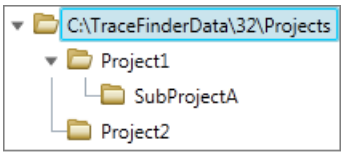
- To create a new batch
- To add samples to the list
- To insert samples into the list
- To import samples into the list
- To remove samples from the list
- To copy a sample
- To reinject a sample
- To edit sample values
- To browse in raw data files
- To customize the column display

❖ 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" on page 396.

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.

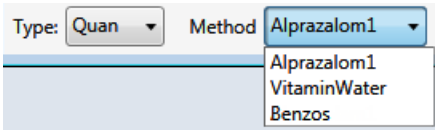
   To create a new folder for the storage location, see "Editing Folders for Batches" on page 398.

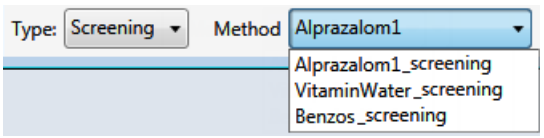
4. Select either **Quan** or **Screening** from the Type list.

   The batch list displays all batches in the selected folder. The Method list displays all methods for the selected type: quantitative or target screening.

5. Select a master method from the Method list.

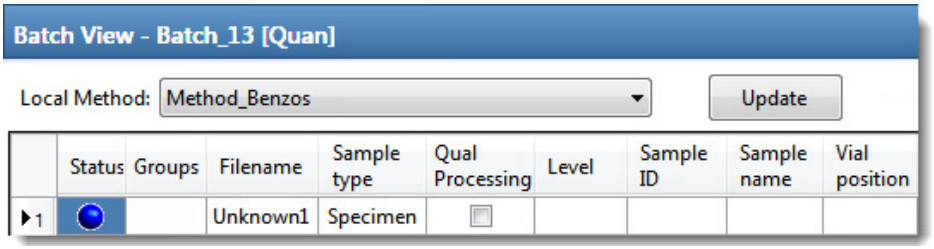
   The list displays all available methods of the selected type, either quantitative or target screening.





6. Click **Create**.

   A new batch opens with one Specimen sample.



   The batch name in the title bar indicates that you are creating either a quantitative or 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, 1 .

   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, Specimen 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 1 .

The application inserts the Specimen samples above the selected sample.

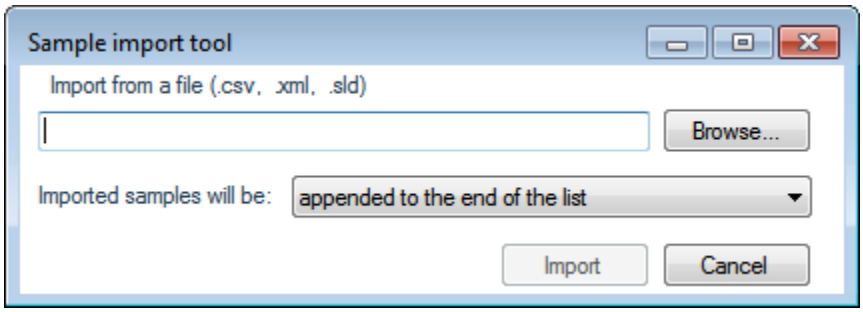
Inserted samples

	Status	Filename	Sample type	Groups	Qual Processing	Level
1		cal_std_5	Calibrator			5
2		Unknown2	Specimen			
3		Unknown1	Specimen			
4		cal_std_10	Calibrator			10

❖ 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 TraceFinder 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 TraceFinder application makes the following sample type substitutions:

Xcalibur sample type	TraceFinder sample type
Blank	Negative
Std Bracket	Calibrator

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 TraceFinder 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 TraceFinder 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			
Specimen	Hydrolysis	Solvent	QC
Unextracted	Calibrator	Negative	

3. For each Calibrator or QC 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 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 219.
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 Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name columns stay fixed 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 Specimen.

   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.

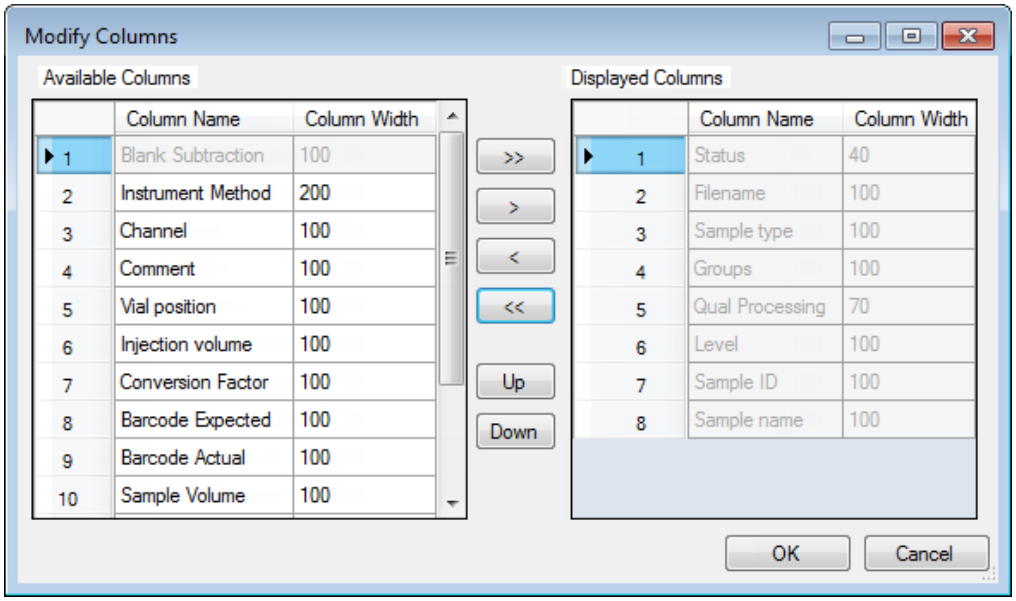


Table 81. Button descriptions for the Modify Columns dialog box

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.
Up	Moves the selected column name in the Displayed Columns pane one row up in the column order.
Down	Moves the selected column name in the Displayed Columns pane one row down in the column order.

Note The application adds a Blank Subtraction column to the fixed columns for target screening batches only.

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 You cannot move the Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, or Sample Name columns.

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.

Create New Batch

Use the Create New Batch dialog box to select a folder and method for your batch and to name the new batch.

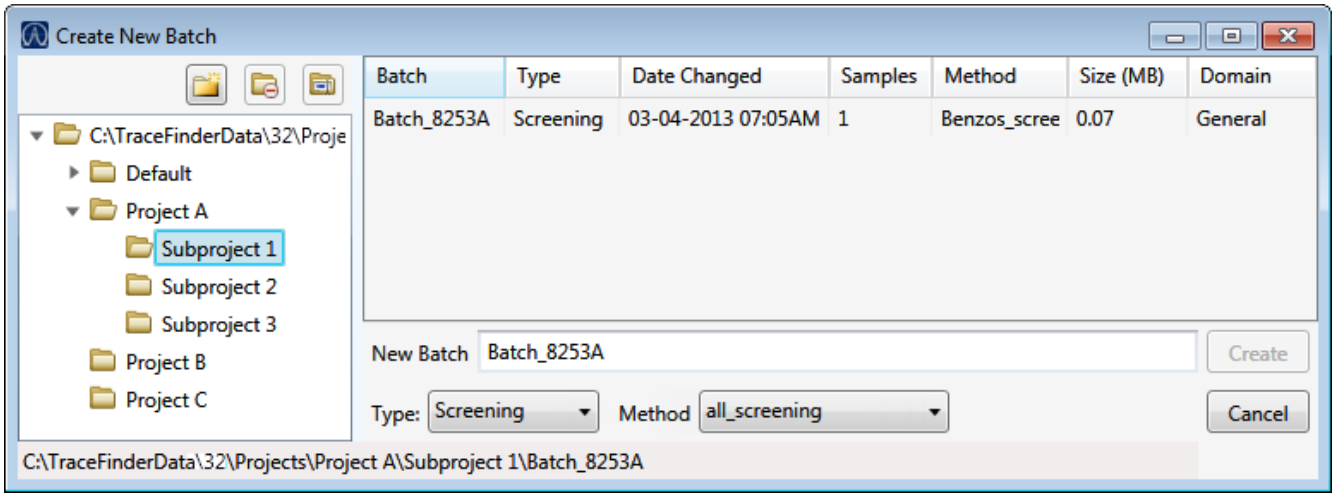


Table 82. Create New Batch dialog box parameters (Sheet 1 of 2)

Parameter	Description
Create New Folder	Adds one of the following: • 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 or Screening.
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.

Table 82. Create New Batch dialog box parameters (Sheet 2 of 2)

Parameter	Description
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 or Screening.
Method	Method used to create the new batch.
Path	Path to the project in the TraceFinderData\32\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\32\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**, **Screening**, or **Any** from the Type list.

   The batch list displays all batches created with the selected type of method.

4. Select a batch from the list.
5. Click **Open**.

   The selected batch opens in the Batch View.

Figure 104. Open Batch dialog box

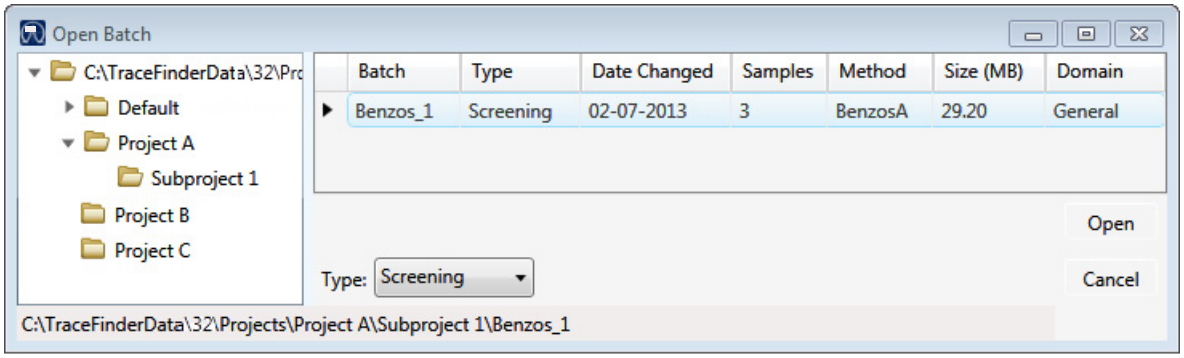


Table 83. Open Batch dialog box parameters (Sheet 1 of 2)

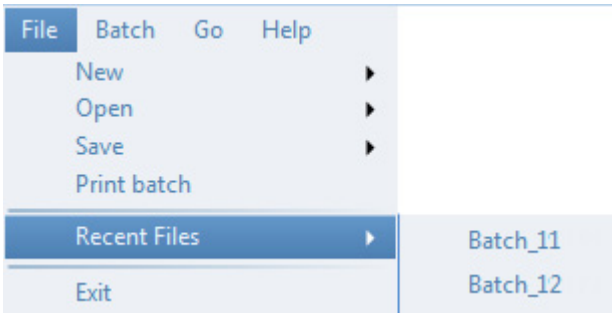
Parameter	Description
Batch	Name of batches in the selected project.
Type	Type of batch: Quan or Screening.
Date Changed	Date the batch was last updated.

Table 83. 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.
Path	Path to the project in the TraceFinderData\32\Projects folder where the batch is stored.
Buttons	
Type	Type of batch to display in the Batch list: Quan, Screening, 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 370.

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 TraceFinder 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_50_INJ001	Calibrator	10
	cal_50	Calibrator	10
	cal_10_INJ001	Calibrator	10
	cal_10	Calibrator	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 403.

For a description of commands on the shortcut menu, see "Batch View shortcut menu commands" on page 384.

❖ 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 403.
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 not selected by default.
   - When any of the submitted samples have not been acquired, this option is selected by default.
3. To process the submitted samples, select the **Process Data** check box.

   You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.
4. (Optional) Select the **Create Reports** check box.

5. (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.

6. (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.

7. (Optional) Click **Show Details** to display additional Acquisition parameters.
8. Select the **Use** check box for the device that you want to use for this acquisition.
9. (Optional) Select the **Start Device** check box to indicate the device that will initiate the communication with the other instruments.

   This is usually the autosampler.

10. (Optional) Select the **Start When Ready** check box to have all instruments start together when they are all ready.

    When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.

11. To start the selected processes, click **OK**.

Figure 105. Submit Options dialog box

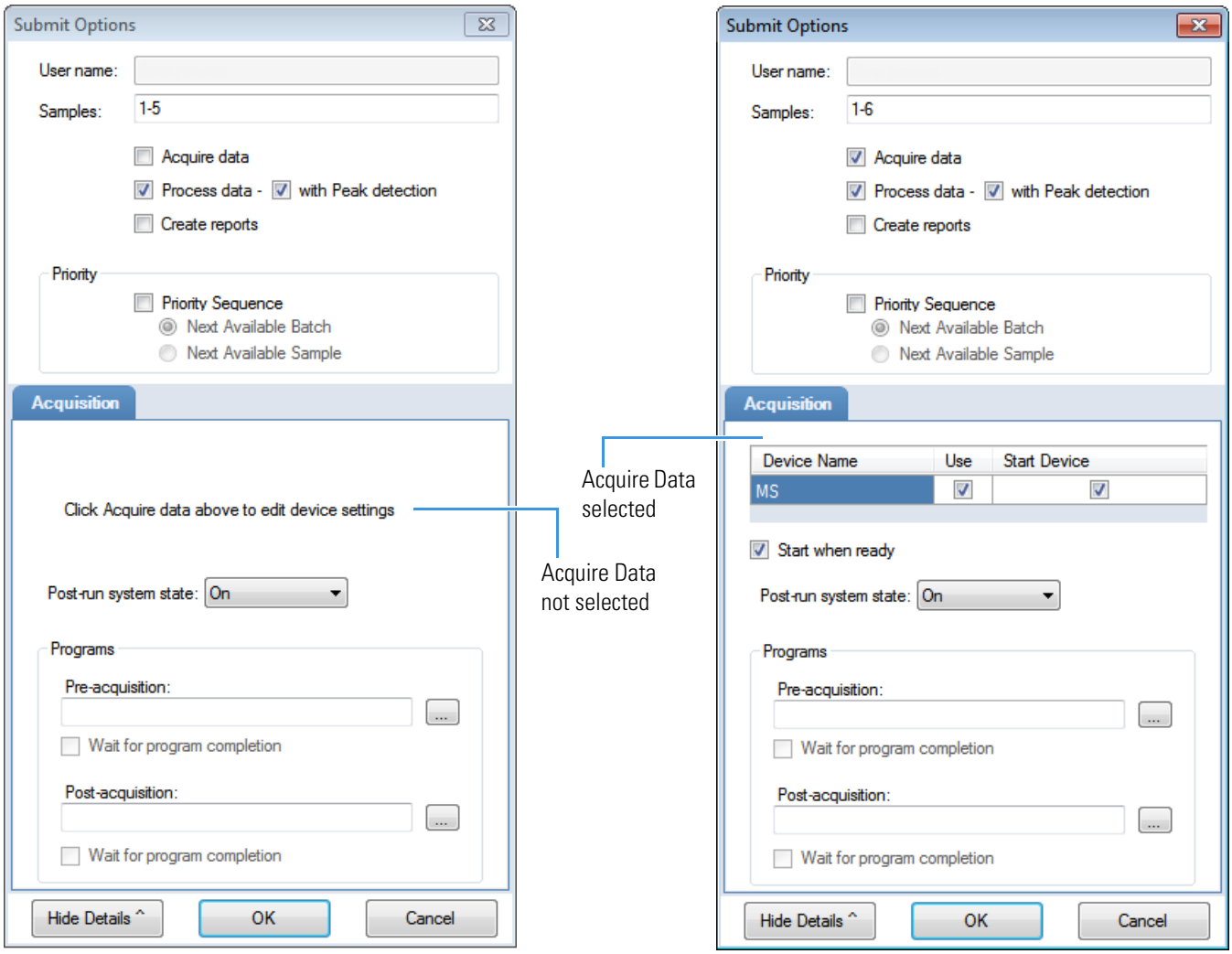


Table 84. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Samples	Range of samples to be submitted for acquisition, processing, or reporting.
Acquire Data	Submits the current batch to acquisition. • When all submitted samples have been previously acquired, this option is (by default) not selected. • When any of the submitted samples has not been acquired, this option is (by default) selected.
Process Data	(Default) Processes the data for the current batch.
With Peak Detection	(Default) Processes the data with peak detection. When cleared, this option lets you reprocess samples without performing peak detection.
Create Reports	Creates reports for the current batch.

Table 84. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
Priority Sequence	With multiplexing activated, places the batch immediately after the currently acquiring batch. Without multiplexing activated, specifies one of the following priority options to place the batch in the queue: • **Next Available Batch** places the batch immediately after the currently acquiring batch. • **Next Available Sample** places the batch immediately after the currently acquiring sample.
Acquisition pane	
Device Name	Lists all configured instruments. If the instrument that you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the TraceFinder application. You cannot configure an instrument while the TraceFinder application is running. Available only when the Acquire Data check box is selected.
Use	Specifies the instruments used for this acquisition. Available only when the Acquire Data check box is selected.
Start Device	Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler. Available only when the Acquire Data check box is selected.
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.

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 folders
- 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 main menu in the Analysis mode.

   The Save Batch As dialog box opens. See "Save Batch As Dialog Box" on page 407.

2. Select a storage location.

   The default storage location is C:\TraceFinderData\32\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 main menu in the Analysis mode.

   The Save Batch As dialog box opens. See "Save Batch As Dialog Box" on page 407.

2. Select a storage location.

   The default storage location is C:\TraceFinderData\32\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 folders

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\32\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 on 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 106. Save Batch As dialog box

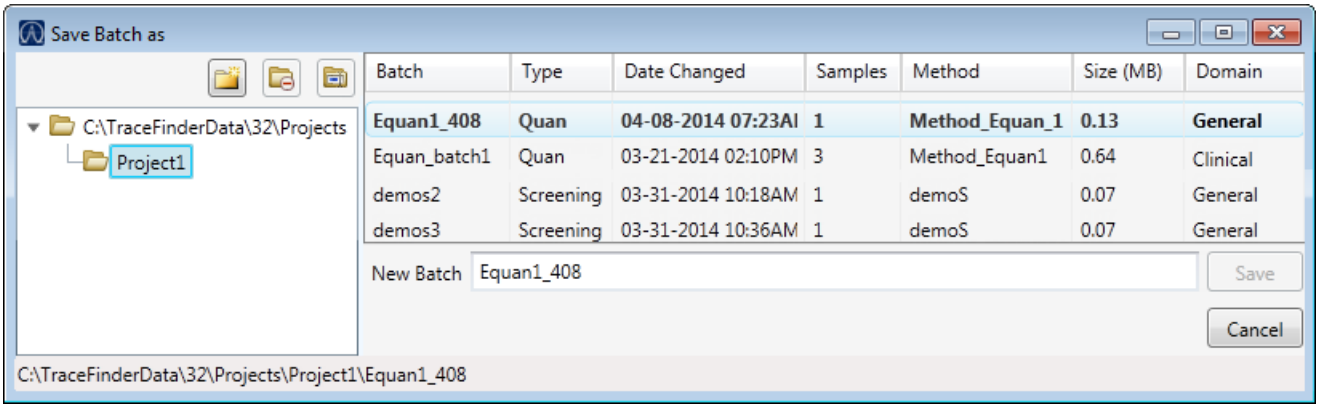


Table 85. Save Batch As dialog box parameters (Sheet 1 of 2)

Parameter	Description
Create New Folder	Adds one of the following: • 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 or Screening.
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 85. 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.
Path	Path to the project in the TraceFinderData\32\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: • 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 Negative 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 244.

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 open the Auto Samples page

Click **Auto Samples** in the Batch View navigation pane.

The Auto Samples page opens. See Auto Samples page.

❖ To add an auto sample type

1. 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 371.

2. To change the sample type to a Negative, click the Sample Type column and select Negative from the list.

3. 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.

4. In the Number of Injections column, type the number of injections available in the designated Solvent or Negative vial.

   After auto sample injections have occurred, you can return to this page to view the number of Injections Used in each vial.

5. In the Vial Position column, type the vial position for the Solvent or Negative sample.

Figure 107. 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 86. 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 Negative. Default: Solvent
Injection Volume	The injection volume used for the sample acquisition as specified on the Samples page. 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 Negative vial.
Vial Position	Vial position for this sample type as specified on the Samples page.

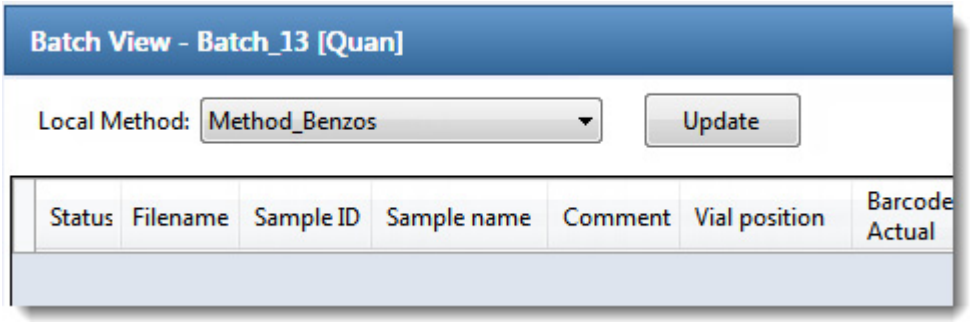
Reference Samples Page

The Reference Samples page displays the reference samples that you selected for this batch.

❖ To specify a chromatogram reference sample

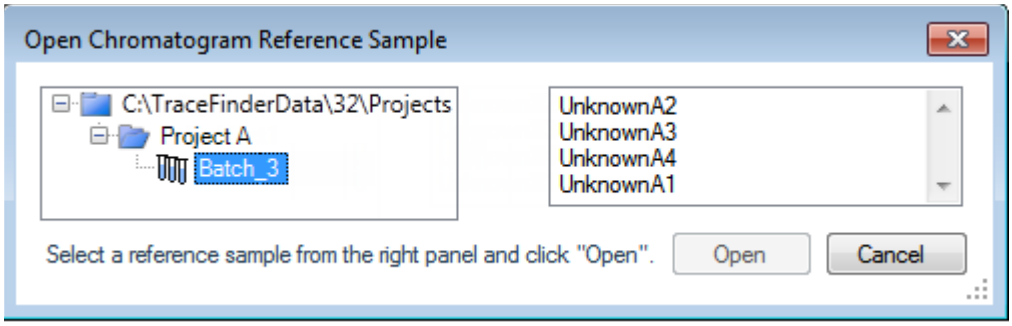
1. In the Batch View, click **Reference Samples**.

   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 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.

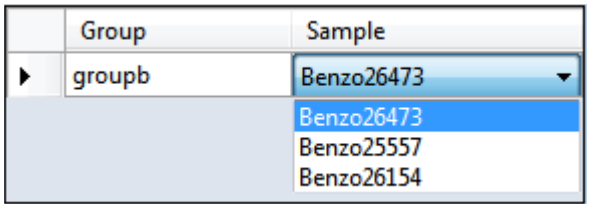
7. Click **Open**.

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.



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 on the sample peak plots.

For information about specifying the method to use for creating a threshold guide, see "Threshold" on page 237.

For information about creating groups, see "Groups" on page 375.

For information about using the threshold guide in the Comparative View, see "Comparative View" on page 436.

Working in Data Review for Quantitation Methods

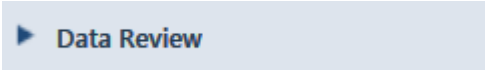
In the Data Review view, you can view the data generated by the quantitation master method. Use Data Review to verify the data for a compound before you generate reports.

❖ To open the Data Review view

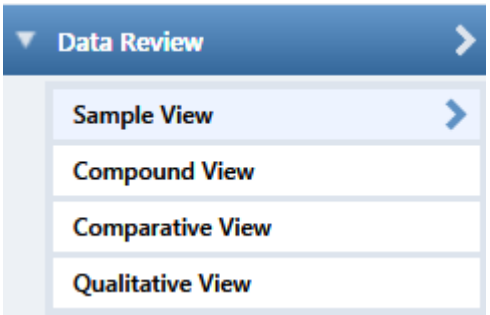
1. Click **Analysis** in the navigation pane.

   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.

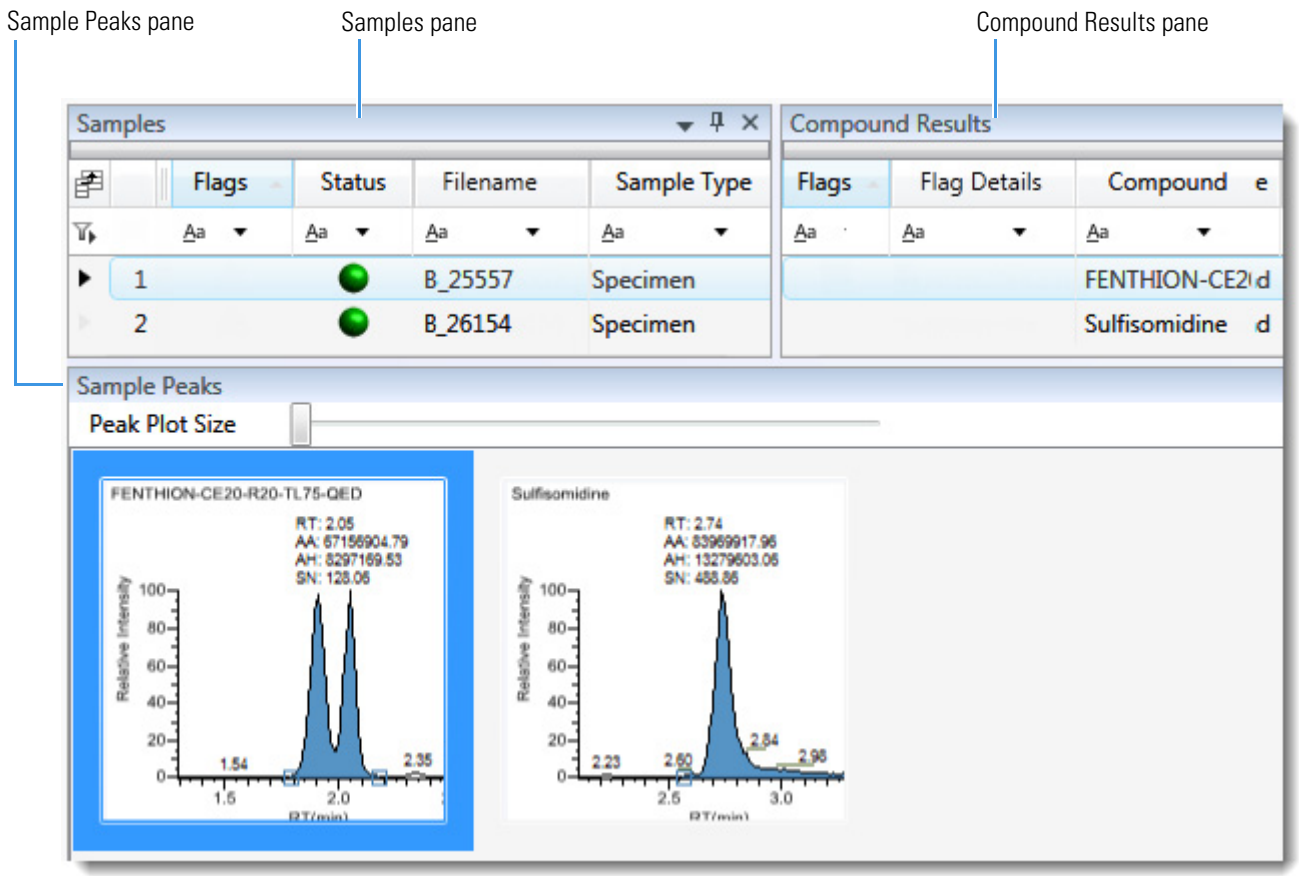
This section includes the following topics:

- 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:



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

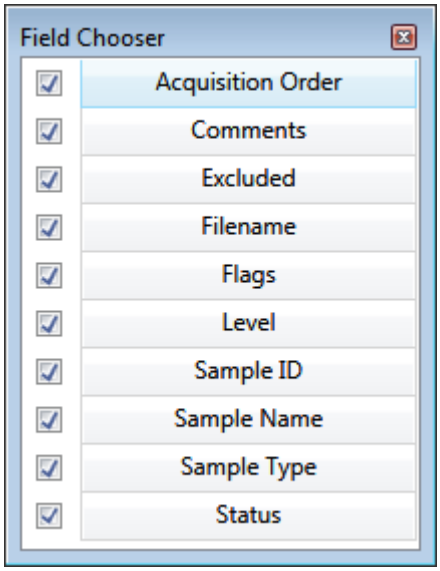
Samples Pane

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 108. Samples pane

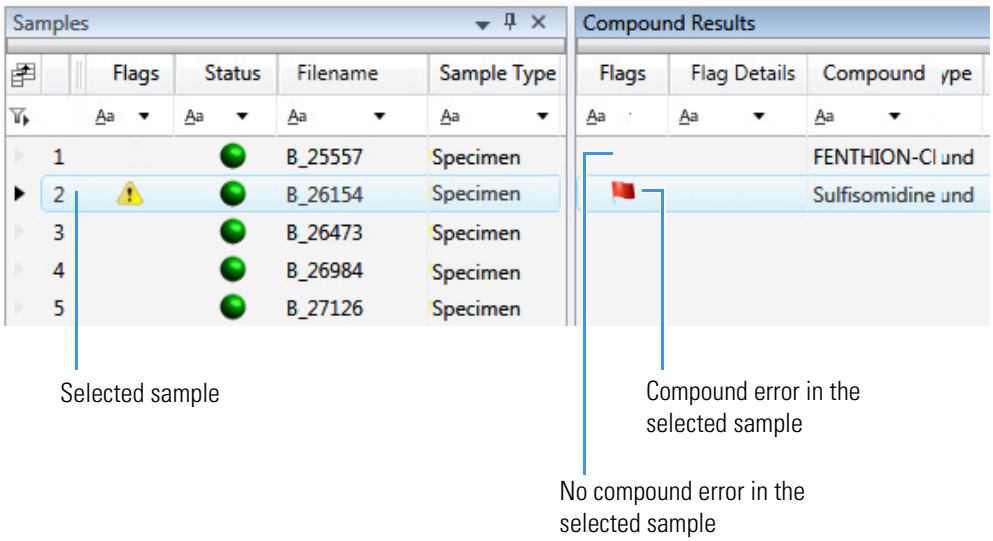


Table 87. Samples pane columns

Column	Description
Flags	Caution flag displayed when a compound in the sample has an error. See "Caution Flags" on page 420.
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.
Sample Name	A user-defined name that identifies a sample.
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative.
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.

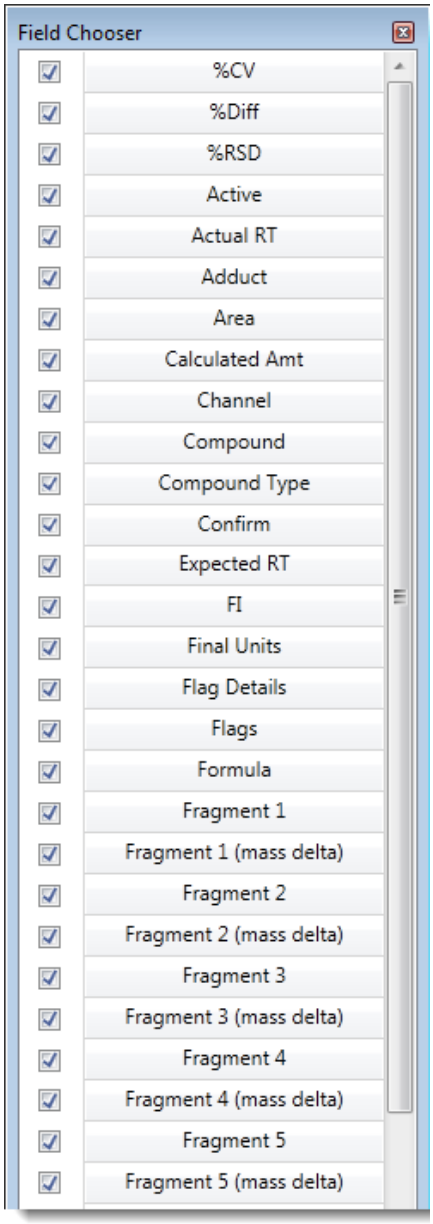
Compound Results Pane

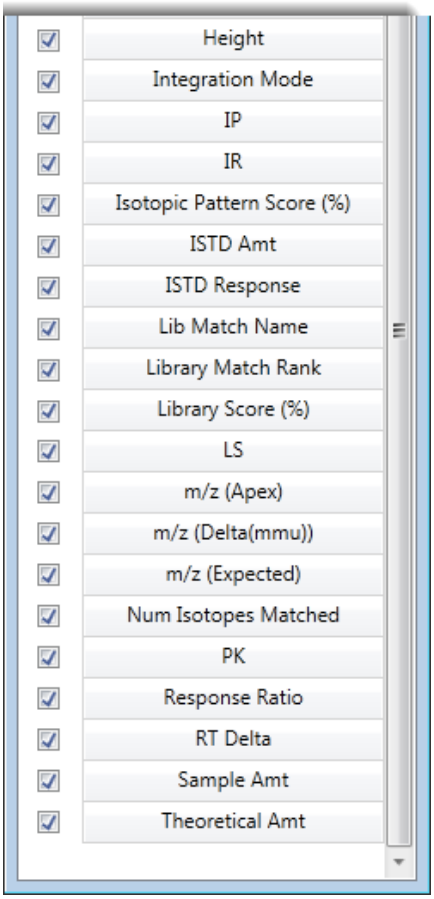
Use the Compound Results pane in the Sample View to select a specific compound in the selected sample. The associated Sample Peaks Pane highlights the selected compound.

❖ 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 immediately 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 109. Compound Results pane

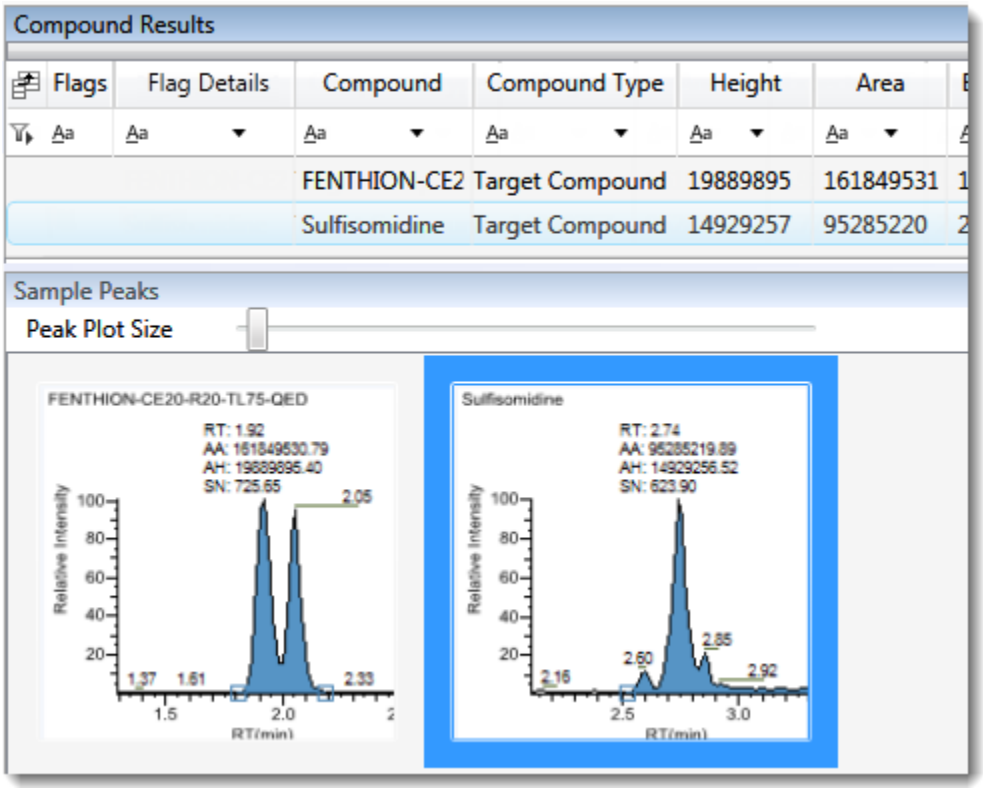
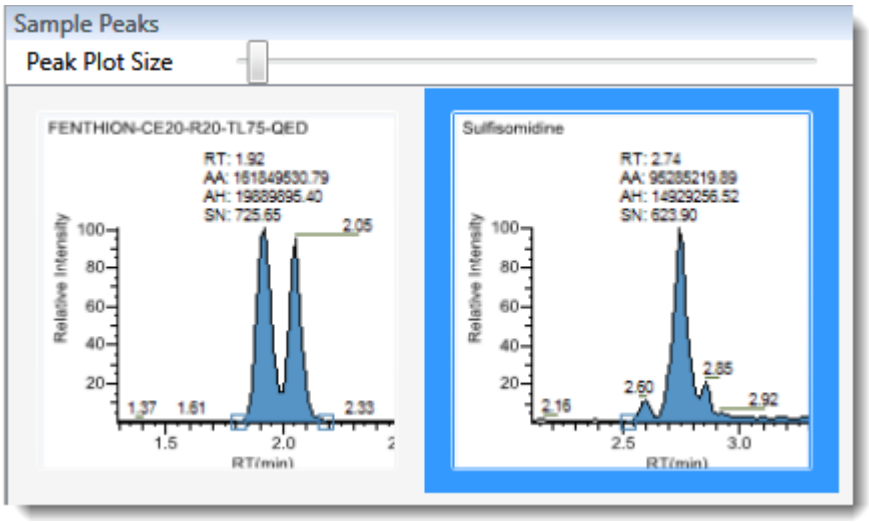


Table 88. Compound Results pane columns

Column	Description
Flags	Caution flag displayed when the compound has an error. See "Caution Flags" on page 420.
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 459.	

Sample Peaks Pane

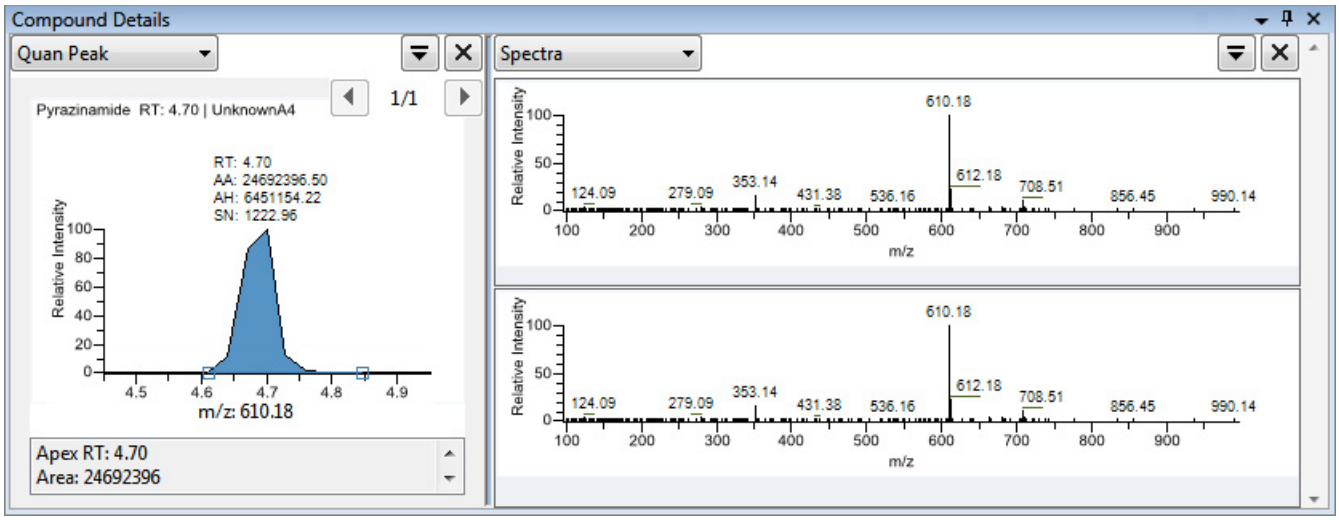
The Sample Peaks pane in the Sample View displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the Compound Results pane. The application highlights the chromatogram for the compound that is currently selected in the Compound Results pane.



❖ 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 468.

Caution Flags

In the Sample View, the application displays caution flags in both the Samples pane and the Compound Results pane.

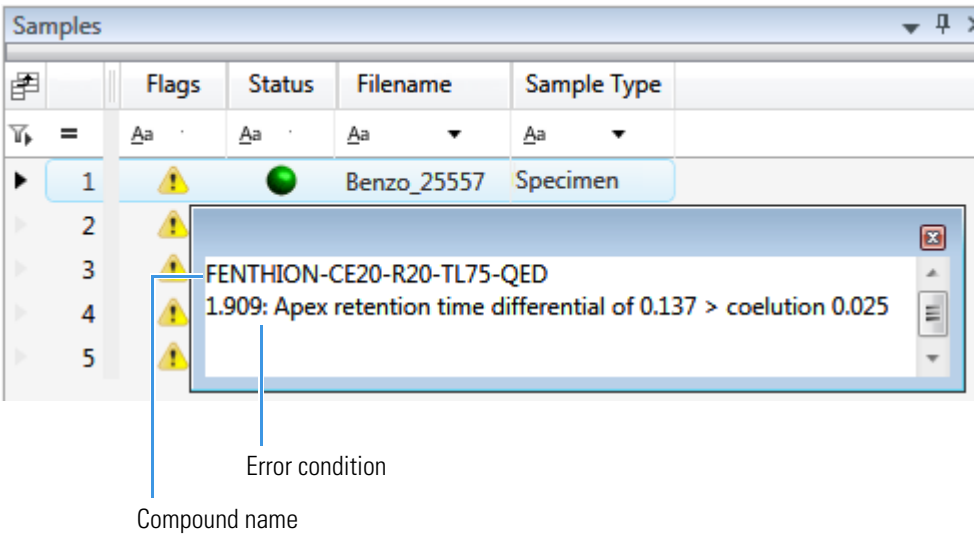
This section includes the following topics:

- Flags in the Samples Pane
- Flags in the Compound Results Pane
- Error Indicators in the Sample Peaks Pane

Flags in the Samples Pane

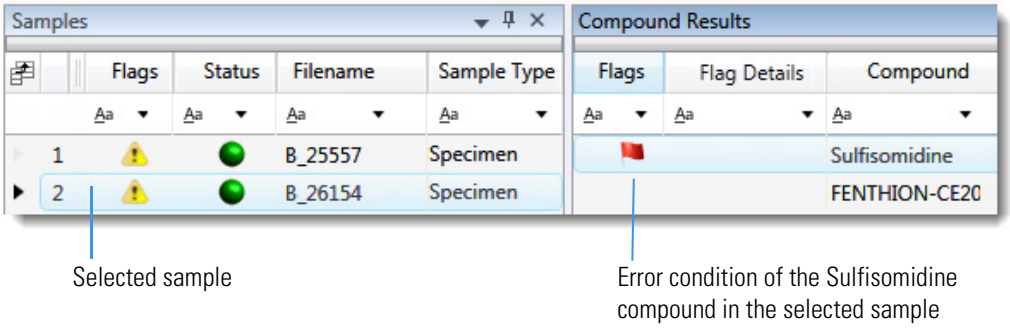
The Flags column in the Samples pane displays a caution flag if any compound in the sample is not in compliance with the method criteria.

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.

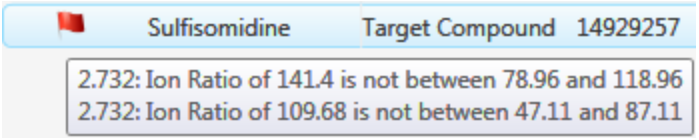


Flags in the Compound Results Pane

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.



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 230.
- 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 231.
- 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 231.
- 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.

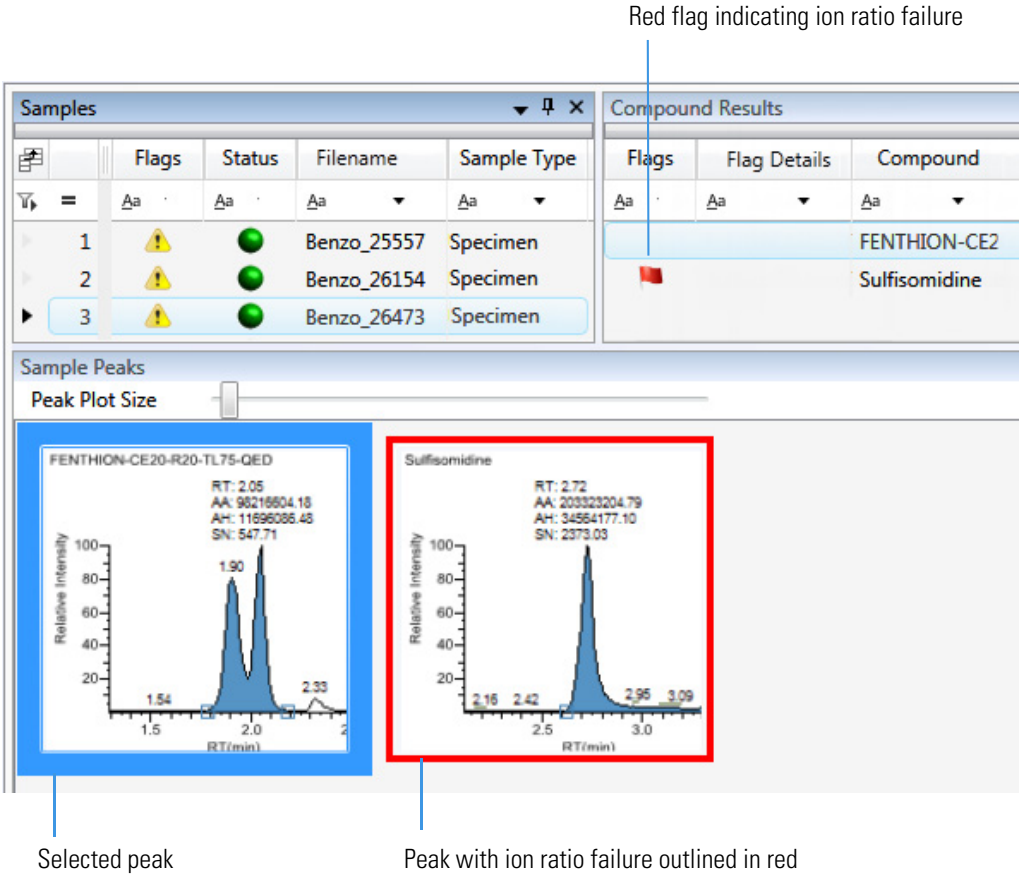
No flag for compounds that have no errors or where no report options are selected.

Note These criteria for flag states do not apply to Negative 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 110. Ion ratio failure flag



Viewing Sample View Panes

The Sample View display uses multiple panes to display data: Sample Results, Compound Results, Sample Peaks, and Compound Details. You can display, hide, or move any of these panes.

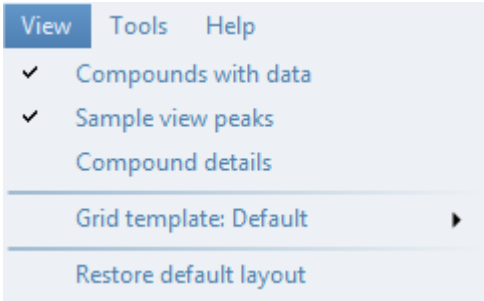
❖ To display or hide a Sample View pane

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 Sample Results pane is required for the Sample View display. You cannot hide the Sample Results pane.

Displayed panes are indicated with a check mark.



Data Review Pane Display Features

All Data Review displays have the following procedures in common:

- 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 restore the default layout

❖ To move a docked pane

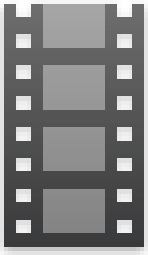
1. Grab the title bar of the pane and begin dragging the pane.

   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.

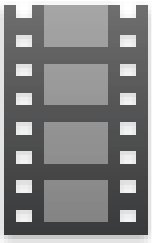
❖ To make a pane floating or dockable

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.

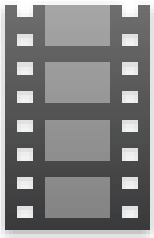
❖ To change a pane from a docked pane to a tabbed pane

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.

❖ To restore the default layout

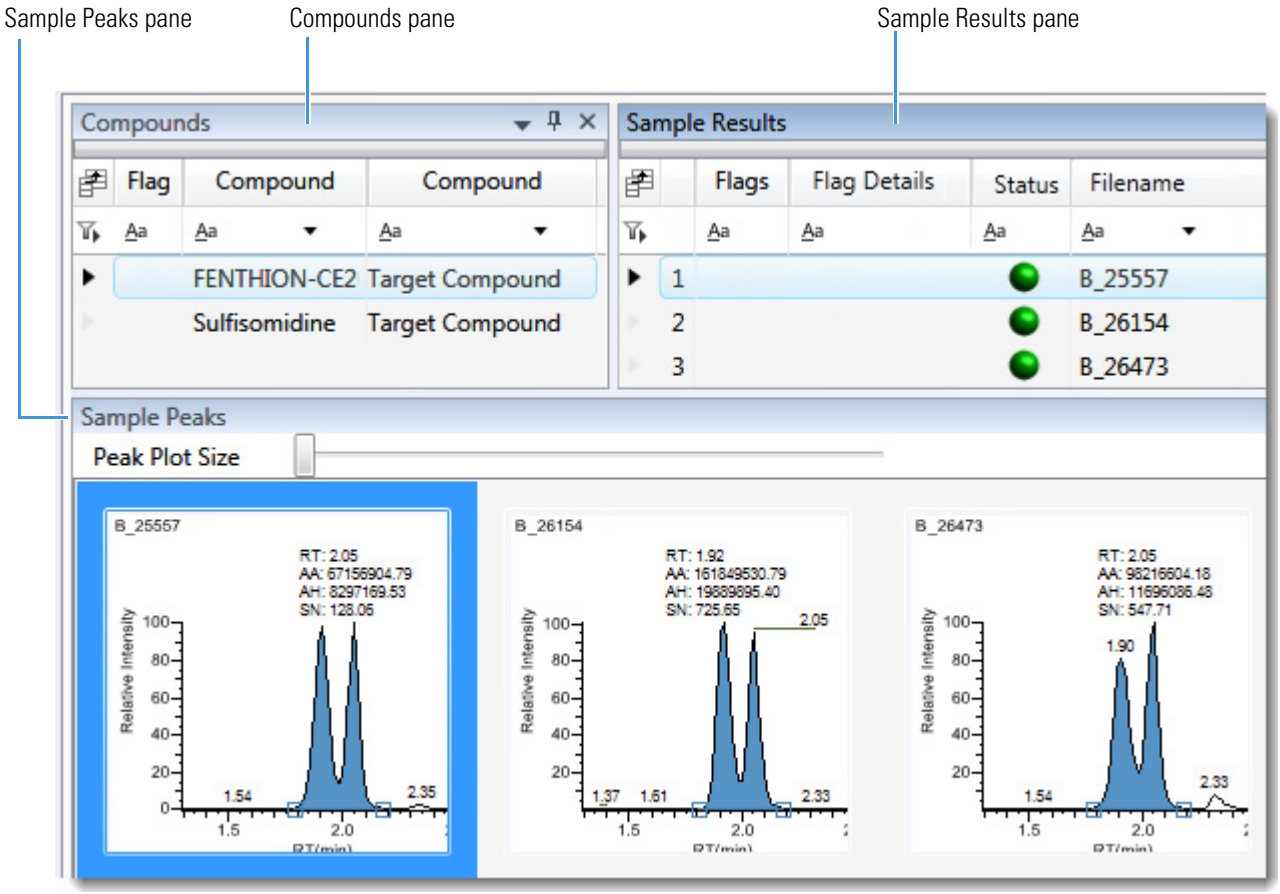
Choose **View > Restore Default Layout**.

The Sample View, Compound View, and Qualitative View each have their own defaults for which panes are displayed and in which location.

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:



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

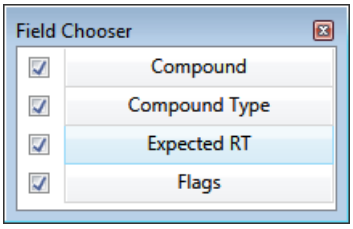
Compounds Pane

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 111. Compounds pane

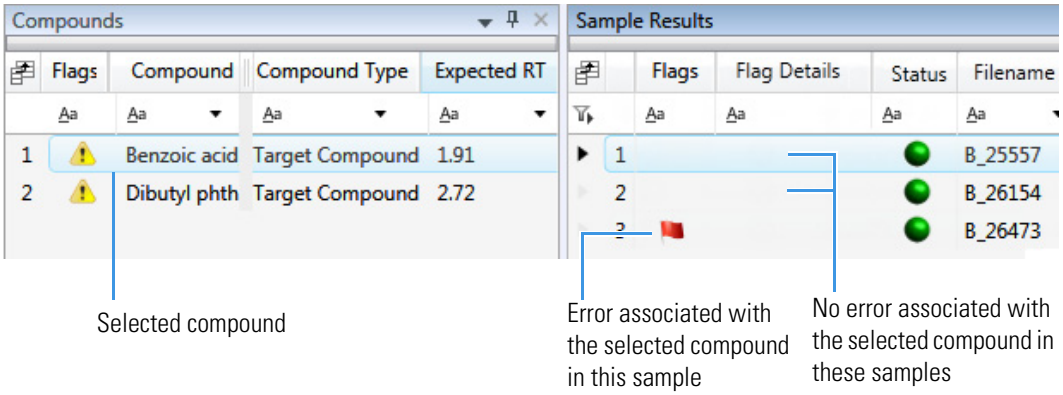


Table 89. Compounds pane columns

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 *peak@RT.*
Compound Type	Specified compound type: Target Compound or Internal Standard.
Expected RT	Expected retention time for the compound.

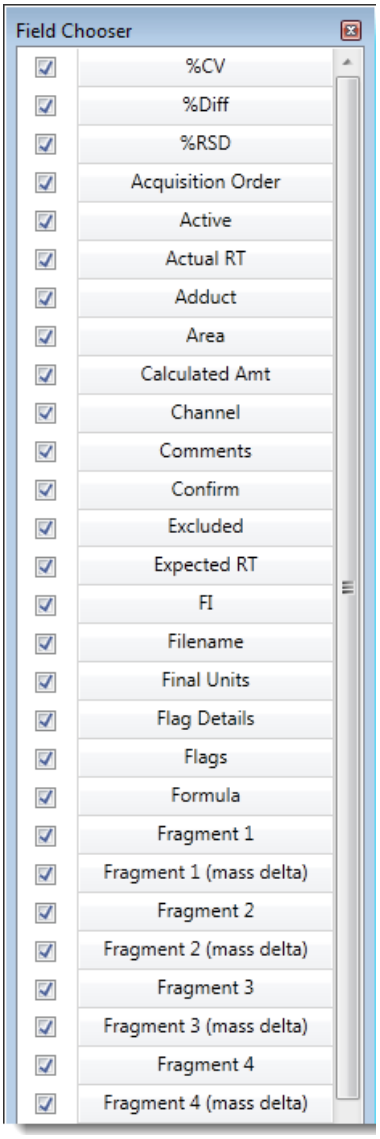
Sample Results Pane

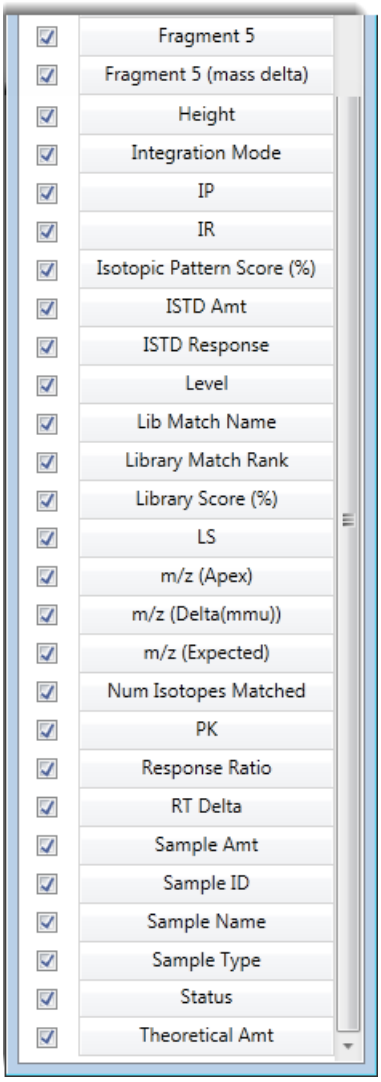
Use the Sample Results pane in the Compound View to select a specific compound in a specific sample. The Sample Peaks pane highlights the selected compound and displays the name of the sample in which the compound was found and the following information about the compound: chromatogram, retention time, 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 112. Sample Results pane

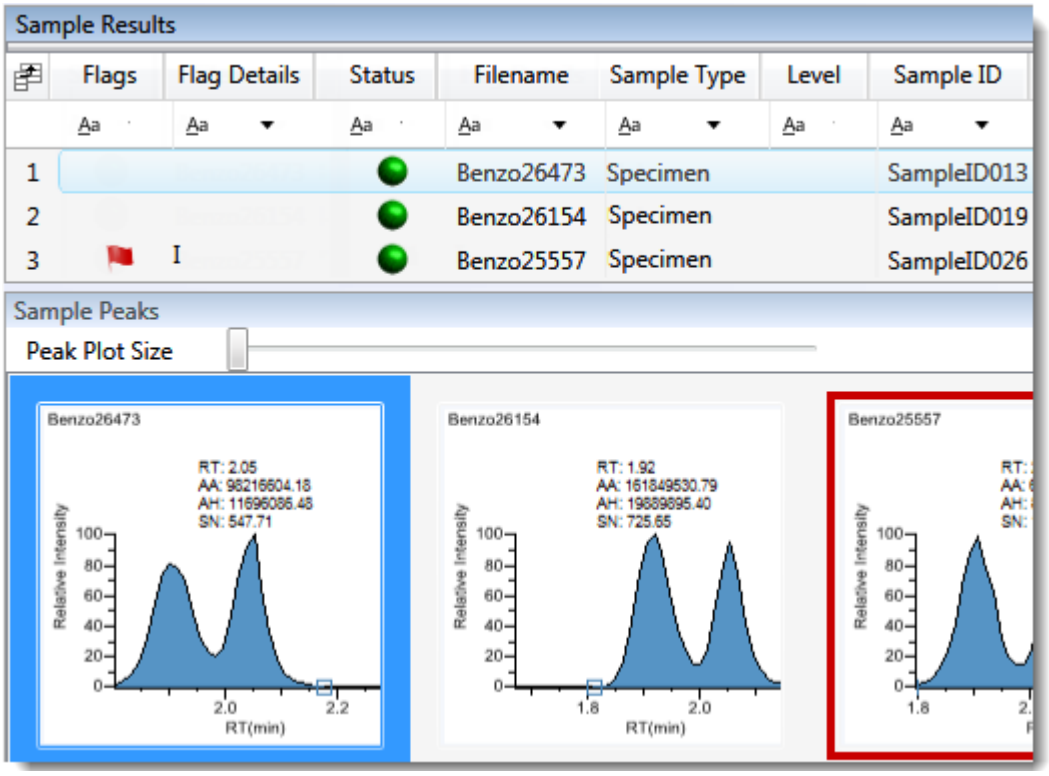


Table 90. Sample Results pane columns (Sheet 1 of 2)

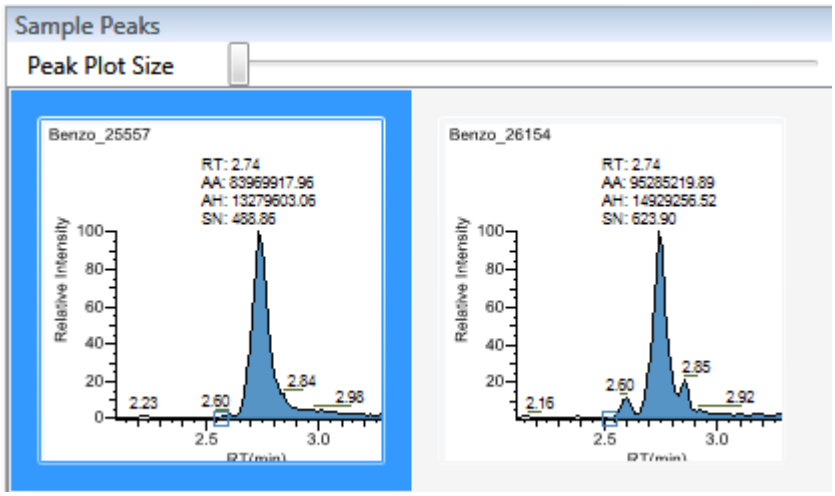
Column	Description
Acquisition Order	Sequentially numbers the samples.
Flags	Caution flag displayed when a compound within the sample has an error.
Flag Details	Indicates the type of error: • I: Confirming ion coelution failure or Ion ratio failure • A: Amount error • B: Matrix blank error • H: Peak not found

Table 90. Sample Results pane columns (Sheet 2 of 2)

Column	Description
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.
Filename	A user-defined name that identifies a sample.
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative.
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 459.	

Sample Peaks Pane

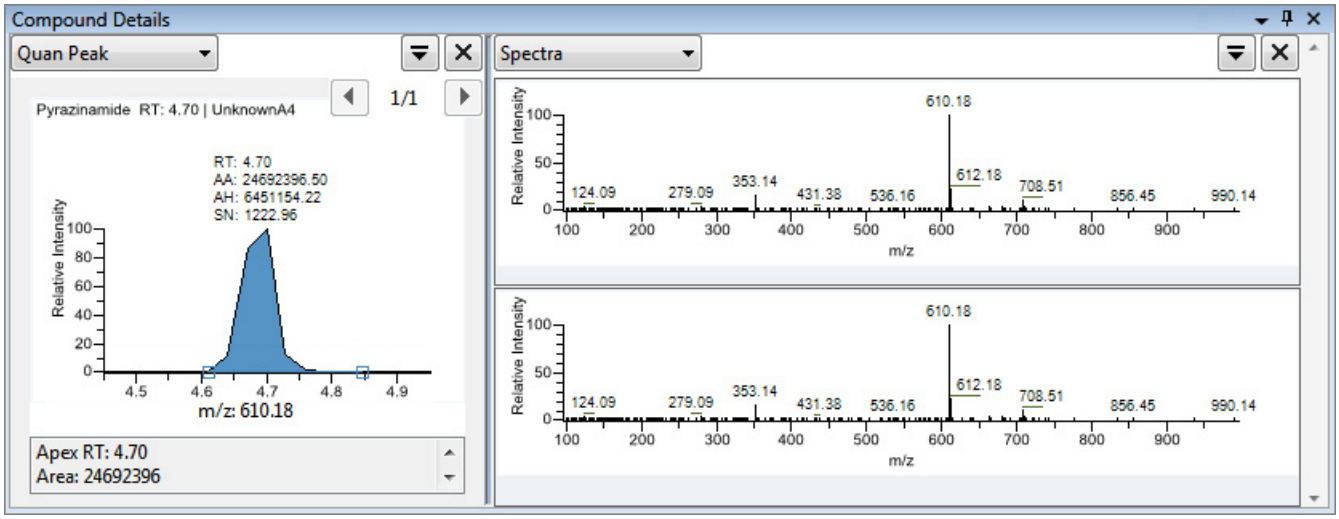
The Sample Peaks pane in the Compound View displays the compound chromatogram, retention time, area, height, and signal-to-noise ratio associated with the selected compound in each of the samples in the batch. The application highlights the compound chromatogram for the sample that is currently selected 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 468.

Caution Flags

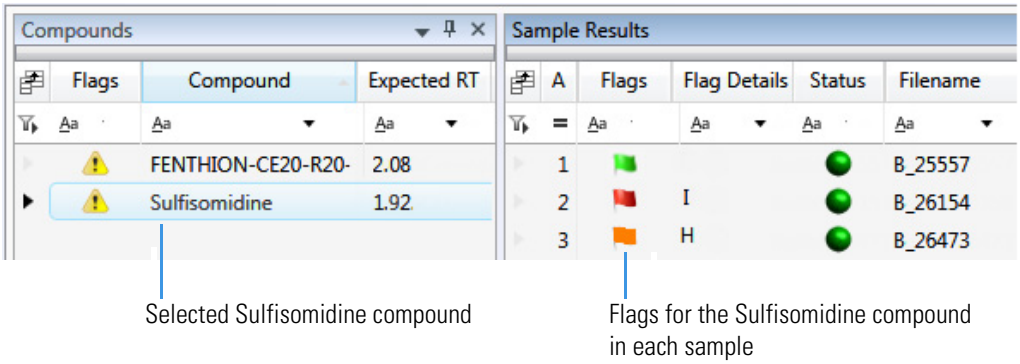
In the Compound View, the application displays caution flags in both the Compounds pane and in the Sample Results pane.

This section includes the following topics:

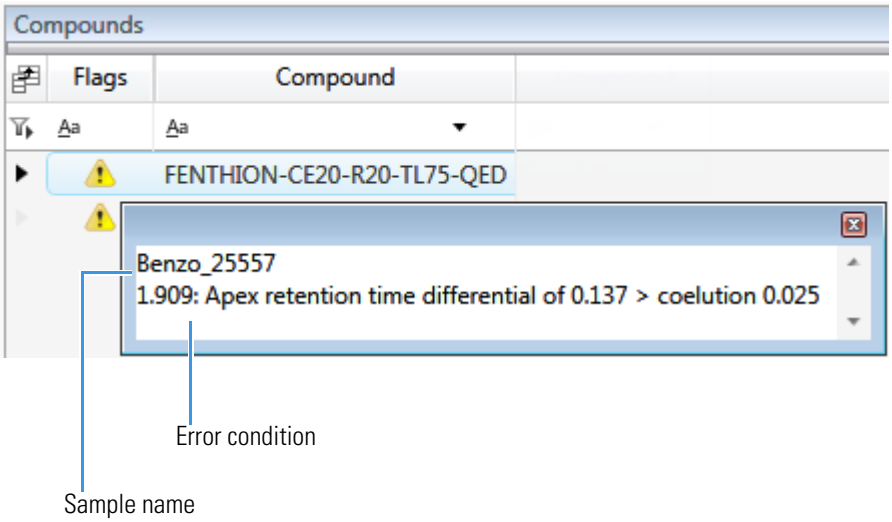
- Flags in the Compounds Pane
- Flags in the Sample Results Pane
- Error Indicators in the Sample Peaks Pane

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.



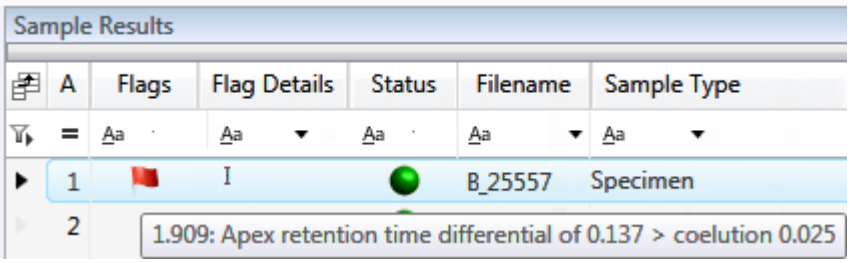
Click the caution flag icon, , to display the details. Information in the pop-up box shows the sample where the compound is in error and describes the exact error condition.



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.



Flags in the Sample Results pane indicate the following:

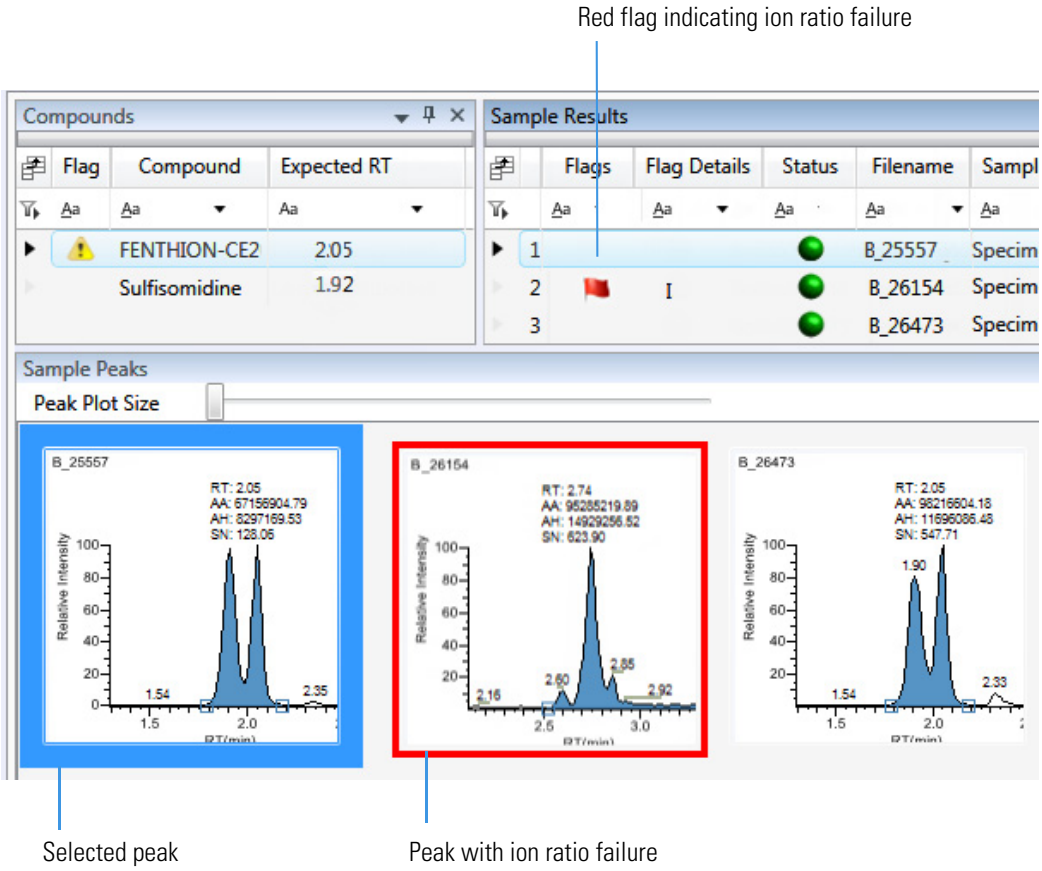
Flag	Description
	A green flag for compounds that are over the LOR amount specified in the method.
	A red flag for compounds that have violated (or are activated by) any of the values set in the method. See "Editing the QAQC Page" on page 230.
	A red flag for compounds that are outside the specified ion ratio range. See Ion ratio failure flag.
	An orange flag for compounds that are not found in Calibrator or QC 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 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 Negative 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 113. Ion ratio failure flag



Viewing Compound View Panes

The Compound View display uses multiple panes to display data: Compounds, Sample Results, Sample Peaks, and Compound Details. You can display, hide, or move any of these panes.

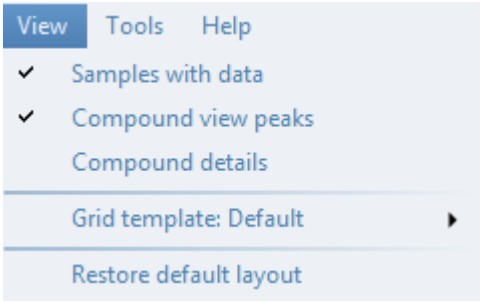
❖ To display or hide a Compound View pane

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.

Displayed panes are indicated with a check mark.



For procedures about creating docked, floating, or tabbed panes, see "Data Review Pane Display Features" on page 424.

Comparative View

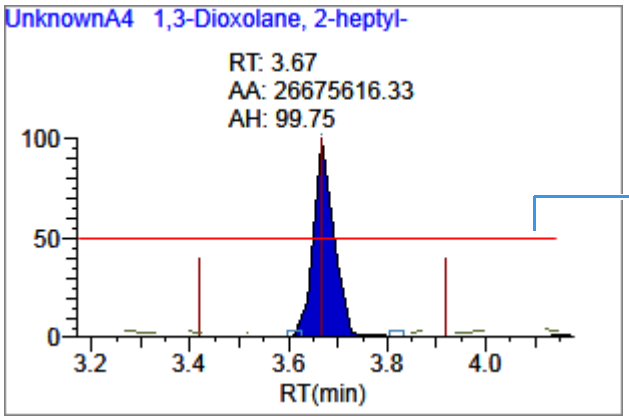
The Comparative View uses three panes to display a list of all compounds available in the method, all samples in the current batch, and the sample peak plots for all compounds found in the samples with the horizontal threshold guide.

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. 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 on 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.

This section includes 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 237.

For information about creating groups, see "Groups" on page 375.

For information about specifying a threshold sample, see "Threshold Samples Page" on page 412.

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 375.

❖ 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 441.

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 114. Number of Rows equals 1 and Number of Columns equals 1

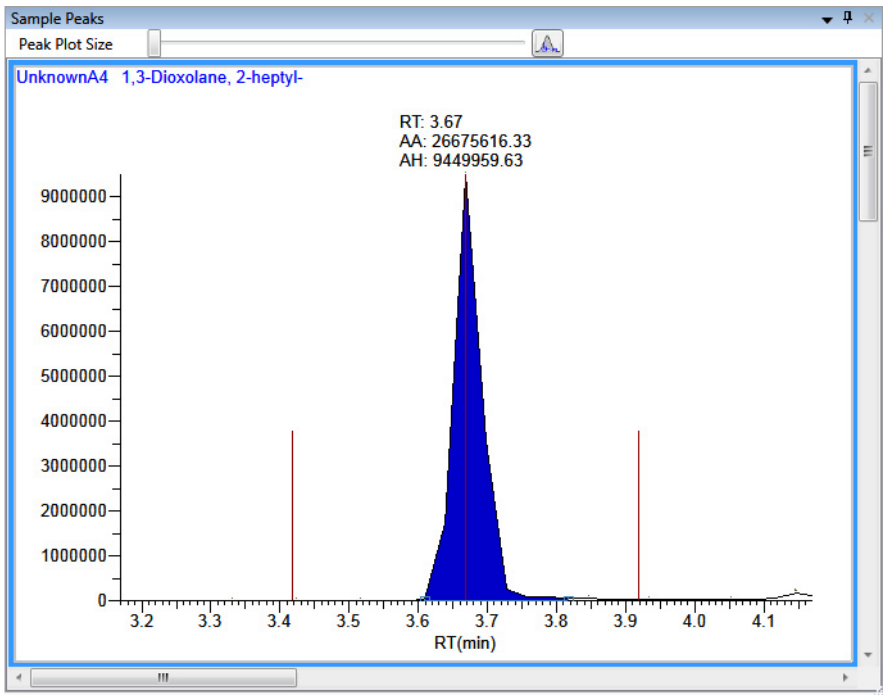
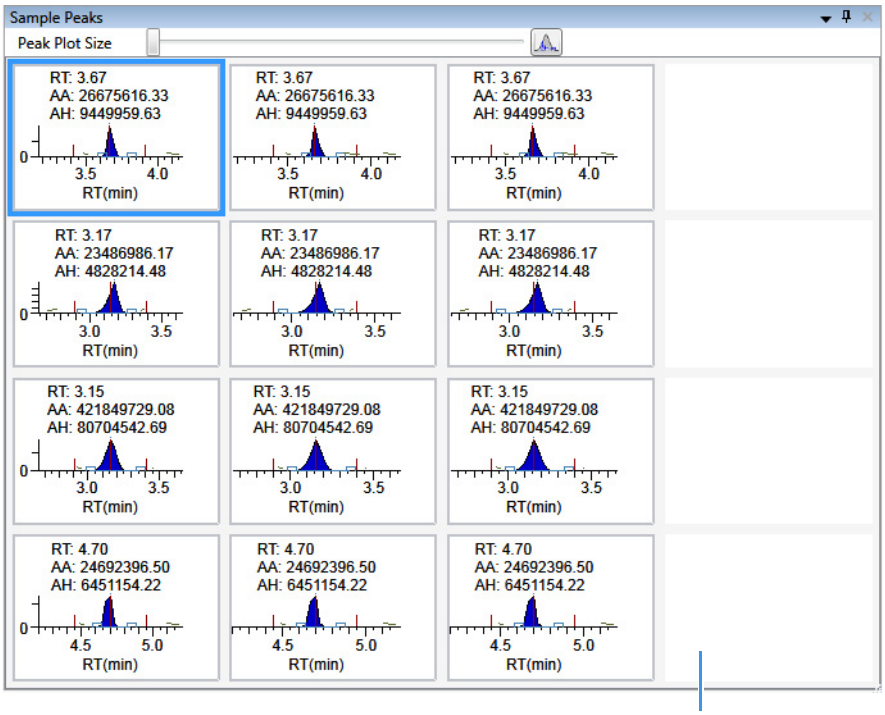


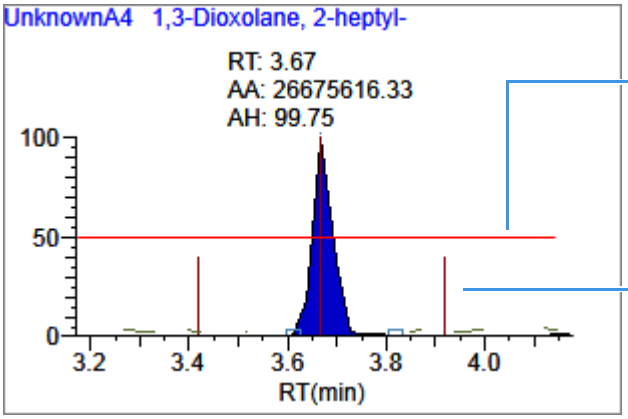
Figure 115. Number of Rows equals 4 and Number of Columns equals 4



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:

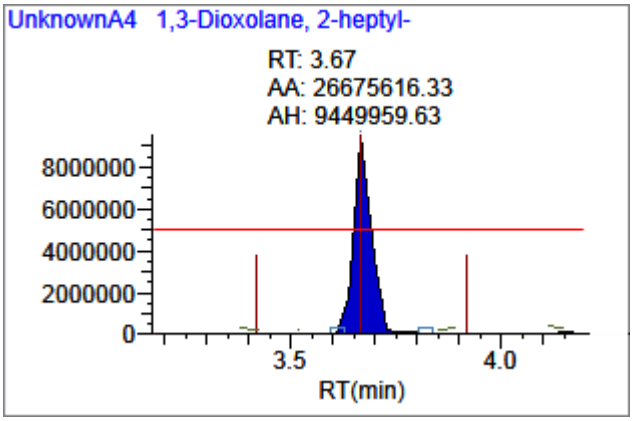
   - **Relative**: Displays the *y*-axis scale from 0 to 100.



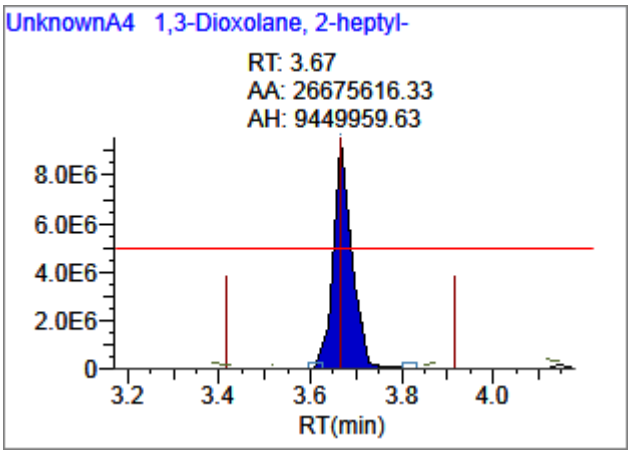
Horizontal bar indicates the threshold value as specified in the method.

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 on 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.

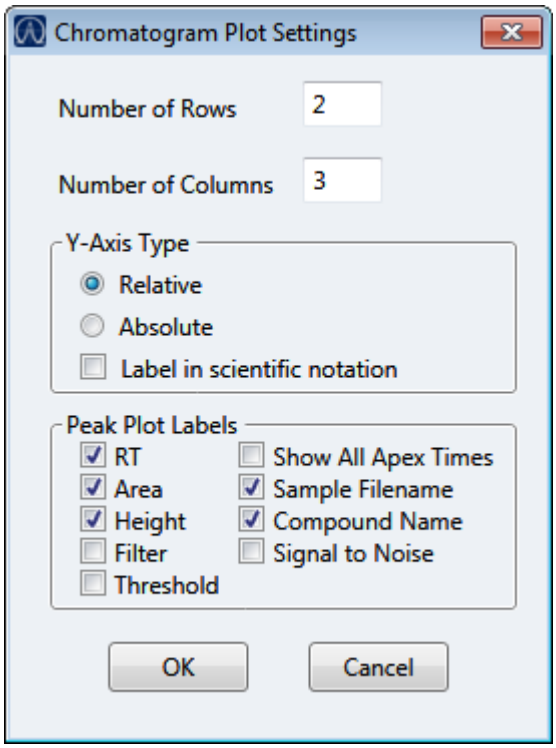
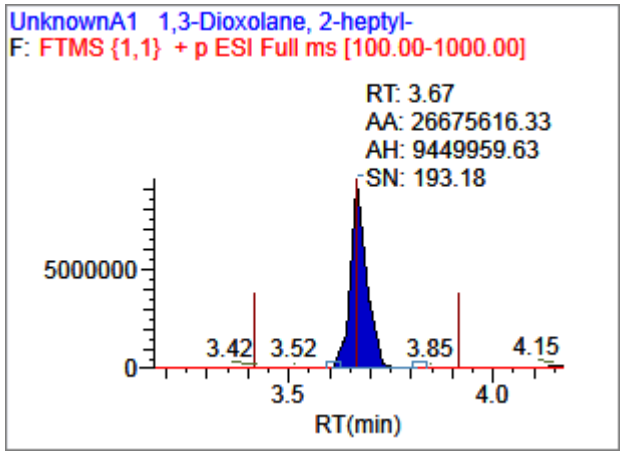


Table 91. Chromatogram Plot Settings dialog box parameters (Sheet 1 of 2)

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

Table 91. Chromatogram Plot Settings dialog box parameters (Sheet 2 of 2)

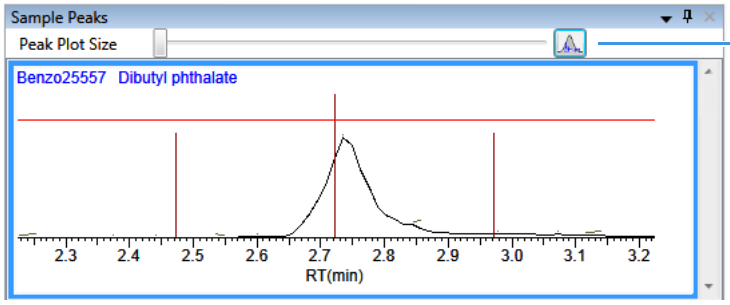
Parameter	Description
Y-Axis Type	Displays the *y*-axis scale as Relative (to the most intense peak), Absolute, or in scientific notation.
Peak Plot Labels	Displays or hides the following peak labels: • RT • Area • Height • Filter • Threshold • Show All Apex Times • Sample Filename • Compound Name • 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.

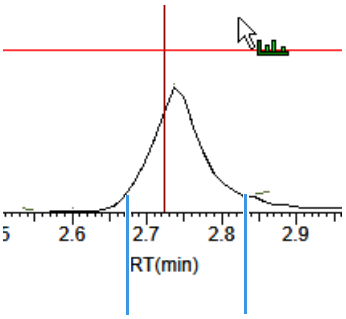


The cursor changes to look like this:

2. To integrate a peak, do the following:
   a. Drag the cursor to describe the beginning and ending base points for the new peak.

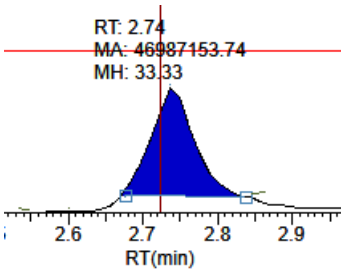
   > **Note** You must drag the cursor inside the *x* axis and *y* axis.

   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 described 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.

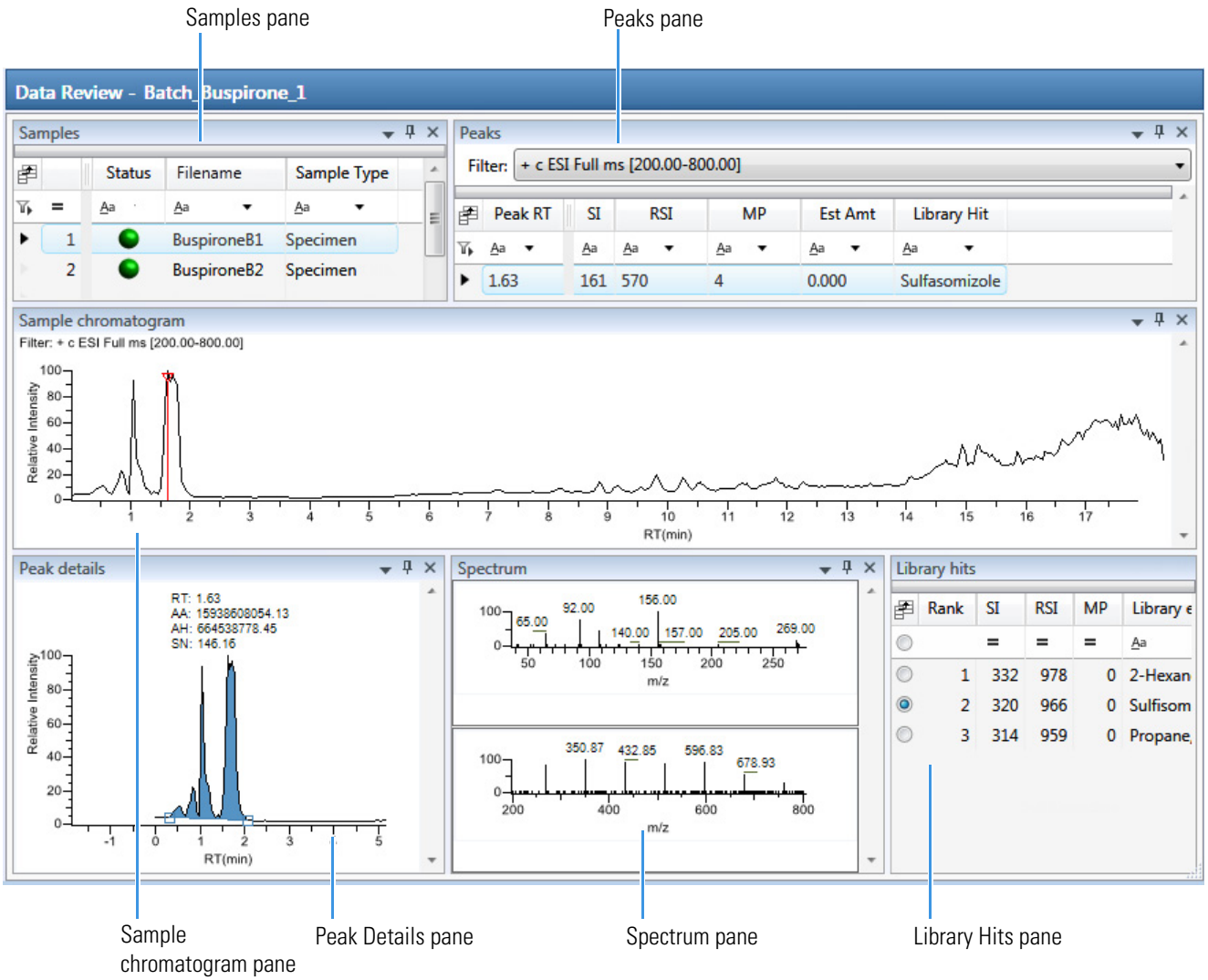
Qualitative View

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 381.

These are the default panes and their locations:



The Qualitative View displays data in the following panes:

- Samples Pane
- Peaks Pane
- Sample Chromatogram Pane
- Peak Details Pane
- Spectrum Pane (Library and Data)
- Library Hits Pane

Displaying Qualitative View Panes

The Qualitative View display uses multiple panes to display data: Samples, Peaks, Sample Chromatogram, Peak Details, Spectrum, and Library Hits. You can display, hide, or move any of these panes.

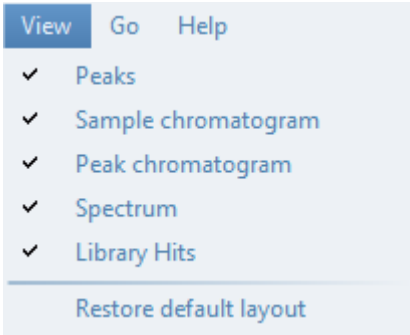
❖ To display or hide a Qualitative View pane

From the View menu, choose to display or hide the following:

- **Peaks**
- **Sample Chromatogram**
- **Peak Chromatogram**: Displays or hides the Peak Details pane.
- **Spectrum**
- **Library Hits**

Note The Samples pane is required for the Qualitative View display. You cannot hide the Samples pane.

Displayed panes are indicated with a check mark.



For procedures about creating docked, floating, or tabbed panes, see "Data Review Pane Display Features" on page 424.

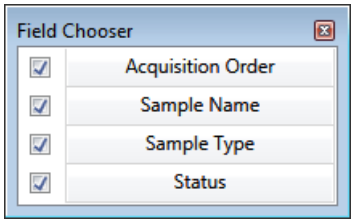
Samples Pane

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 116. Samples pane

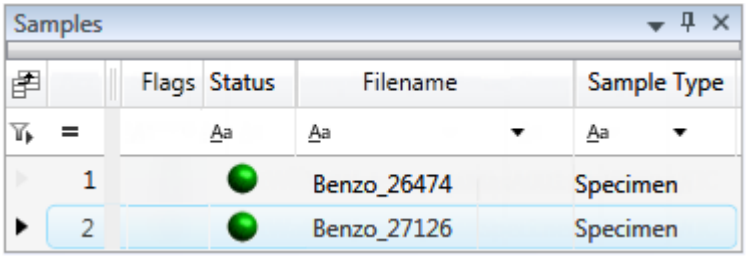


Table 92. Samples pane columns (Sheet 1 of 2)

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 420.
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.

Table 92. Samples pane columns (Sheet 2 of 2)

Column	Description
Filename	A user-defined name that identifies a sample.
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Solvent, Specimen, QC, Calibrator, Hydrolysis, Unextracted, or Negative.

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 450.

Follow these procedures:

- To display peaks for a specific compound
- To remove a peak
- To hide or display columns in the Peaks pane

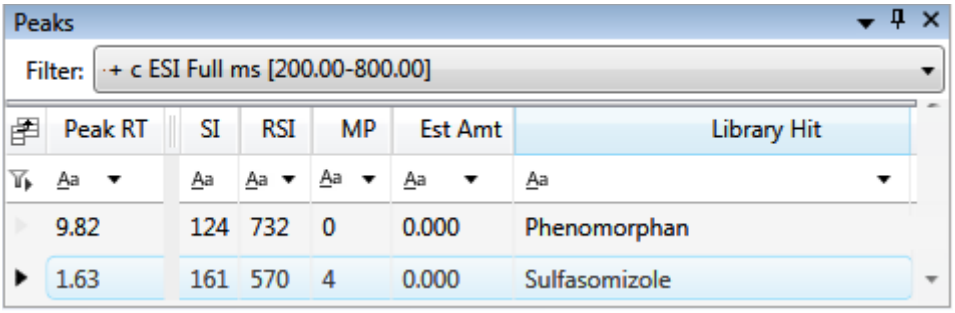
❖ To display peaks for a specific compound

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 257.

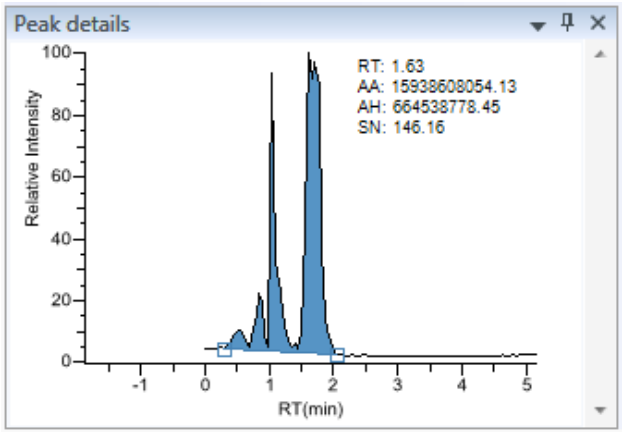
2. In the Peaks pane, select a peak in the sample.



   The TraceFinder application displays the selected peak in the Peak Details 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 117. Peak Details 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 118. Spectrum pane

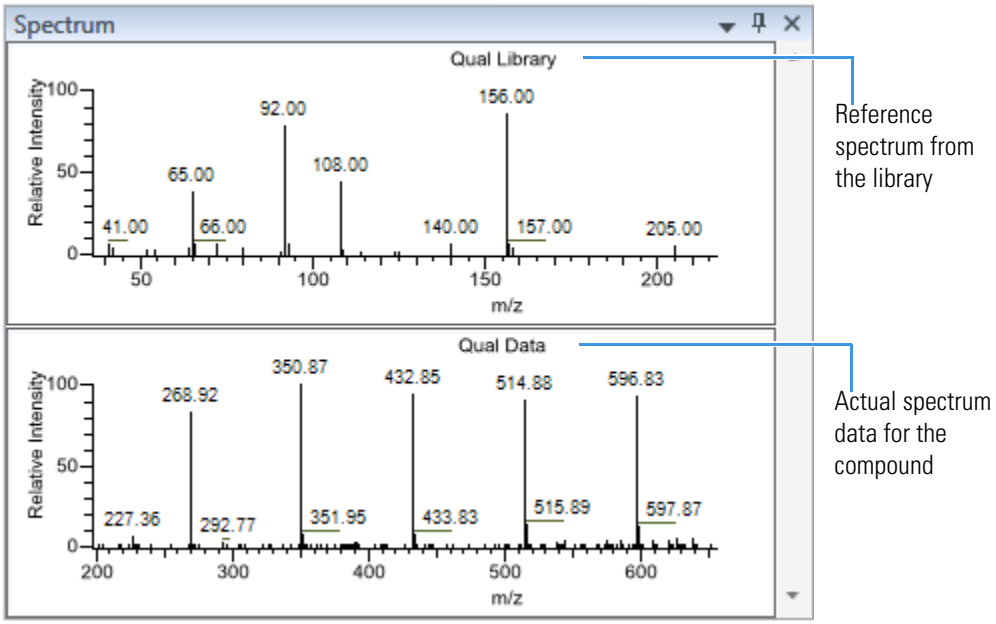
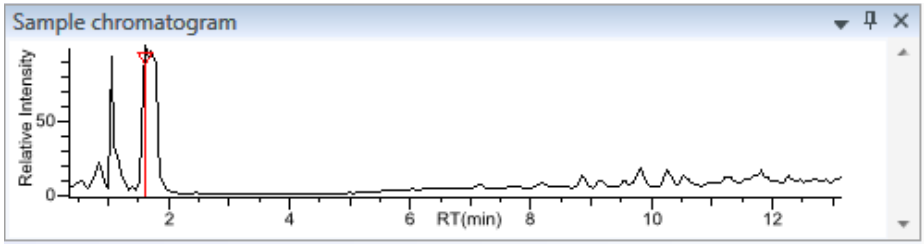


Figure 119. Selected peak in the Sample Chromatogram pane



❖ To remove a peak

1. Select a peak in the Sample Chromatogram pane.
2. Right-click the Peak Details pane and choose **Remove Qual Peak** from the shortcut menu.

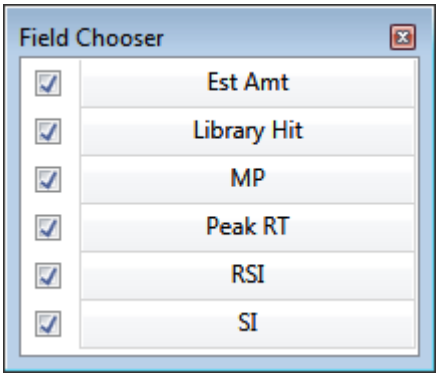
   The TraceFinder application removes the selected peak from all Qualitative View panes.

> **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 451.

❖ 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 120. Peaks pane

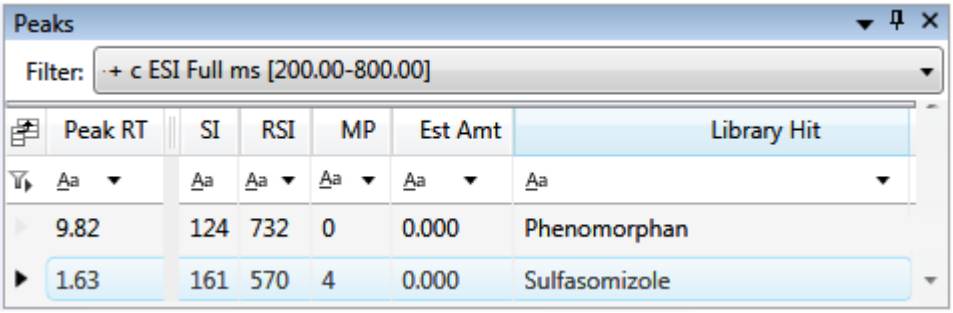


Table 93. Peaks pane parameters

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”. Filter: + c d ESI Full ms [200.00-800.00] Data-dependent filter
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 (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 452.

❖ To zoom in on a peak

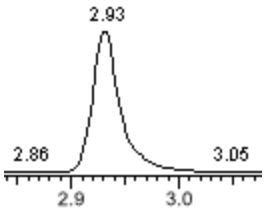
1. In the Sample Chromatogram pane, drag the cursor to delineate a rectangle around the peak.

   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

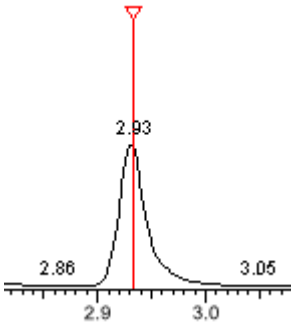
1. Zoom in to better identify which peak to add to the results set.



2. Right-click the Sample Chromatogram pane, and choose **Add Qual Peak** from the shortcut menu.

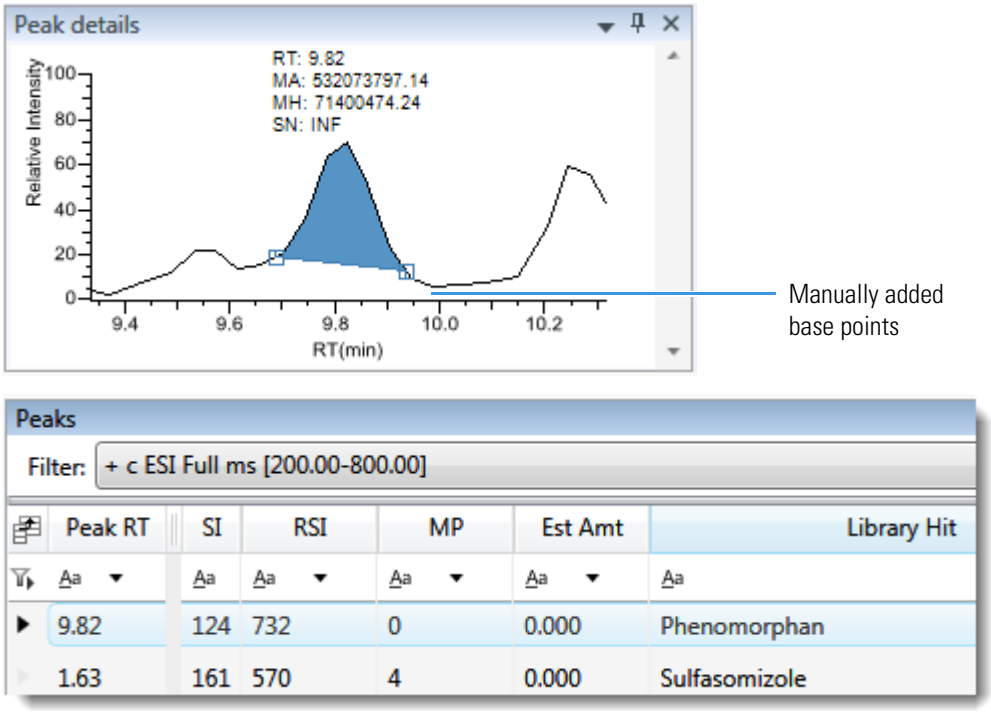
3. Click to indicate the left and right base points for the peak.

   The TraceFinder application marks the peak in the Sample Chromatogram pane.



   The TraceFinder application places the peak delimiter tags at the base point locations and automatically updates the peak values in the Peaks pane and Peak Details pane. See Peak Details pane with a manually added peak.

Figure 121. Peak Details pane with a manually added peak



Sample Chromatogram Pane

Use the features on the Sample Chromatogram pane to display peaks in the selected sample.

Figure 122. Sample Chromatogram pane

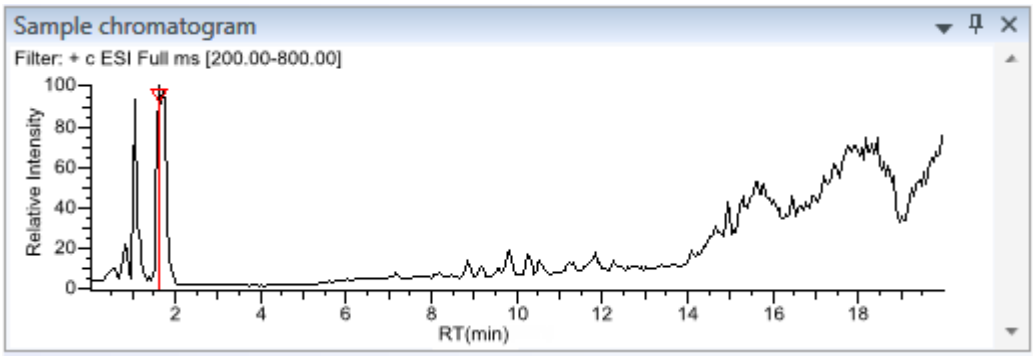


Table 94. Sample chromatogram pane shortcut menu commands

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 Details Pane

The Peak Details pane in the Qualitative View displays the selected peak. For a description of commands on the shortcut menu, see "Peak Details Pane" on page 455.

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.

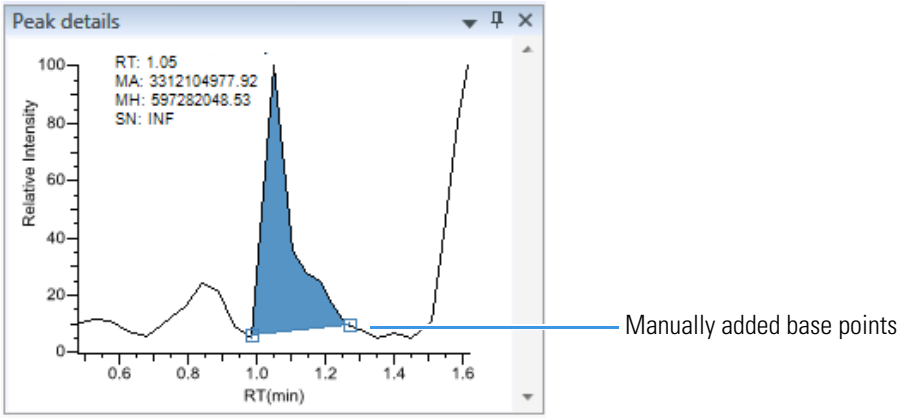
❖ To manually add a peak

1. Right-click anywhere in the Peak Details 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 TraceFinder application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



❖ To remove a peak

Right-click the Peak Details pane, and choose **Remove Qual Peak** from the shortcut menu.

The TraceFinder application removes the peak displayed in the Peak Details pane. All data for this peak are removed from the Qualitative View panes.

❖ To switch between method and manual integration modes

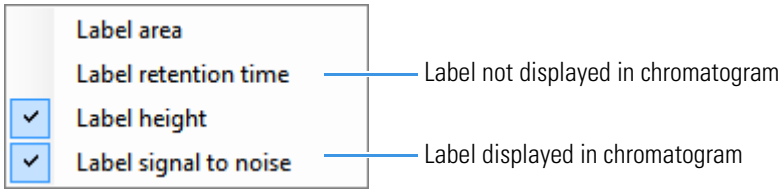
Right-click the Peak Details pane and choose **Method Integration** or **Manual Integration** from the shortcut menu.

Initially, the method and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the Peak Details plots and the result set update as you switch between method and manual modes.

As you switch between modes, each pane reflects the changes. The generated reports for these data identify the manual modifications.

❖ To change the displayed information for detected peaks

1. Right-click the Peak Details 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, select the label type again to clear it.

Peak Details Pane

Use the features in the Peak Details pane to display the selected peak.

Figure 123. Peak Details pane

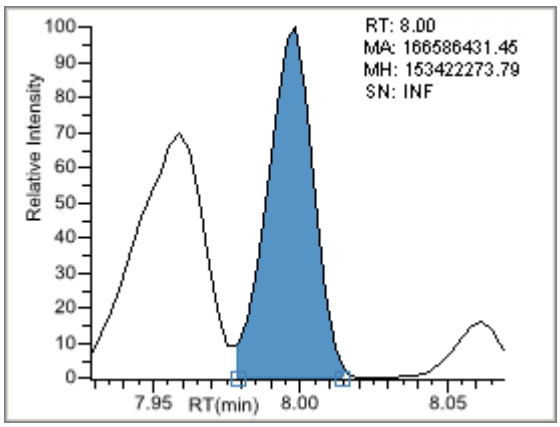


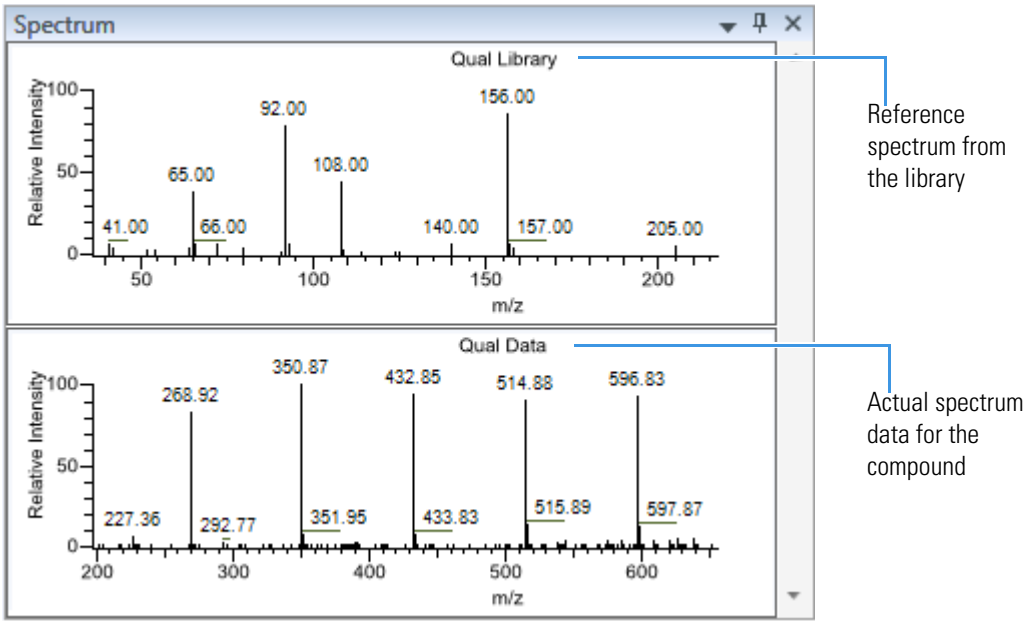
Table 95. Peak Details pane shortcut menu commands

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 Details 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 124. 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:

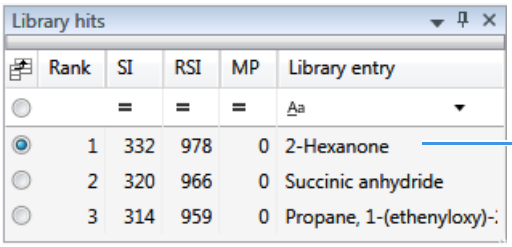
Peak:	Retention Time	Area	Height	Inj Estimate	In-sample Est	Flag
Naphthalene	7.95	13829174	10605061	0.000	0.000	P

P flag

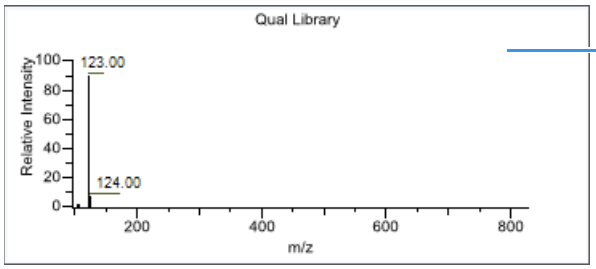
❖ To change the library entry for a selected peak

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.



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 125. Library Hits pane

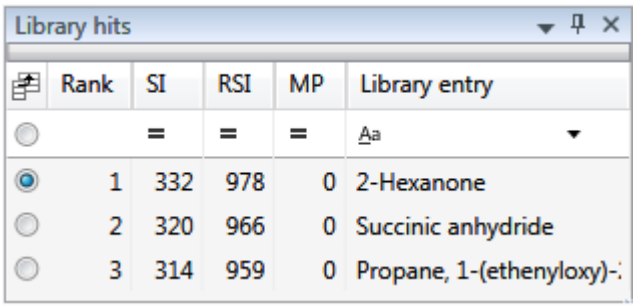


Table 96. Library Hits pane parameters

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 (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 features are common to all quantitative batch data review pages.

- Common Column Parameters
- Inactive and Excluded Compounds
- Compound Details
- Exporting Compounds

Common Column Parameters

Table 97. 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 215. The application uses this %RSD value in Data Review and in the Compound Calibration Report when you acquire multiple samples for the same QC or Calibrator samples.
Active	Displays or hides a compound for a particular sample. • When a compound is marked inactive, the application does not remove its data and calculated values from the result set. Instead, the TraceFinder application masks the appearance of that compound for that particular sample and grays the compound in the compounds list. • 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. In a Sample View, the Active parameter is in the Compound Results pane. In a Compound View, the Active parameter is in the Sample Results pane.
Acquisition Order	Sequentially numbers the samples.

Table 97. Common parameters for Compound Results and Sample Results tables (Sheet 2 of 7)

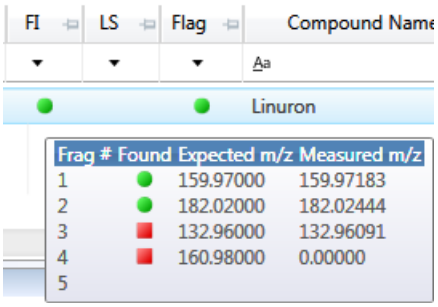
Column	Description
Actual RT	Actual retention time for the compound. Retention time is the time after injection when a compound elutes and the total time that the compound is retained on the chromatograph column.
Adduct	The most intense adduct for the retention time for a compound.
Area	The area obtained 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	Fragment Ions flag. The application displays one of these indicators: • 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. To display a list of fragments and their pass/fail status, hold your cursor over the indicator. 
Filename	Name of the raw data file that contains the sample data.
Final Units	Specifies the calculated amount. Default: 1

Table 97. Common parameters for Compound Results and Sample Results tables (Sheet 3 of 7)

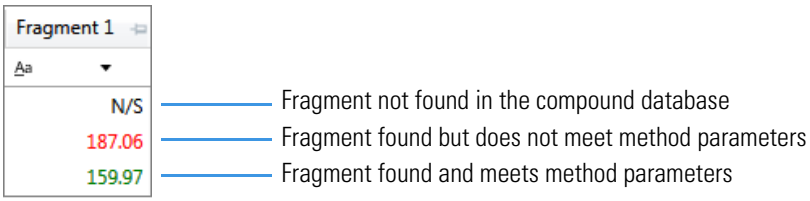
Column	Description
Flag Details	Indicates all errors found in the compound. Type of error: • I: Confirming ion coelution failure • A: Amount error • B: Matrix blank error • PK: Peak not found • LS: Library matching error • IP: Isotope error • FI: Fragment ions error • IR: Ion ratio error
Flags	Caution flag displayed when a compound within the sample has an error.
Formula	The formula for the peak as specified in the compound database.
Fragment *n*	Displays the measured *m/z* for the fragment ion. The application displays a separate column for each found fragment. • For each fragment found in the compound database that passes the filter in the method, the Compounds table displays the *m/z* 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 *m/z* value in red text. • For each fragment that is not found in the compound database, the Compounds table displays N/S (none specified).  **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.
Fragment *n* (Delta (ppm/mmu))	The difference between the expected fragment ion *m/z* from the compound database and the measured fragment ion *m/z*. 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 470.

Table 97. Common parameters for Compound Results and Sample Results tables (Sheet 4 of 7)

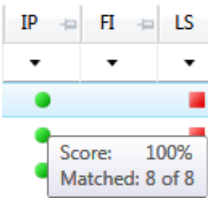
Column	Description
IP	Isotopic Pattern flag. The application displays one of these indicators: • A green circle (pass) when the score percentage is higher than the specified fit threshold percentage. • A red square (fail) when the score percentage is lower than the specified fit threshold percentage. • A blank when the parameter is not scored. To display the score of matched isotopes, hold your cursor over the indicator. 
IR	Ion Ratio flag. The application displays one of these indicators: • 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	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. • 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 97. Common parameters for Compound Results and Sample Results tables (Sheet 5 of 7)

Column	Description
Library Match Rank	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 • 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. 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: • The criteria passes when the library score is higher than or equal to the score threshold. The values in this column are in green text. • The criteria fails when the library score is lower than the score threshold. The values in this column are in red text. 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 (%)	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. 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: • The criteria passes when the library score is higher than or equal to the score threshold. The values in this column are in green text. • The criteria fails when the library score is lower than the score threshold. The values in this column are in red text. 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. Range: 1 to 100%
LS	Library Search flag. The application displays one of these flags: • A green circle when the library search is successful. • A red square when the library search is not successful.
m/z (Apex)	Mass-to-charge ratio found in the spectra for the peak. Assumes that the charge is 1. When the application successfully integrates the peak, this column displays the charged *m/z* value for the compound, which is the highest intensity in the apex scan. When the application cannot successfully integrate the peak, this column displays N/F.

Table 97. Common parameters for Compound Results and Sample Results tables (Sheet 6 of 7)

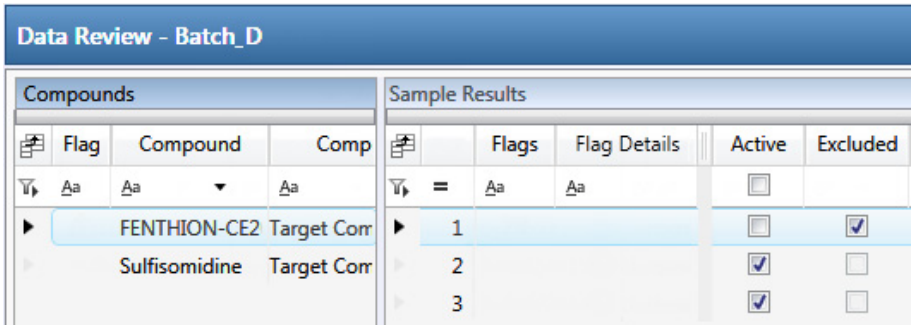
Column	Description
m/z (Delta (mmu))	Difference between the *m/z* (Expected) and *m/z* (Apex). Assumes that the charge is 1. When the *m/z* (Apex) column displays *m/z* value for the compound, this column displays the delta *m/z* corresponding to the highest intensity in the apex scan. • When the mass tolerance is specified in ppm in the master method, then *m/z* (Delta) = 1 000 000 × ([*m/z* (Apex) – *m/z* (Expected)] × *m/z* (Expected)). • When the mass tolerance is specified in mmu in the master method, then *m/z* (Delta) = 1000 × *m/z* (Apex) – *m/z* (Expected)).
m/z (Expected)	Mass-to-charge ratio from the compound database. Assumes that the charge is 1. • 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. For details about defining adducts for the compound database, see "Specifying Adducts" on page 52. For details about adding adducts to compounds, see "Editing Compounds in the Database" on page 89. **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.
Num Isotopes Matched	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 • 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	Peak found The application displays one of these flags: • A green circle when the peak is found. • A red square when the peak is not found.
Response Ratio	The ratio of the Response value to the IS Response value. If the Response is specified as Area in the processing method, the units of both Response and IS Response are counts-sec. If the Response is specified as Height in the processing method, the units of both Response and IS Response are counts.
RT Delta	Difference between the expected retention time and the measured retention time.

Table 97. 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 TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative.
Status	Status indicators for each sample indicate if the sample is currently acquiring, not acquired, acquired, or processed. Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.
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.



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 it marked inactive, the application does not remove its data and calculated values from the result set. Instead, the TraceFinder application masks the appearance of that compound for that particular sample and grays the compound 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.

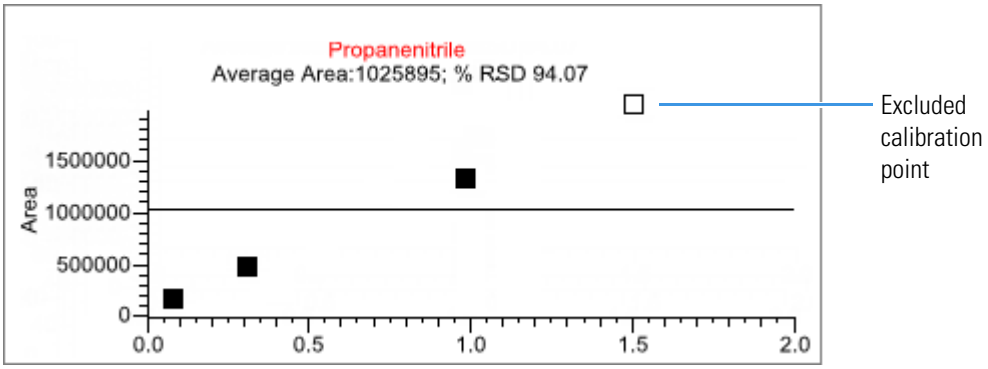
❖ To exclude a calibration point

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

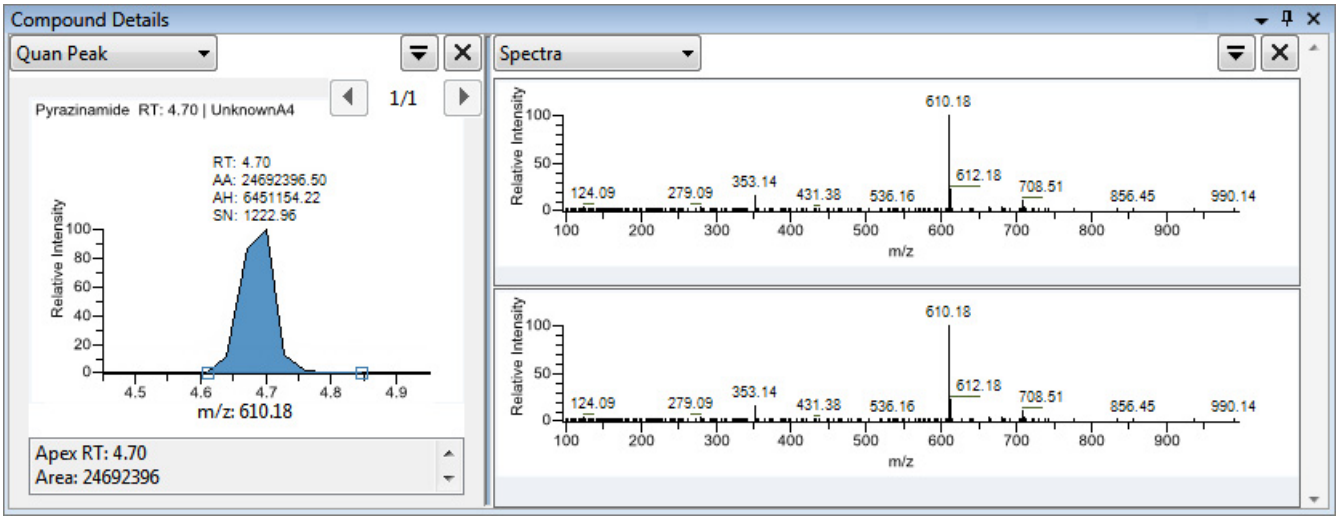
Use the Compounds Details pane to display any of the following types of data:

- 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.

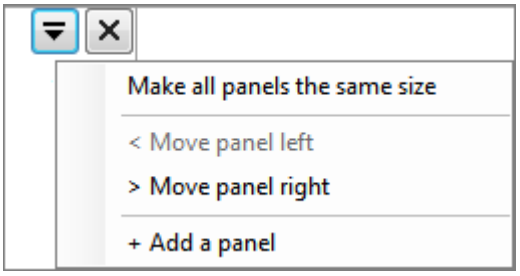
2. In the second pane, select the additional type of data that you want to display.

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.

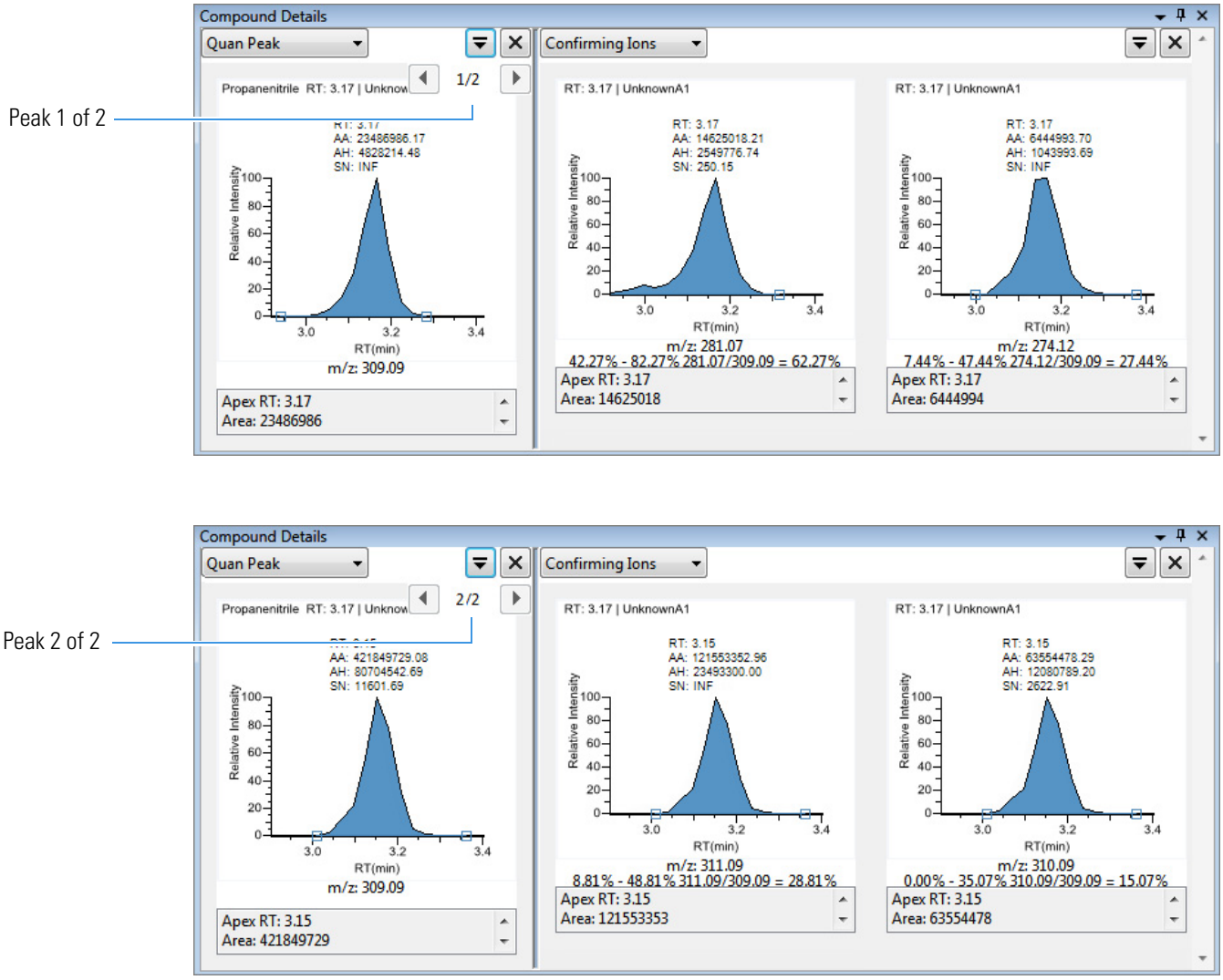
   The delineated area expands to fill the view.

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 indicator in the upper right corner of the Quan Peak pane displays which of the multiple quantitative peaks you are viewing. The Quan Peak pane uses a unique shortcut menu. See "Quan Peak pane shortcut menu commands" on page 474.

Figure 126. Quantitative peak pane with multiple quantitative peaks



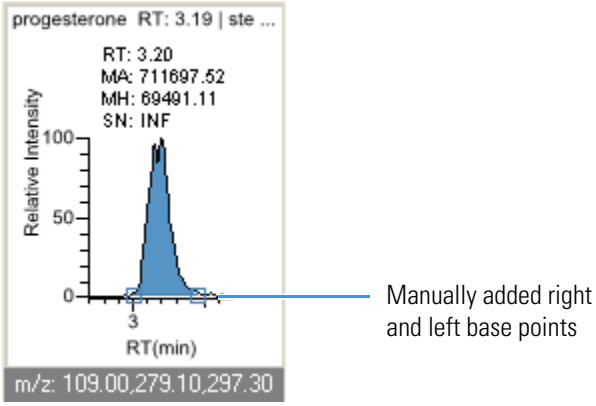
Follow these procedures to modify the quantitative or confirming ion peak data:

- 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 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 **Method Integration Settings** or **Manual Integration Settings** from the shortcut menu.

Initially, the method and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the chromatogram plots and the result set update as you switch between method and manual modes.

As you switch between modes, each pane reflects the changes. The generated reports for these data identify the manual modifications.

❖ To change the displayed information for detected peaks

1. Right-click the 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, select 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

1. 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 TraceFinder 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 127. Peak Detection Settings dialog box

2. Edit any of the detection settings.

   For detailed descriptions of all detection settings, see "Detection" on page 160.

3. To save your changes to this compound, click **Apply**.

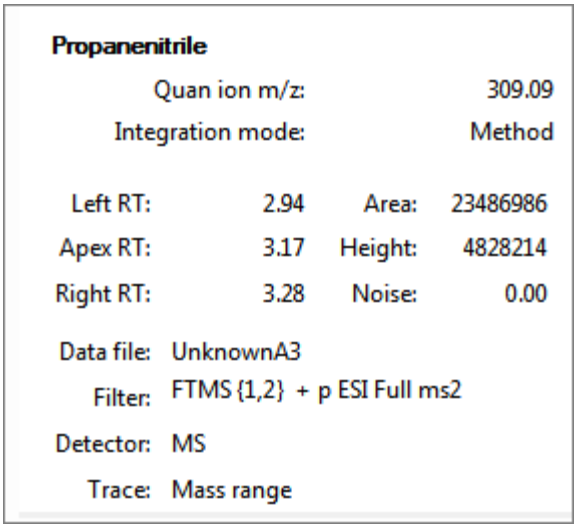
   - When you are editing a single sample, the application makes changes to the selected compound for this sample. If the sample is a calibration sample type, this update changes the calibration curve which, in turn, affects all calculated amounts.
   - When you are editing the local method, the application makes changes to the selected compound for all samples in this batch.

Note The Peak Detection Settings commands are also available on the Confirming Ions pane.

Table 98. Quan Peak pane shortcut menu commands (Sheet 1 of 2)

Command	Description
Method Integration Settings	**Use Local Method Peak Detection Settings**: Applies the local method integration settings to the selected compound. To edit these peak detection settings, use the Peak Detection Settings > Edit Local Method Peak Detection Settings command. **Use User Peak Detection Settings**: Applies the user-customized method integration settings to the selected compound. To edit these user-customized settings, use the Peak Detection Settings > Edit User Defined Peak Detection Settings command.
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 to Noise).

Table 98. 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:  **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	**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.

Confirming Ions

The Confirming Ions pane displays a graphical view of all qualifying/confirming ions for the selected compound and displays calculated ion ratios and ion ratio acceptance windows. A red border indicates that an ion ratio is outside of its window. The Confirming Ions pane uses a unique shortcut menu. See Confirming Ions pane shortcut menu commands.

> **Note** For compounds with an analog detection type, the application displays "No Confirming Ions are Enabled" in the Confirming Ions pane.

Figure 128. Quantitative peak with multiple confirming ions

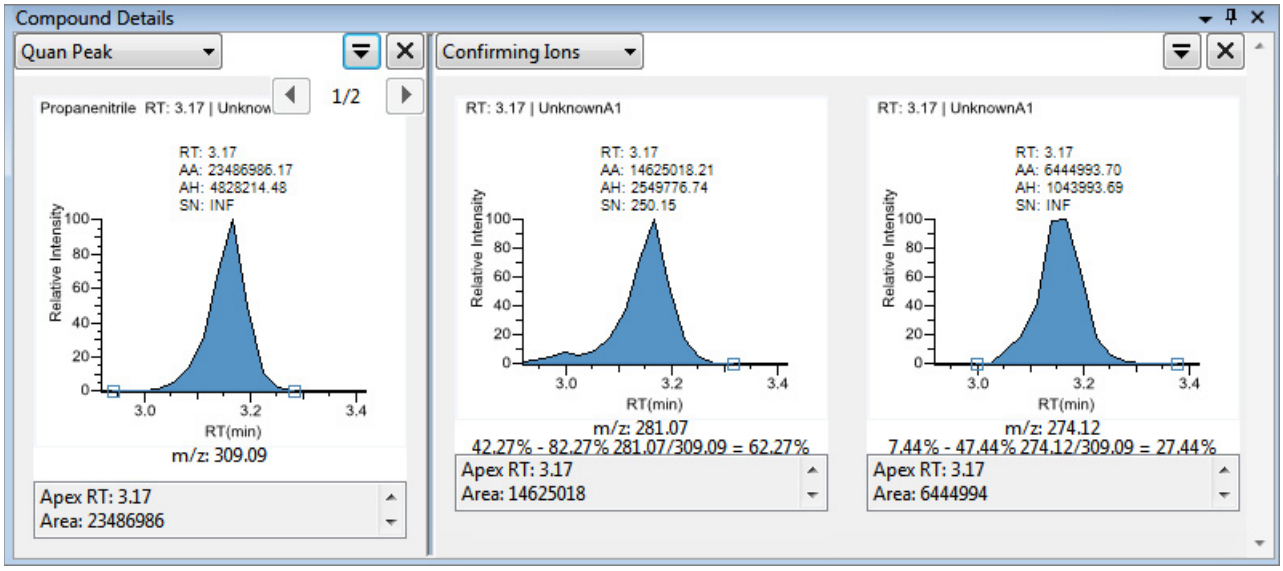
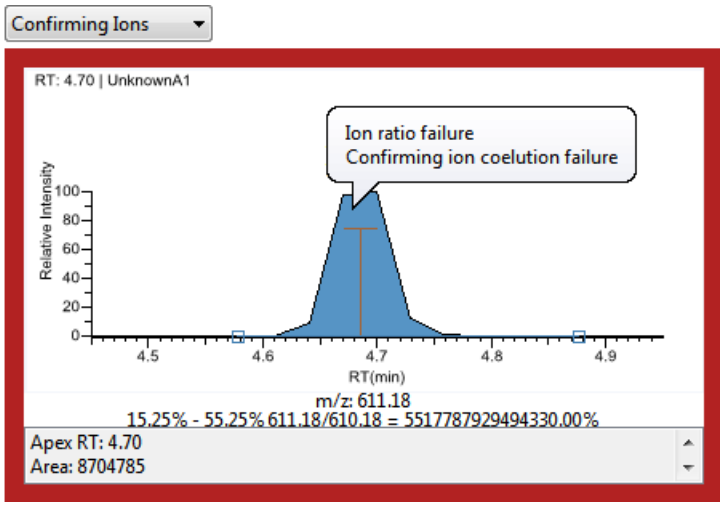


Figure 129. Confirming ion with coelution failure



❖ To manually integrate a confirming ion 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.

   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.

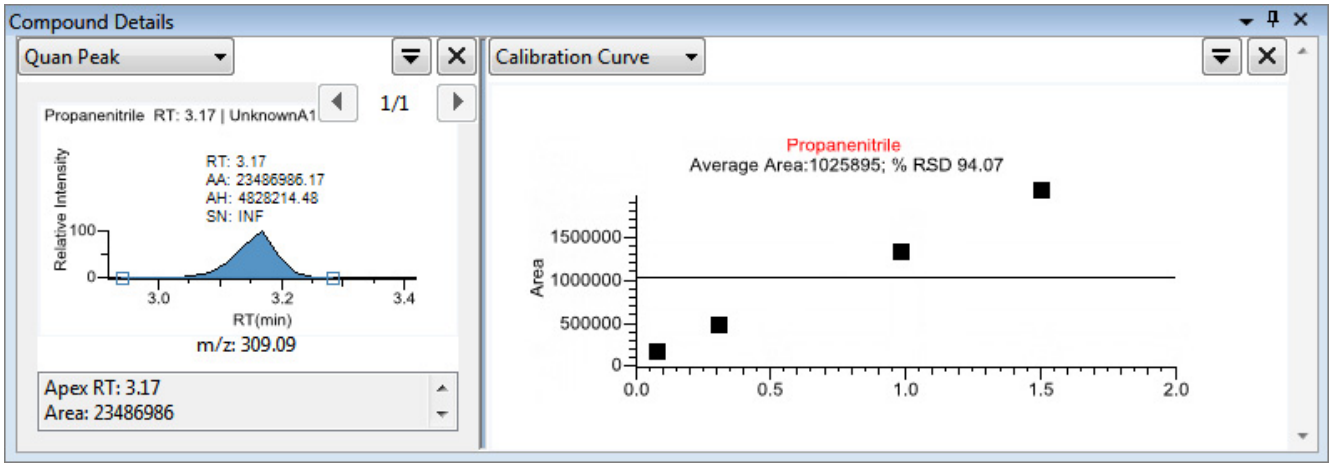
Table 99. Confirming Ions pane shortcut menu commands

Command	Description
Method Integration Settings	Displays the method integration settings.
Manual Integration Settings	Displays the manual integration settings.
Add/Remove/Cancel Quan Peak	Adds a quantitation peak, removes a peak, or cancels an add peak operation in progress.
Range Calc Method: Manual	Selects the method used to calculate the ion ratio range windows: Manual, Average, Weighted Average, or Level.
Range Calc Level	Displays the range based on the calibration level.
Target Ratio	Specifies the theoretical ratio of the confirming ion's response to the quantification ion's response.
Window Type	Specifies the Absolute or Relative calculation approach for determining the acceptable ion ratio range.
Window	Specifies the acceptable ion ratio range as a percentage.
Peak Labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label to Noise).
Show Peak Info	Displays peak information for the selected compound.
Reset Scaling	Resets the original scaling after a zoom operation.
Peak Detection Settings	Opens the Peak Detection Settings dialog box for the selected compound.

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 130. 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.

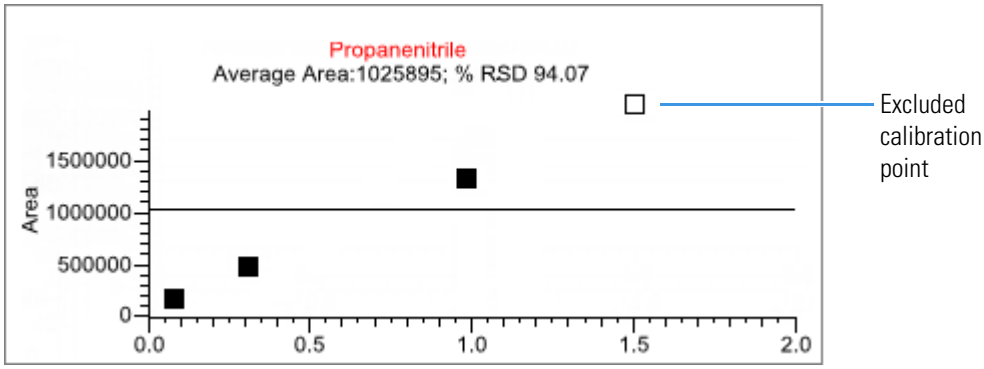


Table 100. Calibration Curve pane shortcut menu commands

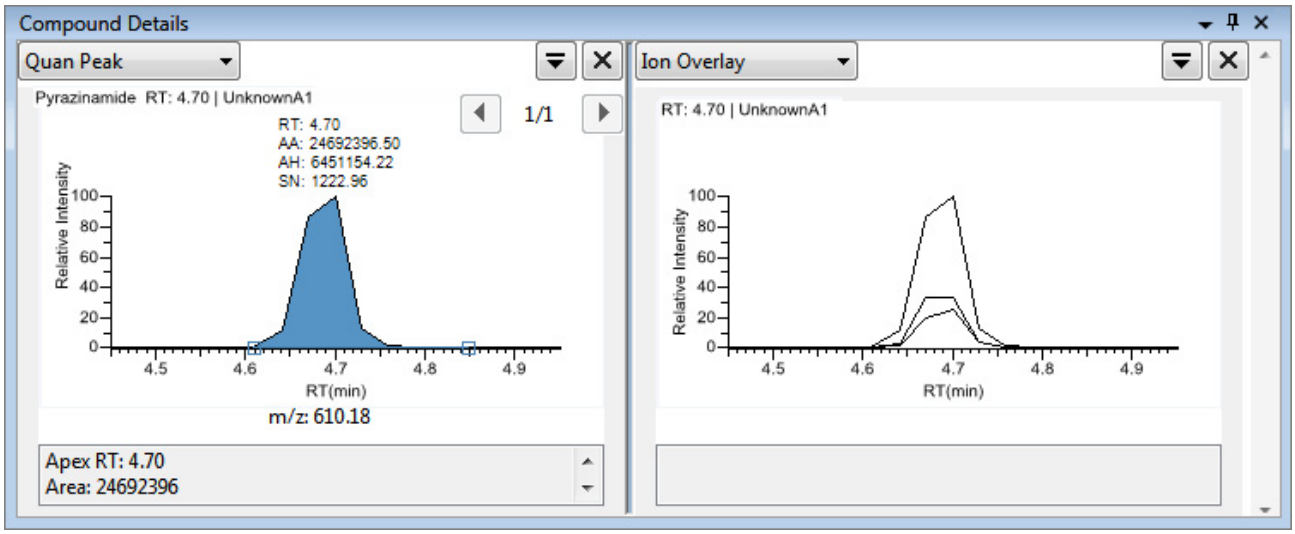
Command	Description
Standard Type	Sets the standard type to External or Internal.
Calibration Curve Type	Sets the calibration curve type to one of the following: • Linear: Allows all settings with this exception: When Origin is set to Include, all Weighting values are grayed out and Weighting is set 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.

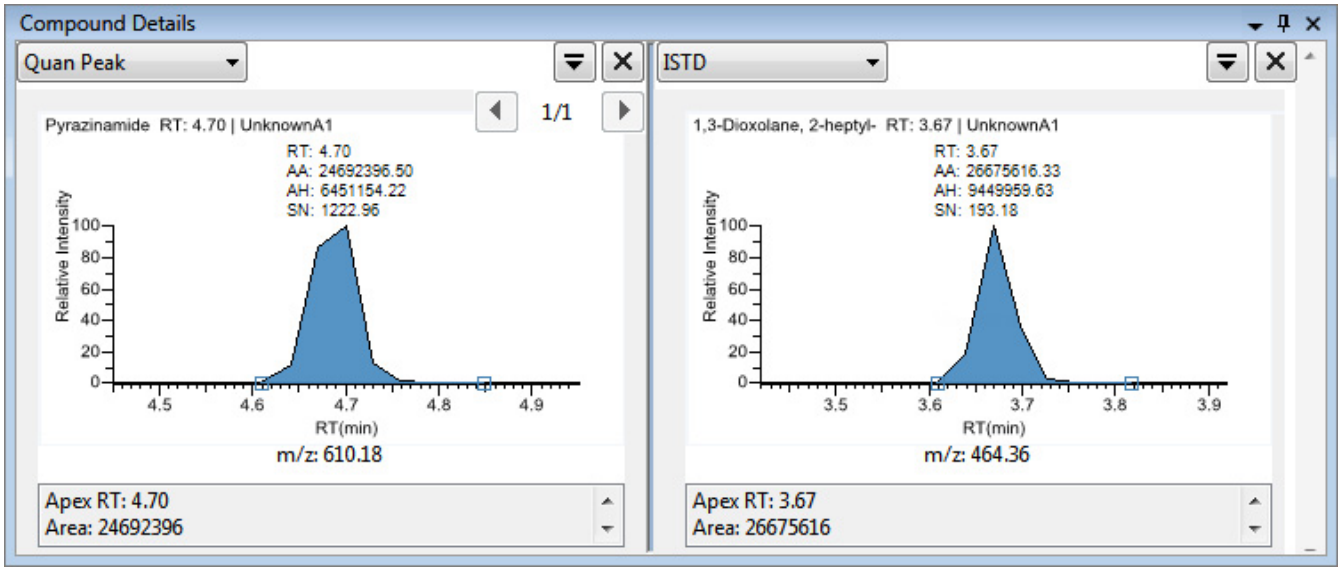
Figure 131. Quantitative peak with confirming ion overlay



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 215.

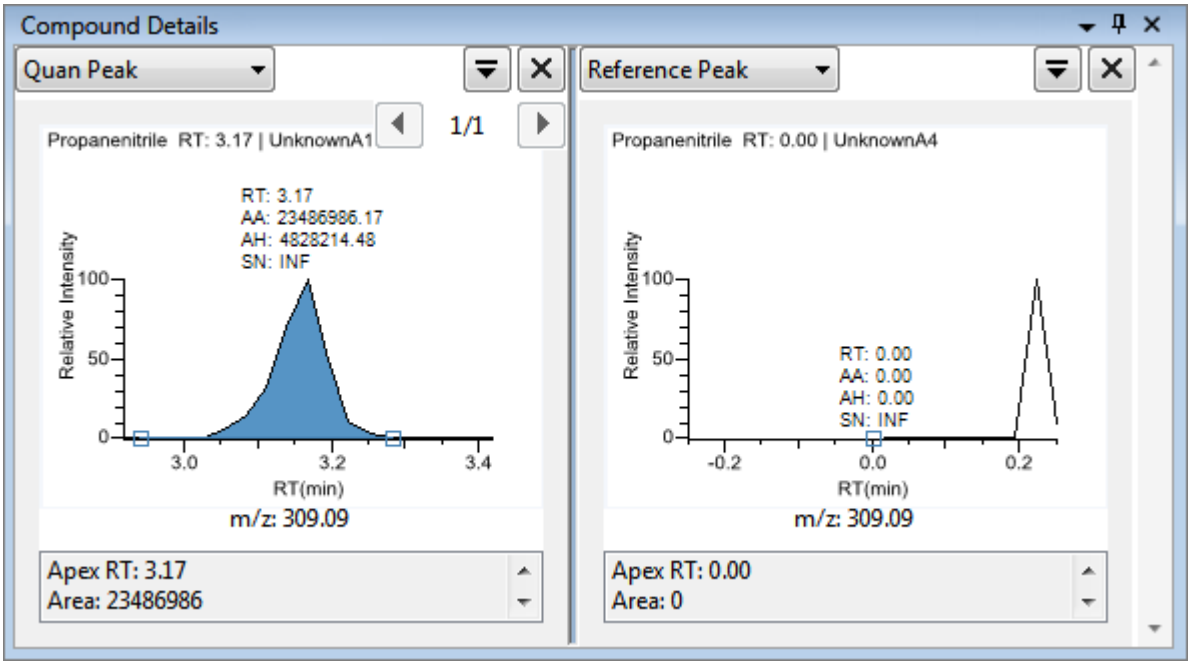
Figure 132. Quantitative peak with an internal standard



Reference Peak

The Reference Peak pane displays the reference peak as specified in the method.

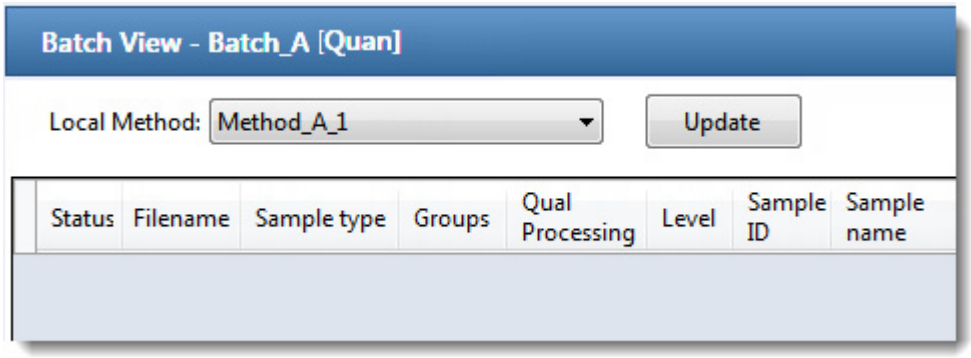
Figure 133. Quantitative peak with a reference peak



❖ **To specify a chromatogram reference peak**

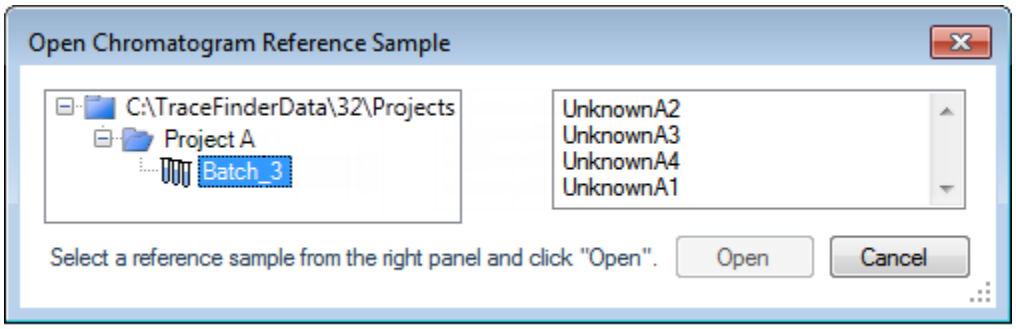
1. In the Batch View task pane, click **Reference Sample**.

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

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

   The TraceFinder application displays all the processed samples in the selected batch. To use a sample as a reference sample, 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.

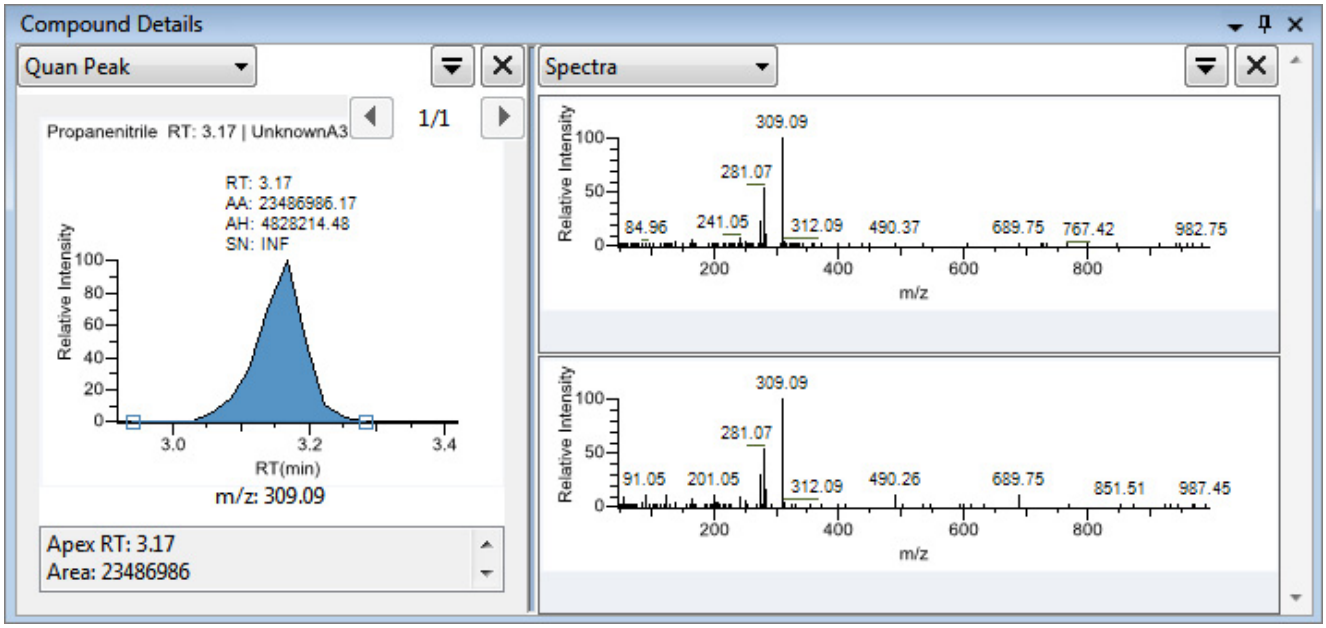
Tip To clear the reference sample from the master method, select **None** in the Set Chromatogram Reference Samples pane.

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.

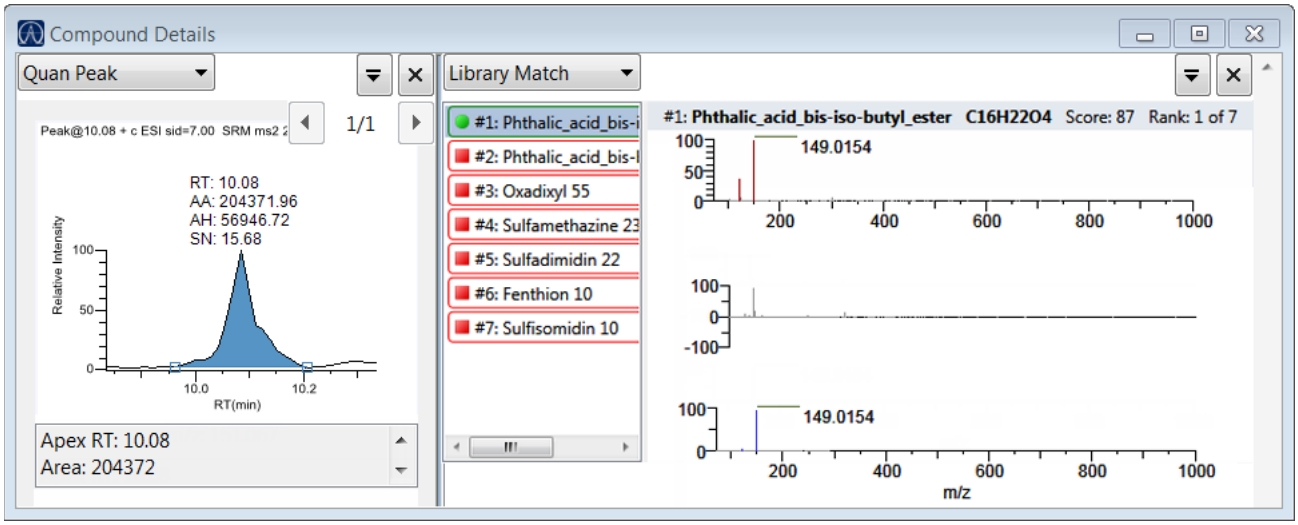
Figure 134. Quantitative peak with data and reference spectra



Library Match

The Library Match pane displays all library matches for the selected compound.

Figure 135. Library Match for selected compound



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 205.

Isotope

The Isotope pane displays all isotopes for the selected compound.

> **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 207.

Figure 136. Isotopes for the selected compound

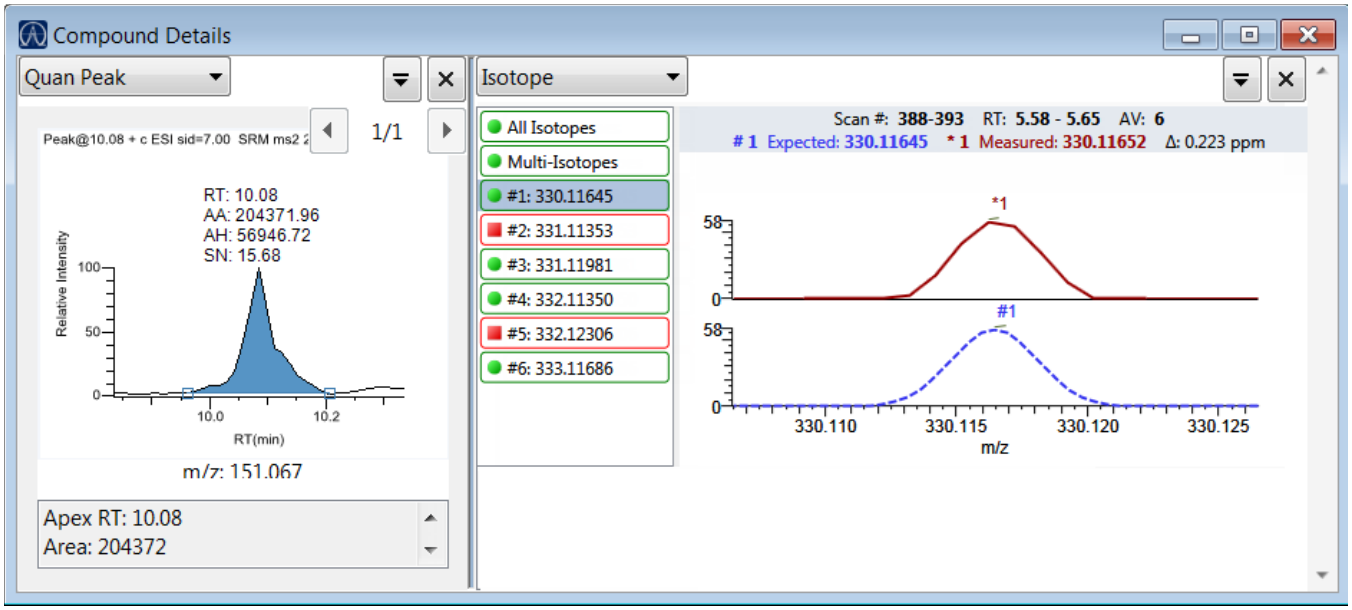
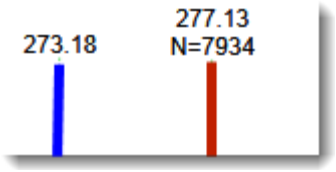
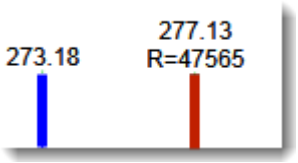


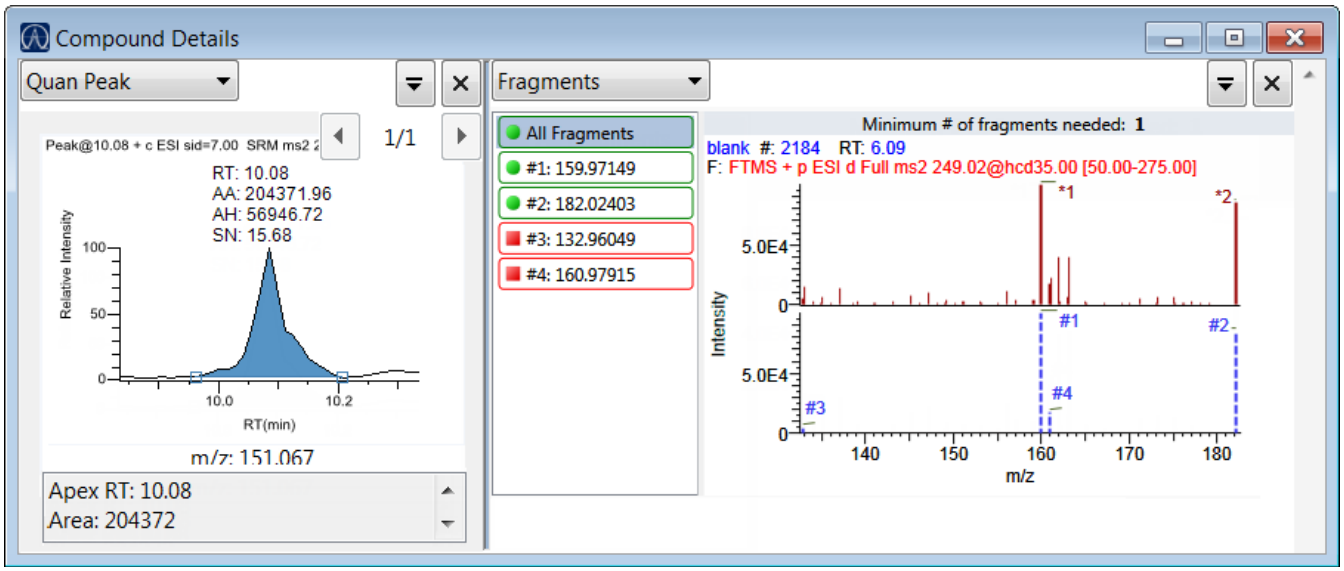
Table 101. Isotopes pane shortcut menu commands

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. 

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 137. 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 Data Review for Target Screening Methods

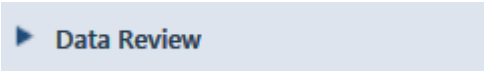
The Data Review view displays the data generated by the target screening master method. Use Data Review to verify the data for a compound before you generate reports.

❖ To open the Data Review view

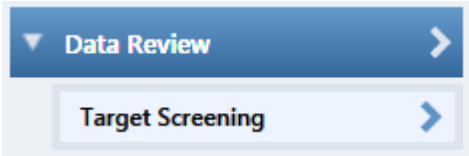
1. Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.

2. Click **Data Review**.



The Data Review navigation pane opens.



In the target screening display, the panes show a list of all samples in the current batch, the compound results for all compounds in the method, and 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 or hide the following:

- **Samples**
- **Target Screening Results**: Displays or hides the Compounds pane.
- **Chromatogram**
- **Spectrum**

Displayed panes are indicated with a check mark.

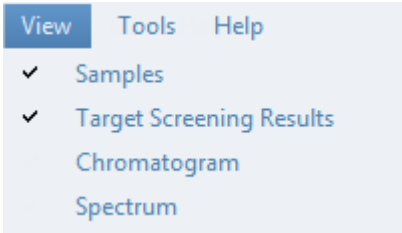
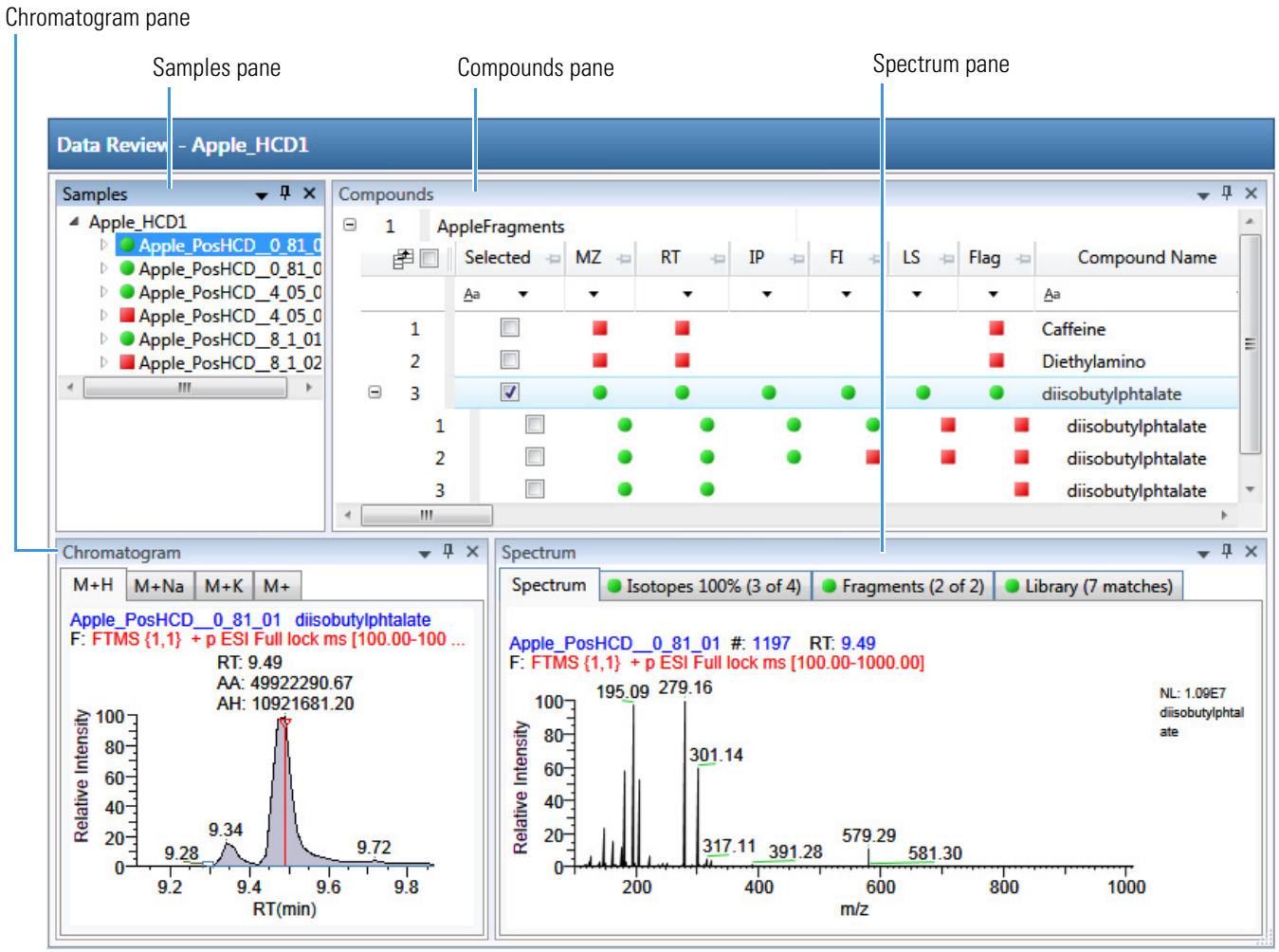


Figure 138. Target Screening panes



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.

For procedures about creating docked, floating, or tabbed panes, see "Data Review Pane Display Features" on page 424.

The target screening display includes the following features:

- Samples Pane
- Compounds Pane
- Chromatogram Pane
- Spectrum Pane

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 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.

Figure 139. Samples pane

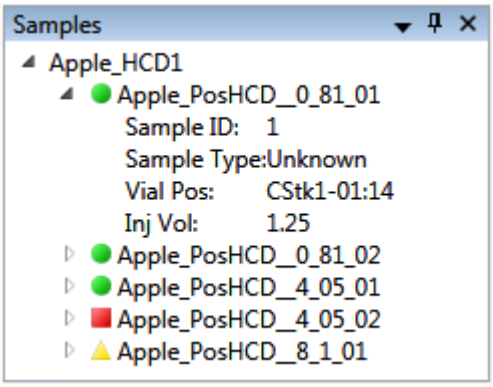


Table 102. Samples pane shortcut menu commands

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 498.

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
3.1312E04
1.9131E05
6.7147E04
1.4341E05

Library Score (%)
12
10
10
11

Displaying Multiple Adducts

When the TraceFinder 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	☑	●	●	●	●	●	●	diisobutylphtalate	diisobutylphtalate@RT 9.49	C16H22O4	M+H
1	☐	●	●	●	●	■	■	diisobutylphtalate	diisobutylphtalate@RT 9.49	C16H22O4	M+Na
2	☐	●	●	●	■	■	■	diisobutylphtalate	diisobutylphtalate@RT 9.49	C16H22O4	M+K
3	☐	●	●				■	diisobutylphtalate	diisobutylphtalate@RT 9.49	C16H22O4	M+

Exporting Compounds

Use the functions on the File menu to export data to an Excel spreadsheet, a CSV file, a compound database, or a new quantitation method.

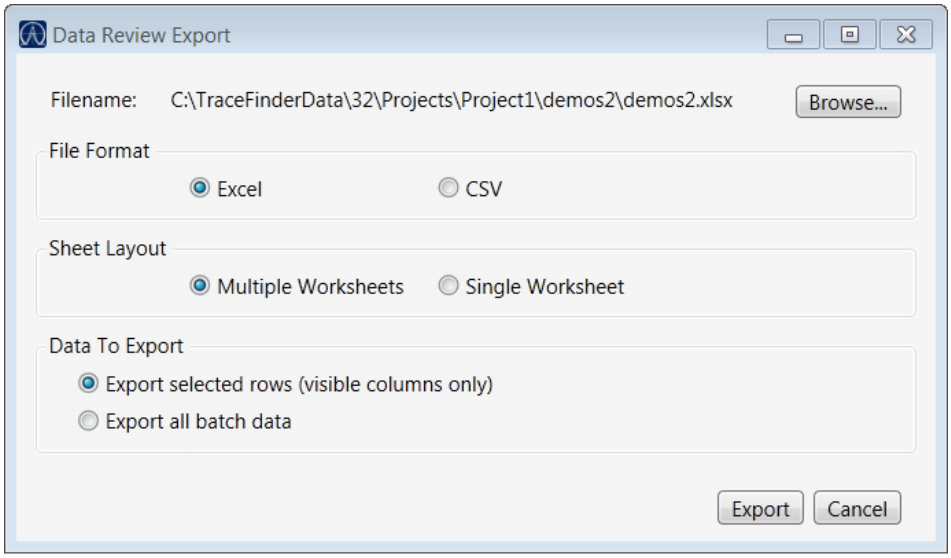
Follow these procedures:

- 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.



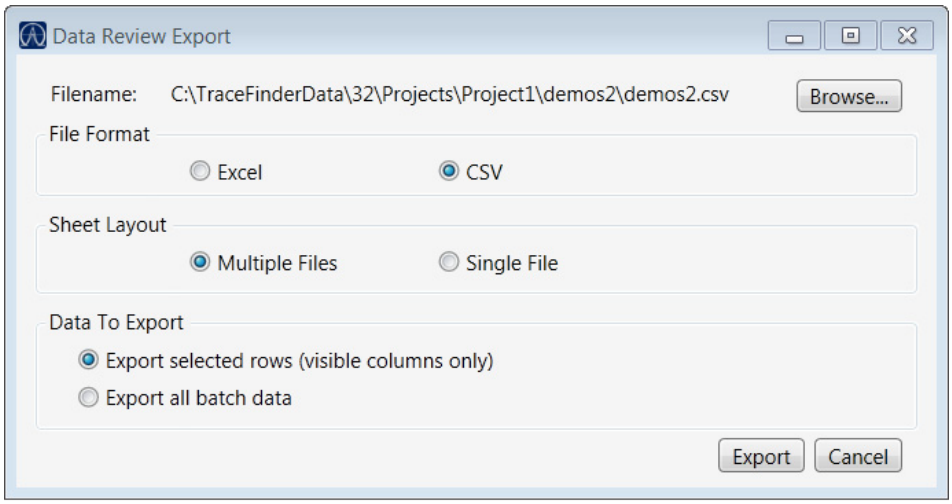
3. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.
4. Type a file name for the XLSX file and click **Save**.
5. In the File Format area, select the **Excel** option.
6. In the Sheet Layout area, select one of the following file formats 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**.

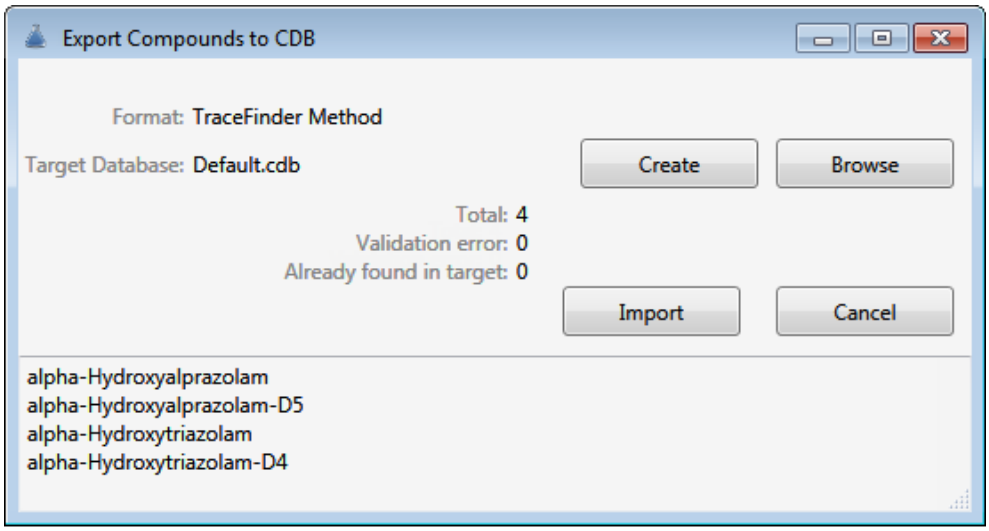
   The application saves the specified compound data to an CSV spreadsheet and opens the folder where you saved the file.

❖ 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.

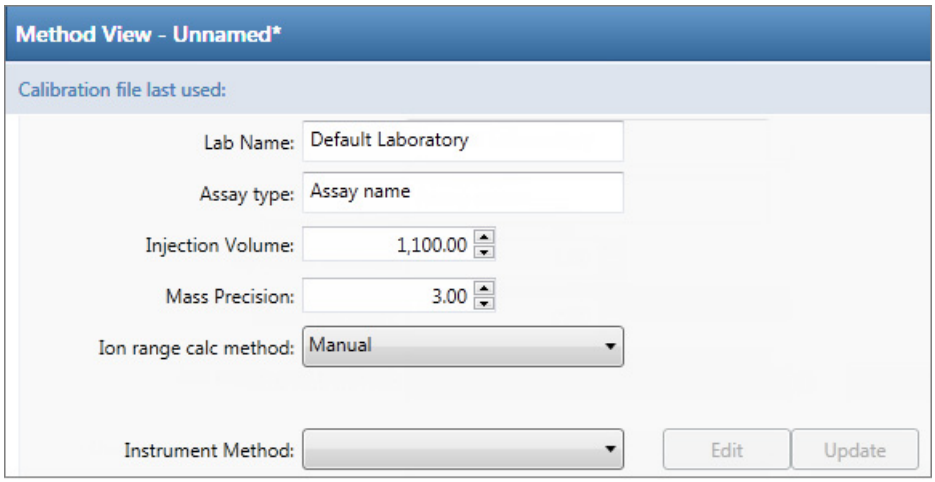
   The application uses the expected *m/z* value for the compound in the updated or new compound database.

   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. Observe that the application exported the selected compounds from the screening method to the new quantitation method.

   The application uses data from the selected compounds as follows:

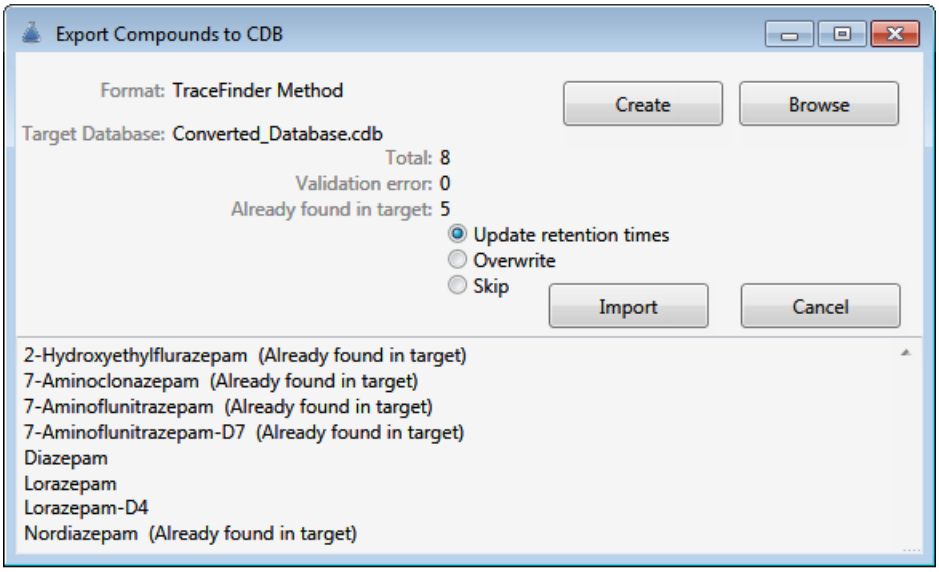
   - Exports quantitation peaks in the order of intensity.
   - Exports measured retention time value for the compounds in the new method.
   - Exports expected *m/z* value for the compounds in the new method.
   - Exports all found fragments to the new method.
   - Adds a filter for both quantitative peaks 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.

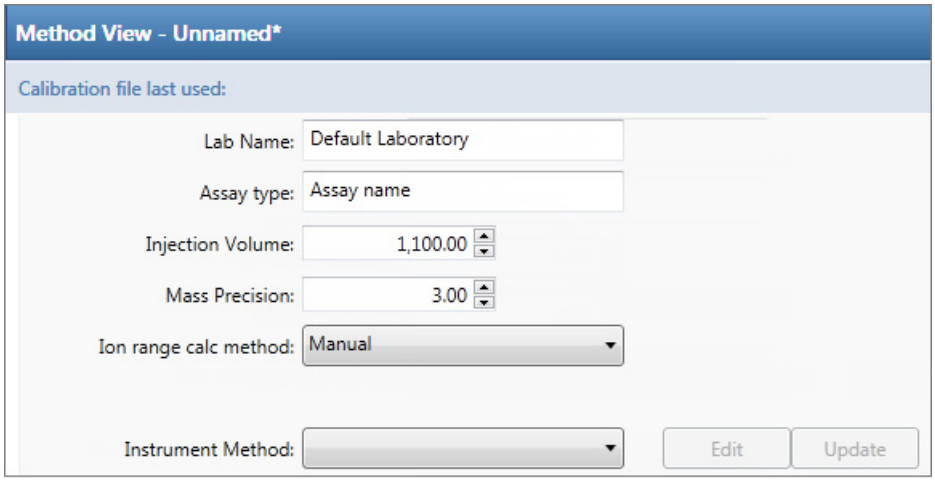
   The compounds list indicates which compounds already exist in the target compound database and which do not.

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.



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 and observe that the new method uses the specified compound database and that the application exported the selected compounds (with the specified options) from the screening method to the new quantitation method.

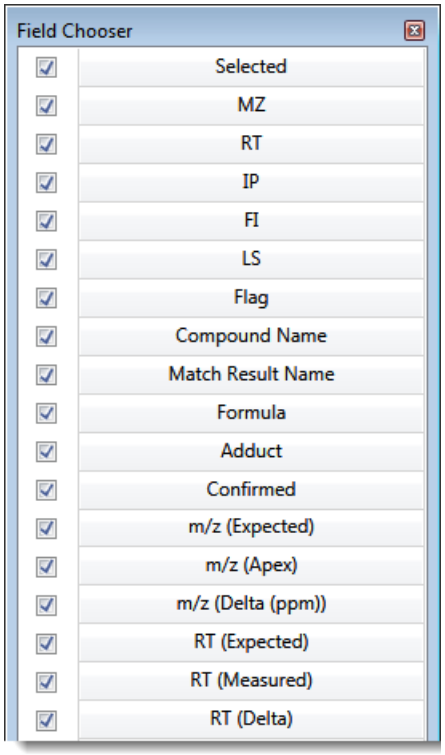
Compounds Pane Columns

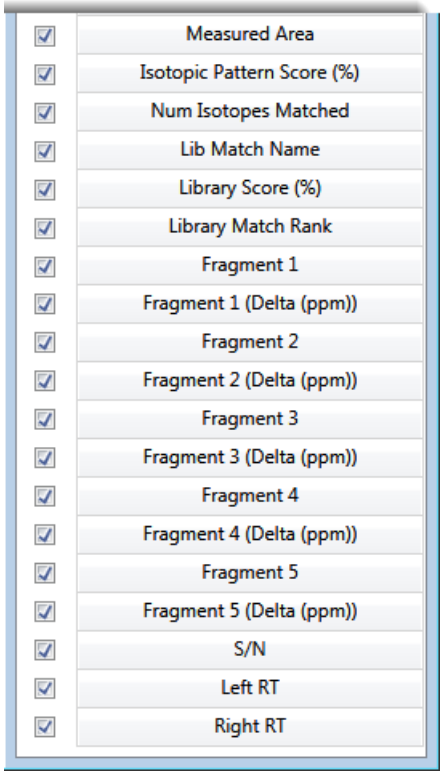
The columns of data in the Compounds pane display all parameter values associated with each compound in the selected sample. See Compounds Pane Parameters.

❖ 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 140. Compounds pane

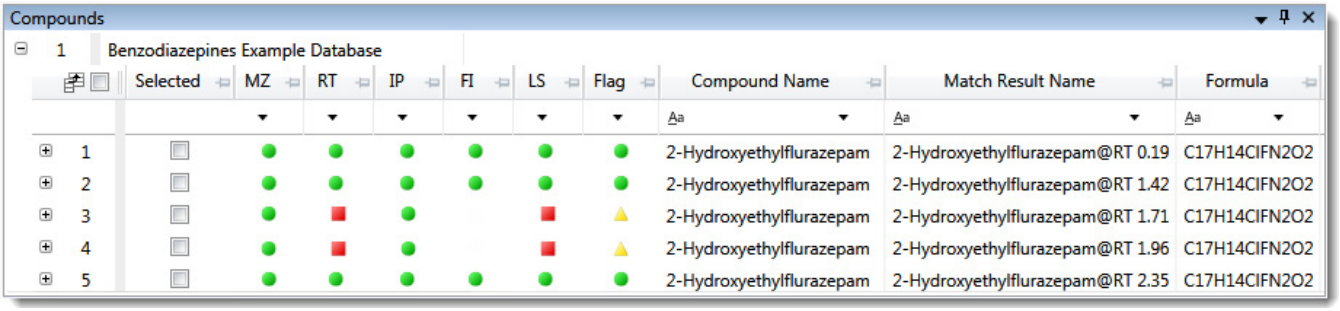


Table 103. Compounds pane parameters (Sheet 1 of 6)

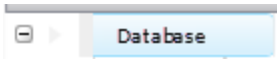
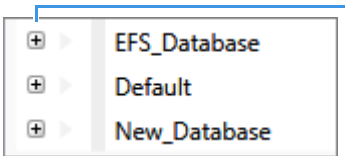
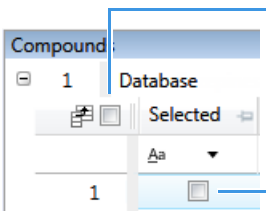
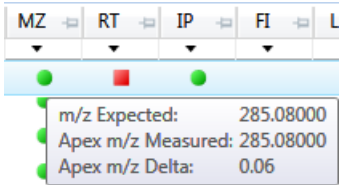
Column	Description
	Displays the current compound database. When you have multiple screening databases, the application lists the results for each database separately.  Expand the list of found compounds in the screening database.
Selected	Identifies individual compounds for export. To select all compounds for export, select the check box in the first column.  Selects all compounds in the Compounds pane. Selects the compound for export.
MZ	Mass-to-charge ratio flag. The application displays one of these indicators: • 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. To display the expected, measured, and delta *m/z*, hold your cursor over the indicator. 

Table 103. Compounds pane parameters (Sheet 2 of 6)

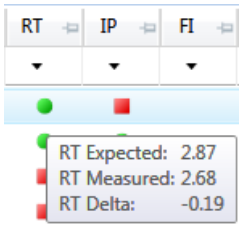
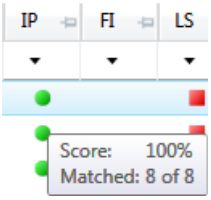
Column	Description
RT	Retention Time flag. The application displays one of these indicators: • A green circle (pass) when the measured retention time value is within the RT Window value specified in the compound database. • A red square (fail) when the measured retention time value is not within the 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 279. To display the expected, measured, and delta retention times, hold your cursor over the indicator. 
IP	Isotopic Pattern flag. The application displays one of these indicators: • 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 103. Compounds pane parameters (Sheet 3 of 6)

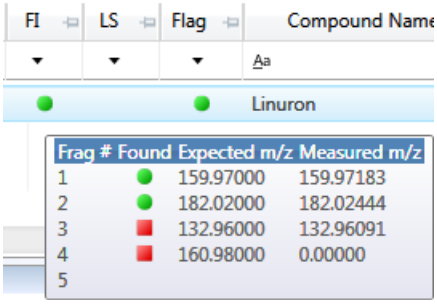
Column	Description
FI	Fragment Ions flag. The application displays one of these indicators: • A green circle (pass) when the measured *m/z* value of any of the fragments is within the mass tolerance specified in the method. On the Isotopes page in the Spectrum pane, the All Isotopes and Multi-Isotopes 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. To display a list of fragments and their pass/fail status, hold your cursor over the indicator. 
LS	Library Search flag. The application displays one of these flags: • A green circle when the library search is successful. • A red square when the library search is not successful.
Flag	Indicates the status of the identification and confirmation criteria. • 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.

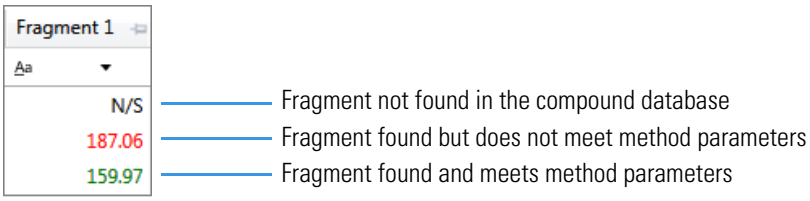
Table 103. Compounds pane parameters (Sheet 4 of 6)

Column	Description
m/z (Expected)	Mass-to-charge ratio from the compound database. Assumes the charge is 1. • 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. For details about defining adducts for the compound database, see "Specifying Adducts" on page 52. For details about adding adducts to compounds, see "Editing Compounds in the Database" on page 89. **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.
m/z (Apex)	Mass-to-charge ratio found in the spectra for the peak. Assumes the charge is 1. When the application successfully integrates the peak, this column displays the charged *m/z* value for the compound, which is the highest intensity in the apex scan. When the application cannot successfully integrate the peak, this column displays N/F.
m/z (Delta)	Difference between the *m/z* (Expected) and *m/z* (Apex). Assumes the charge is 1. When the *m/z* (Apex) column displays *m/z* value for the compound, this column displays the delta *m/z* corresponding to the highest intensity in the apex scan. • When the mass tolerance is specified in ppm in the master method, then *m/z* (Delta) = 1 000 000 × ([*m/z* (Apex) – *m/z* (Expected)] × *m/z* (Expected)). • When the mass tolerance is specified in mmu in the master method, then *m/z* (Delta) = 1000 × *m/z* (Apex) – *m/z* (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 103. Compounds pane parameters (Sheet 5 of 6)

Column	Description
Num Isotopes Matched	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 • 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	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. • 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 (%)	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. 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: • The criteria passes when the library score is higher than or equal to the score threshold. The values in this column are in green text. • The criteria fails when the library score is lower than the score threshold. The values in this column are in red text. 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. Range: 1 to 100%

Table 103. Compounds pane parameters (Sheet 6 of 6)

Column	Description
Library Match Rank	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 • 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. 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: • The criteria passes when the library score is higher than or equal to the score threshold. The values in this column are in green text. • The criteria fails when the library score is lower than the score threshold. The values in this column are in red text. 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.
Fragment *n*	Displays the measured *m/z* for the fragment ion. The application displays a separate column for each found fragment. • For each fragment found in the compound database that passes the filter in the method, the Compounds table displays the *m/z* 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 *m/z* value in red text. • For each fragment that is not found in the compound database, the Compounds table displays N/S (none specified).  **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.
Fragment *n* (Delta (ppm/mmu))	The difference between the expected fragment ion *m/z* from the compound database and the measured fragment ion *m/z*. The application displays a separate delta column for each identified fragment.
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 141. Chromatogram pane

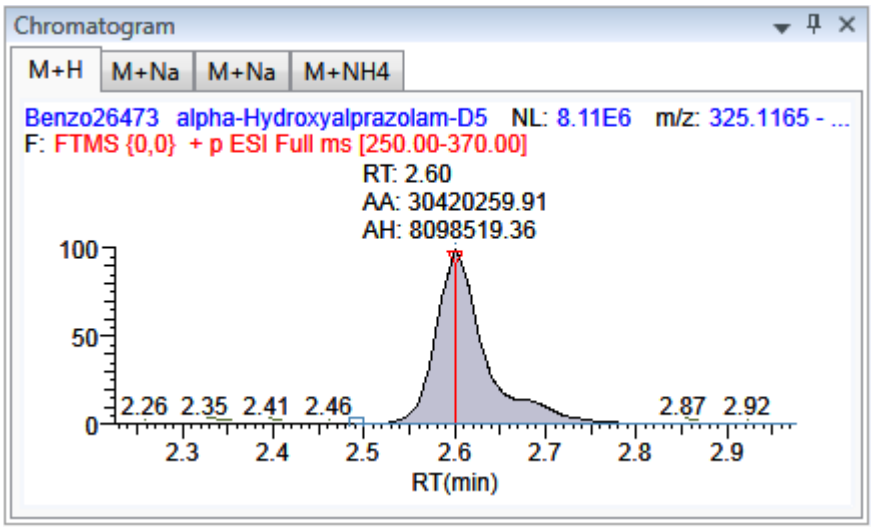


Table 104. Chromatogram pane shortcut menu commands

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 279.

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 142. Spectrum page

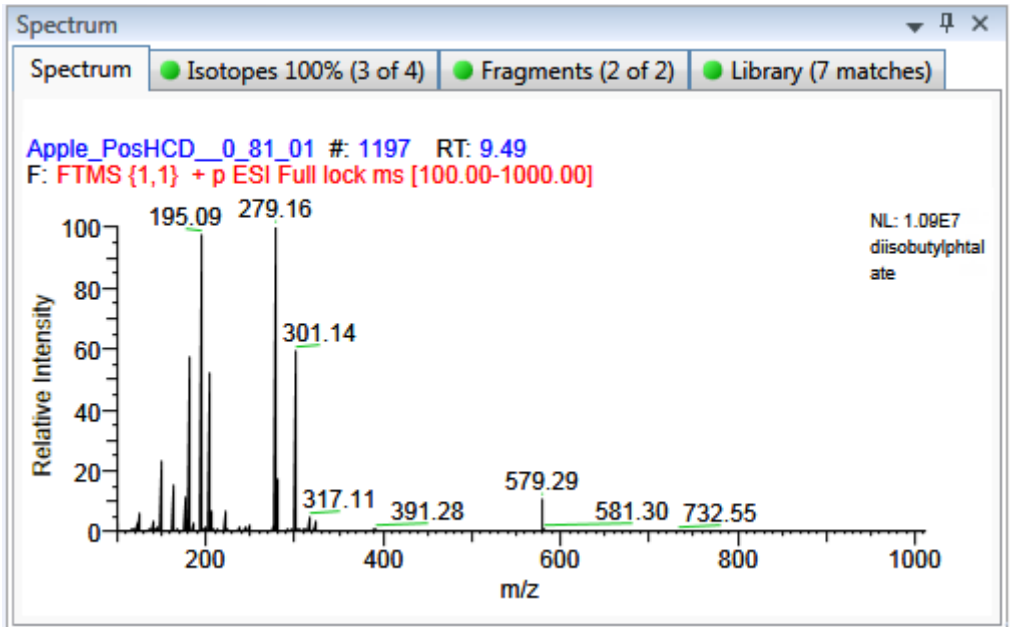


Table 105. Spectrum page shortcut menu commands

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 279.

The Isotopes page displays the isotopes in one of three ways:

- All Isotopes
- Multi-Isotopes
- Individual Isotopes

All isotopes pages use a shortcut menu to specify how you want the data displayed. See " Isotopes page shortcut menu commands" on page 512.

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:

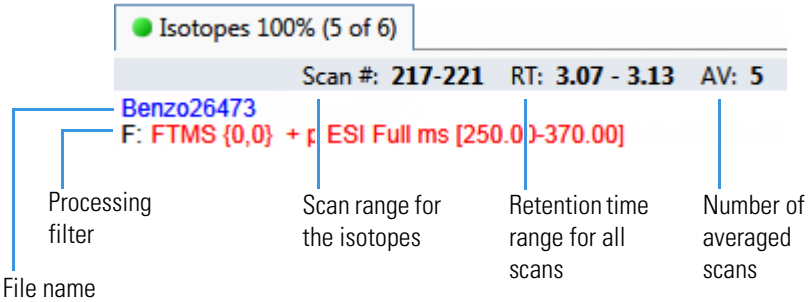
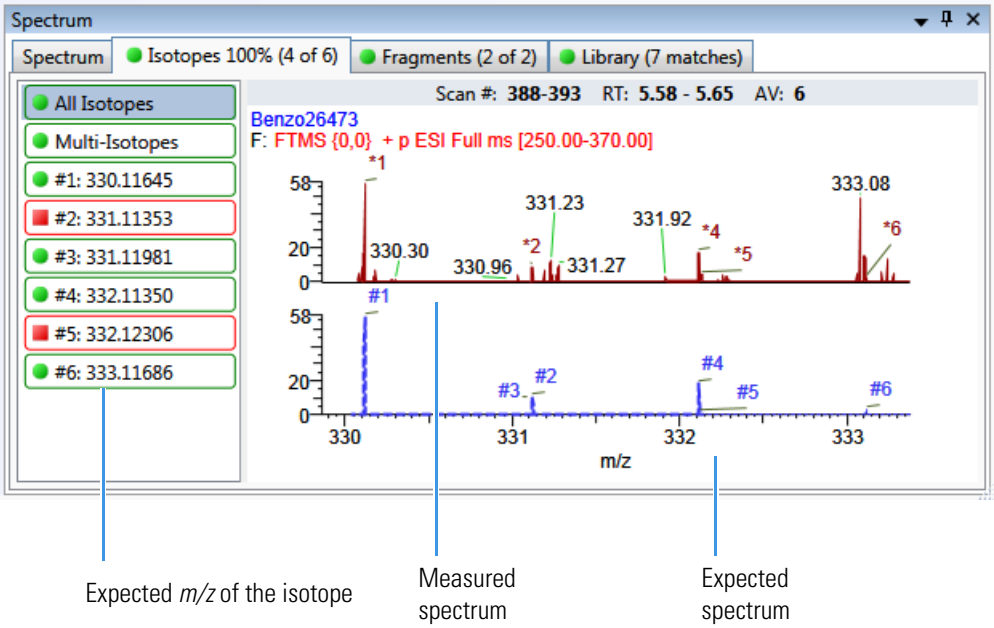


Figure 143. Isotopes page with stacked spectra for all isotopes

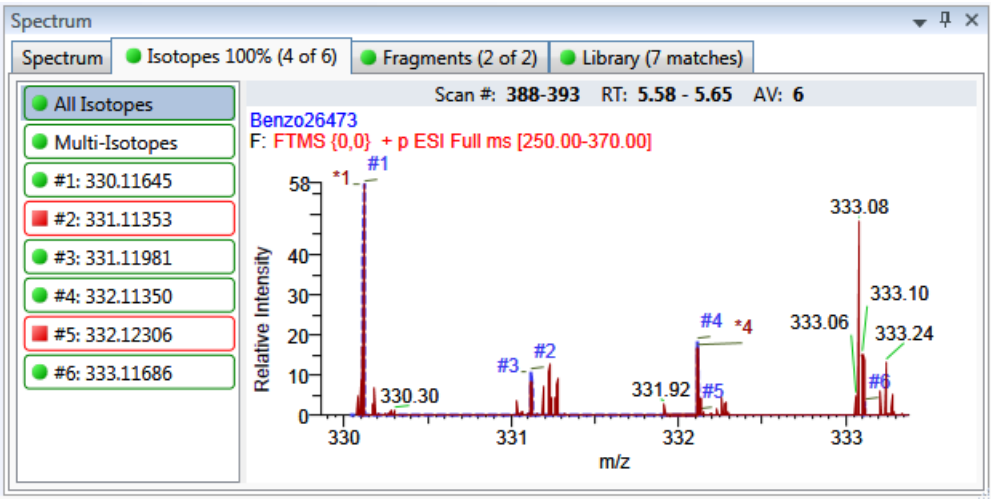


Expected *m/z* of the isotope

Measured spectrum

Expected spectrum

Figure 144. Isotopes page with overlaid spectra for all isotopes



Expected spectrum in blue

Measured spectrum in red

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:

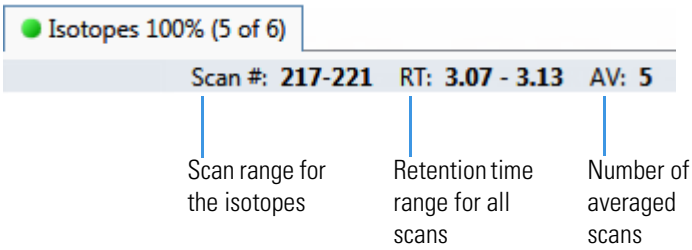
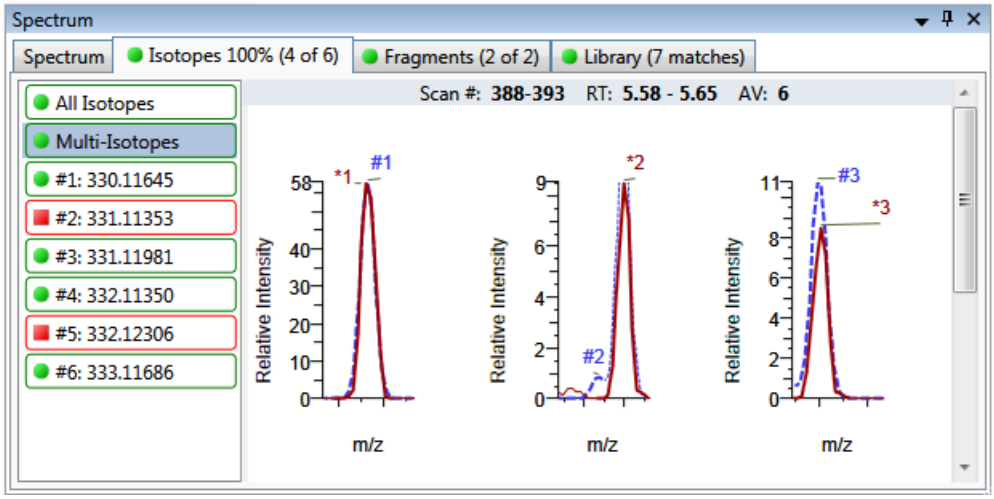
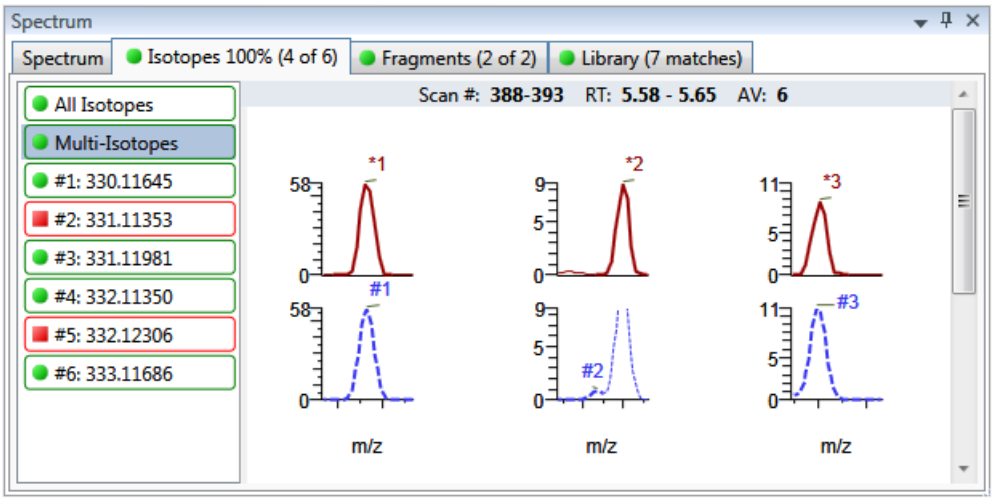


Figure 145. Isotopes page with overlaid spectra for multi-isotopes



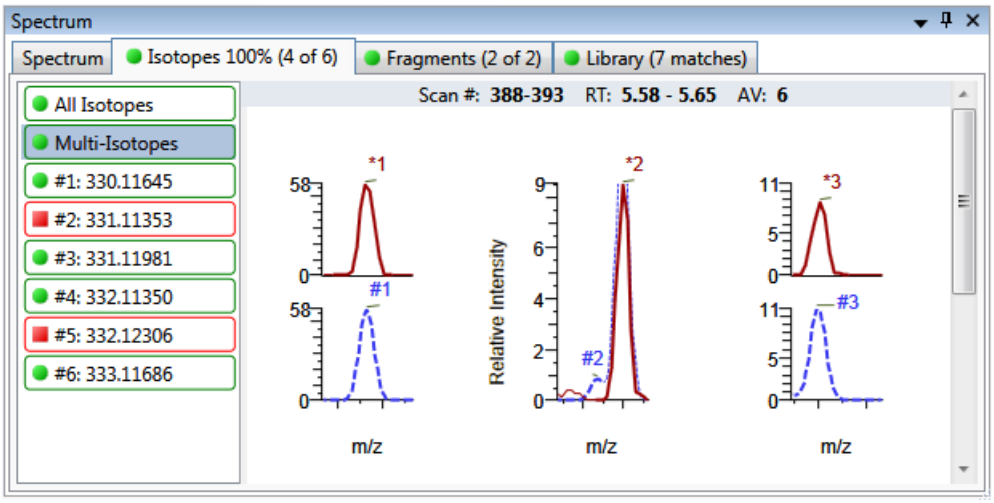
Expected spectrum in blue Measured spectrum in red

Figure 146. Isotopes page with stacked spectra for multi-isotopes



Expected spectrum in blue Measured spectrum in red

Figure 147. 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:

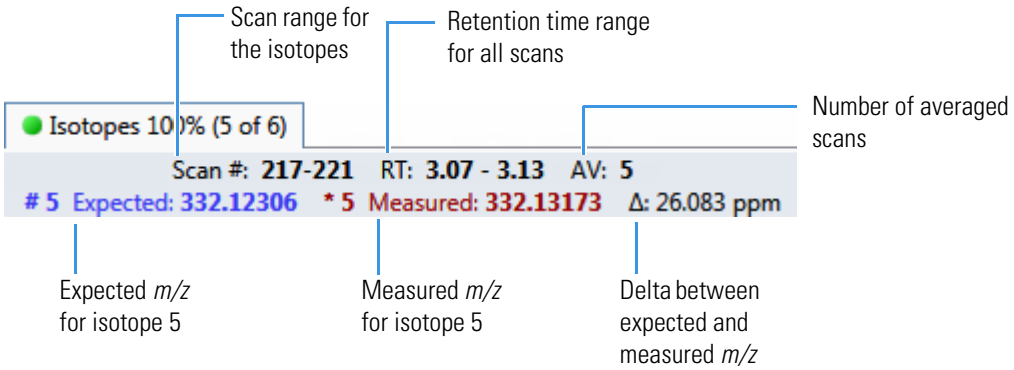
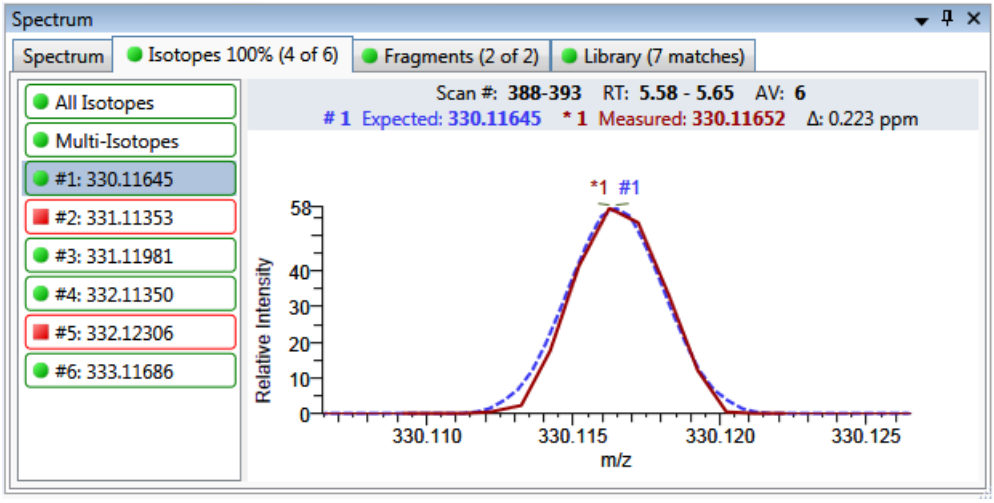
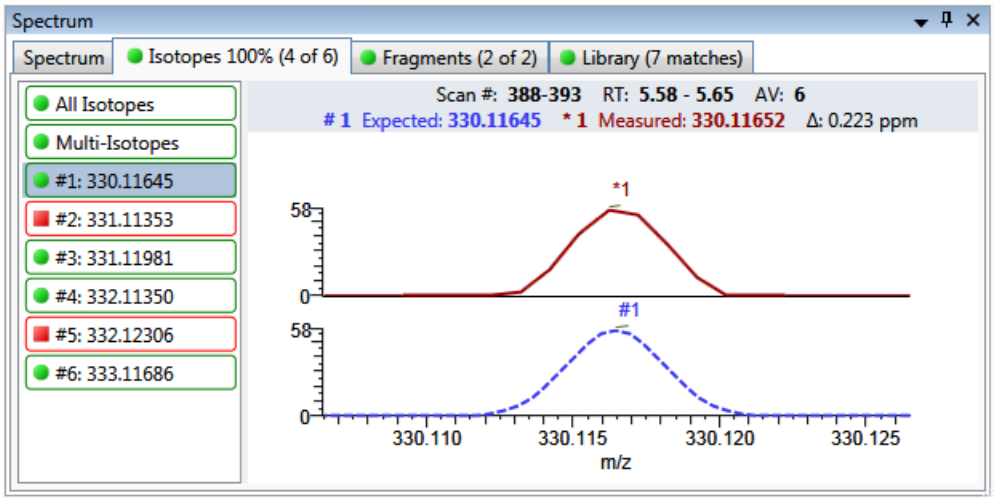


Figure 148. Isotopes page with overlaid spectra for a single isotope



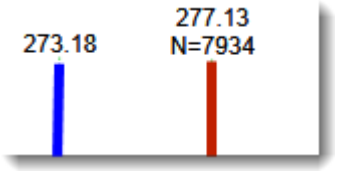
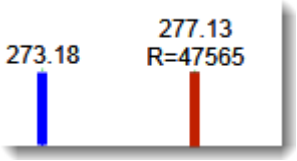
Expected spectrum in blue Measured spectrum in red

Figure 149. Isotopes page with stacked spectra for a single isotope



Expected spectrum in blue Measured spectrum in red

Table 106. 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 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 279.

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 96.

The Fragments page 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 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:

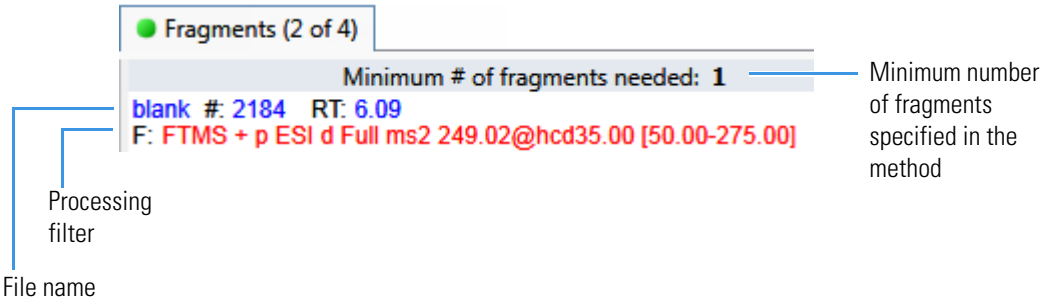


Figure 150. Fragments page with overlaid spectra for all fragments

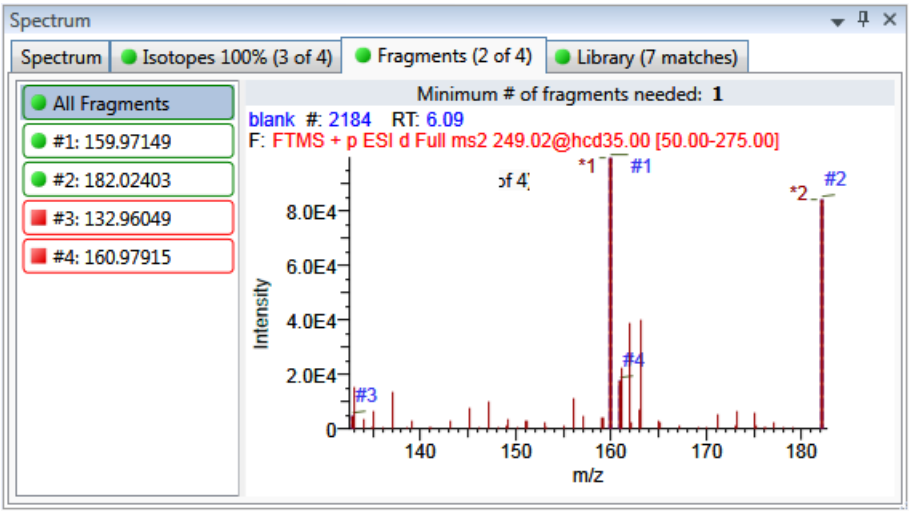
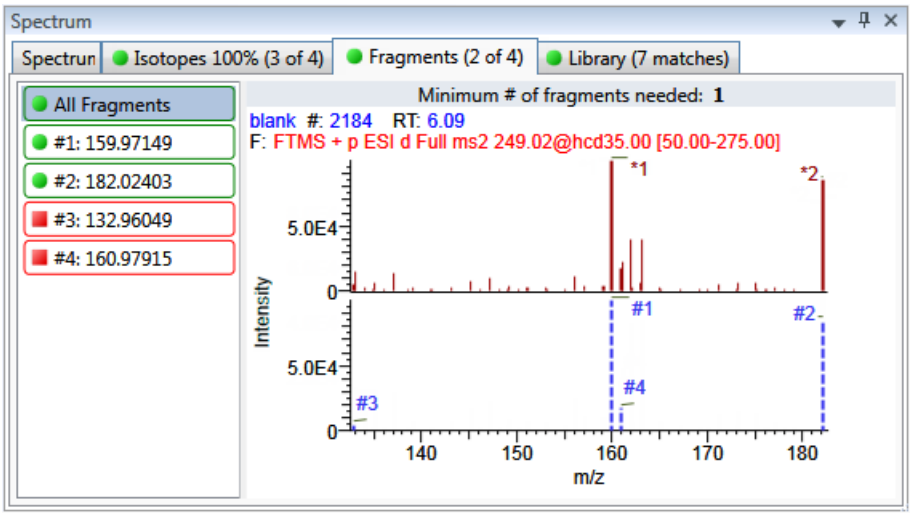


Figure 151. Fragments page with stacked spectra for all fragments



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:

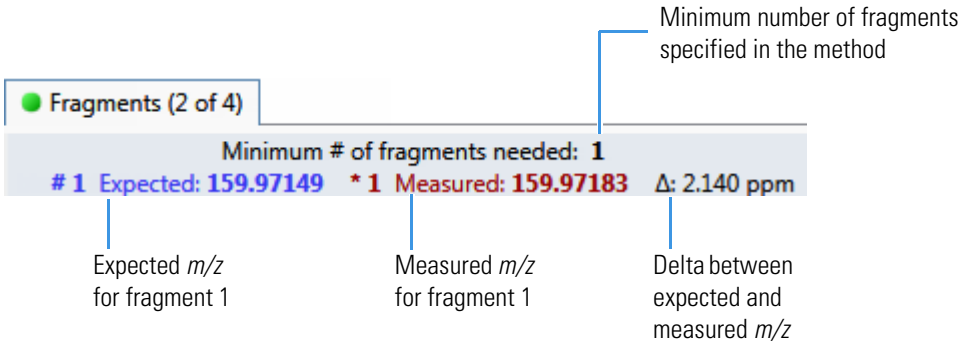


Figure 152. Fragments page with overlaid spectra for a single fragment

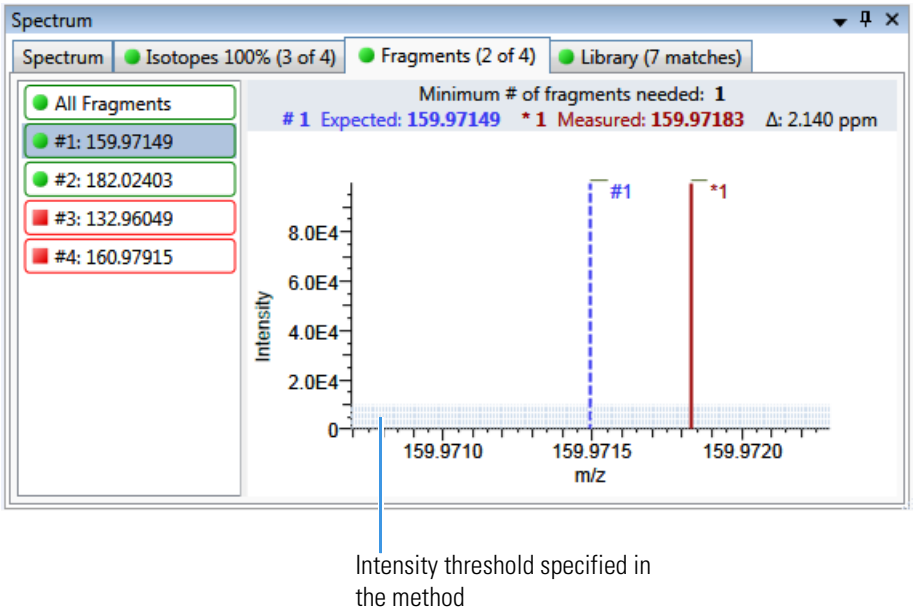


Figure 153. Fragments page with stacked spectra for a single fragment

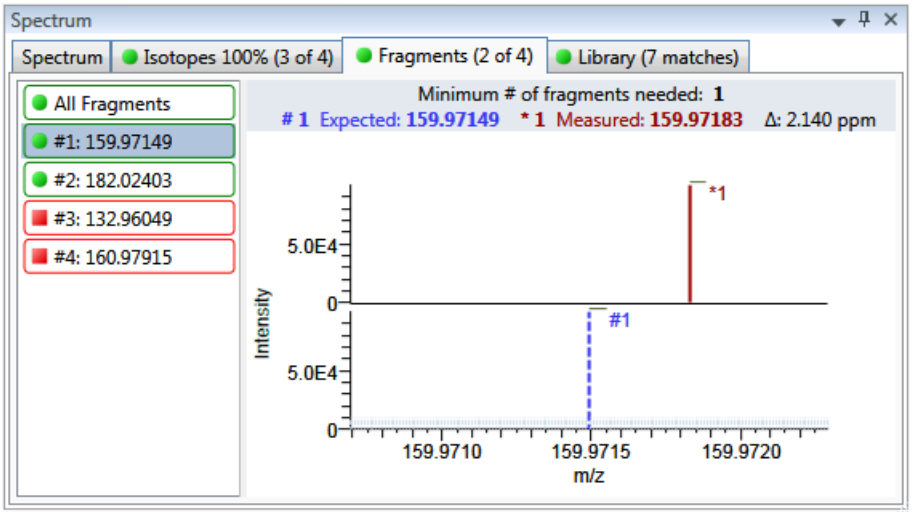


Table 107. Fragments page shortcut menu commands

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 Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.

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 279.

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:

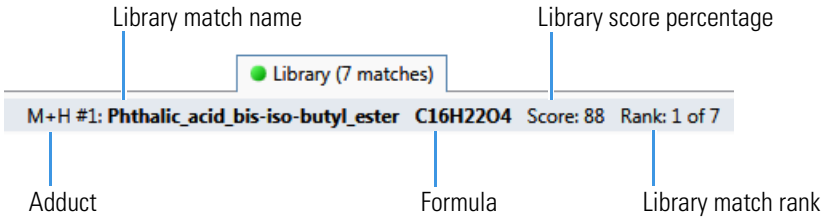


Figure 154. Library page with stacked spectra

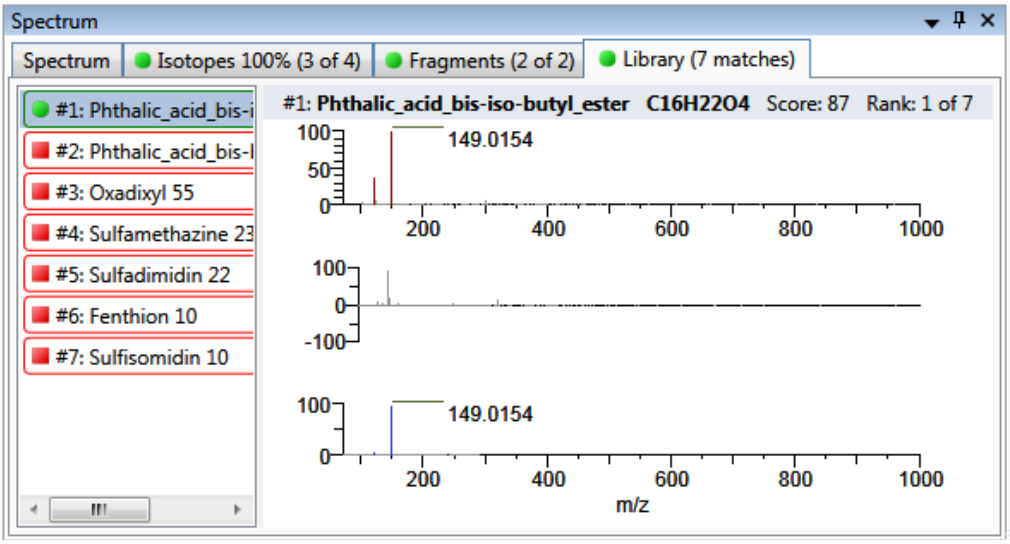


Figure 155. Library page with overlaid spectra

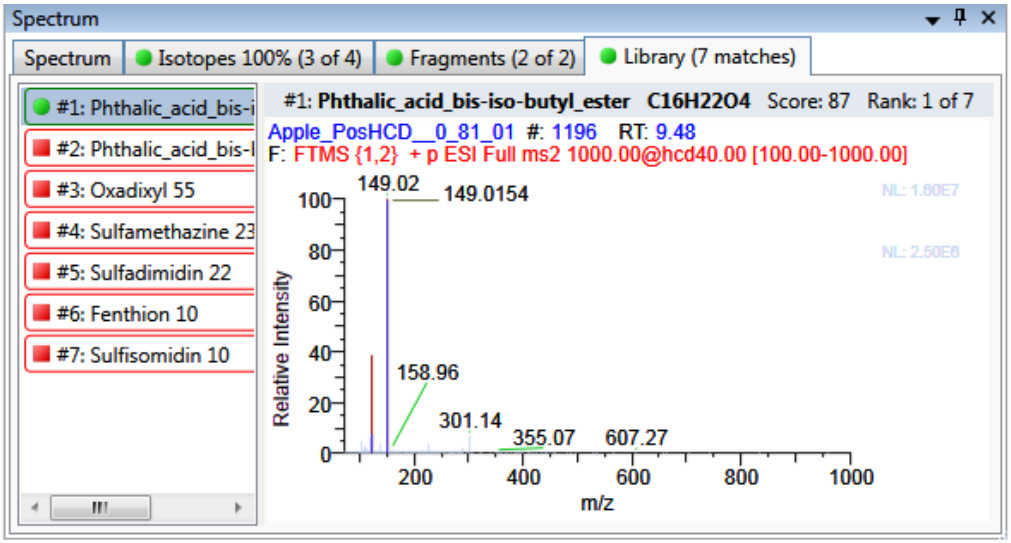


Table 108. Library page shortcut menu commands

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 Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.

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. In the Analysis navigation pane, click **Local Method**.

   The Local Method view for the currently selected batch opens.

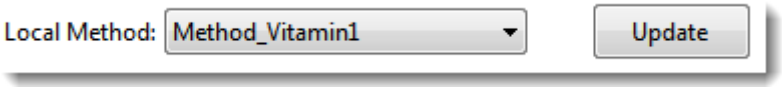
   You can edit many of the method parameters in a local method. Editing the local method does not affect parameters in the master method.

   For detailed descriptions of quantitation method parameters, see "Editing a Master Method" on page 144 (Chapter 5).

   For detailed descriptions of target screening method parameters, see "Editing a Master Method" on page 275 (Chapter 6).
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 156. Local Method view of a quantitation method

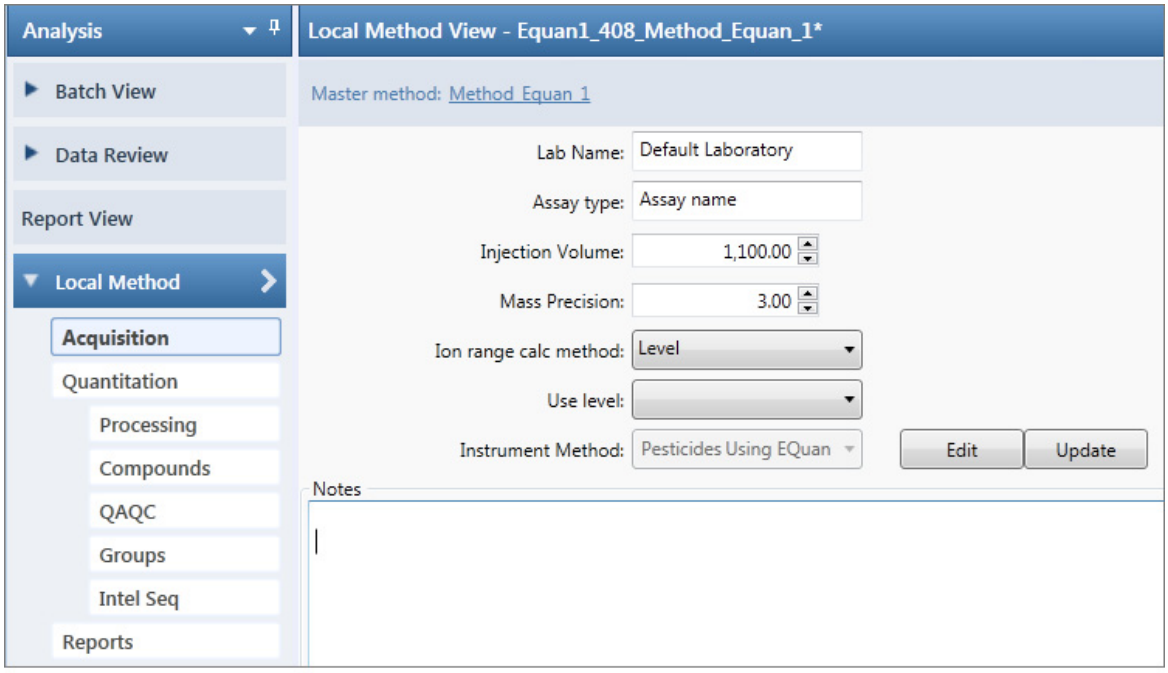
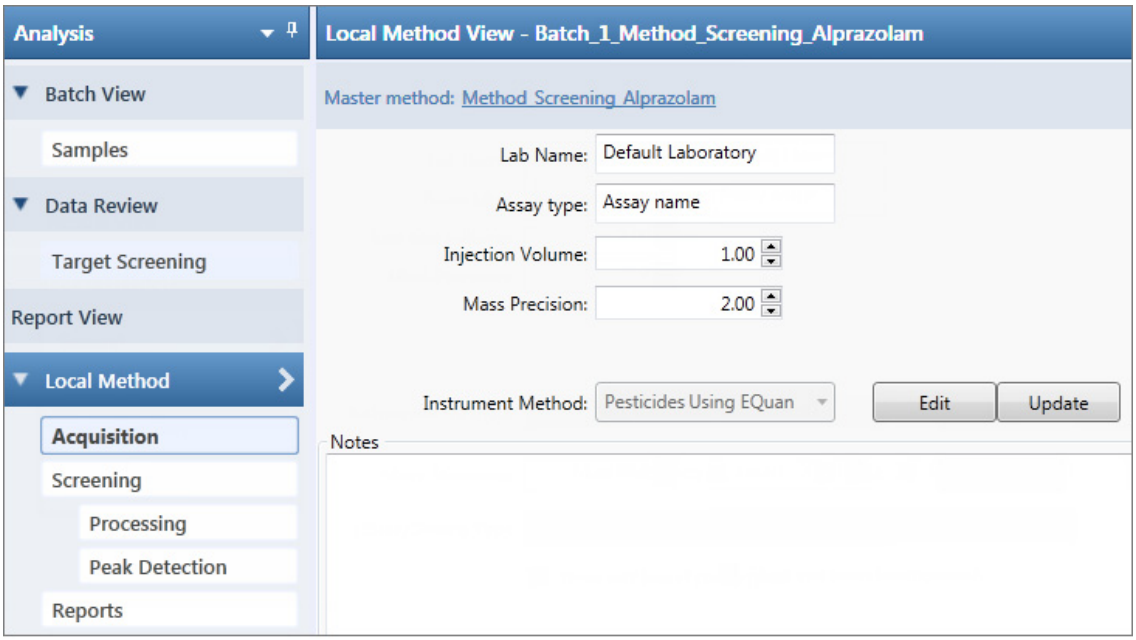


Figure 157. Local Method View of a screening method



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.

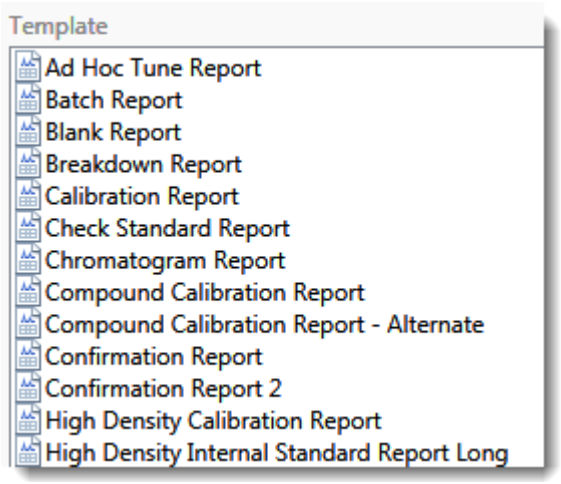
The application opens the Reporting view. For detailed descriptions of all parameters, see "Report View" on page 525.

❖ 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 72.

   Figure 158. Example template list



2. Click **Preview**, Preview.

   The application opens the Report Designer, showing the report information for the current batch in the selected report template format.

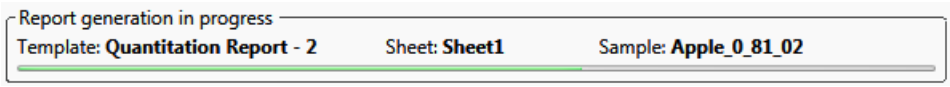
   For details about using the Report Designer, see "Working in the Report Designer" on page 527.

❖ 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 525.
   - Saves the report files to the …\TraceFinderData\32\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:

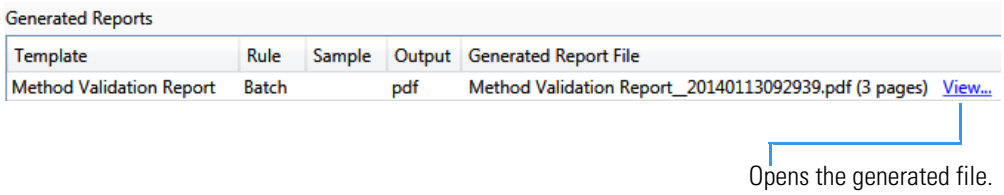
   - Creates a report for the current batch using the selected report template format.
   - Prints the report to your default printer.
   - Adds information about the generated report to the Generated Reports pane.

     For details about the Generated Reports pane, see "Report View" on page 525.
   - Saves the report files to the …\TraceFinderData\32\Projects*batch*\ReportOutput folder.

❖ To display a generated report

In the Generated Reports pane, click **View** for the report you want to see.

Figure 159. Generated Reports pane showing a PDF report



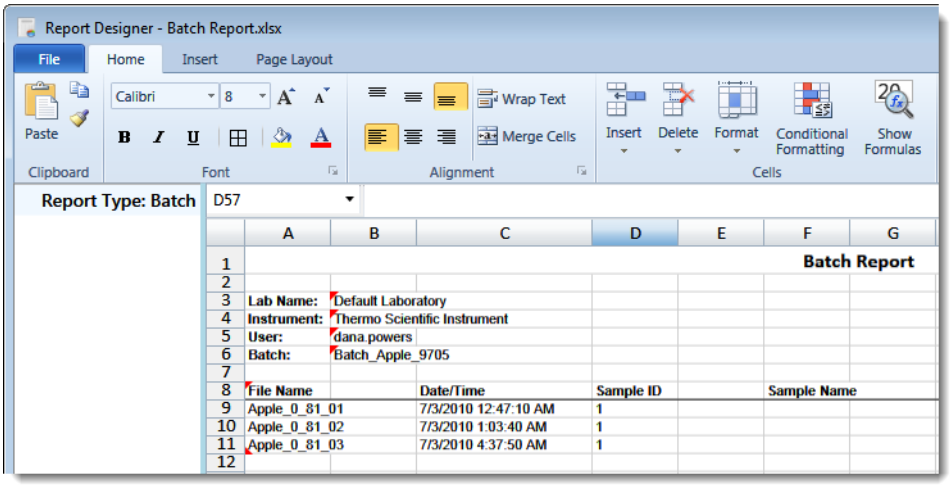
The application opens the output file.

❖ To edit a report template

1. In the Template pane, select a report template.
2. Click **Design**, Design .

   The application opens the Report Designer showing the template in an Excel spreadsheet.

   Figure 160. Report Designer showing the template for the selected report



3. Use the features in the Report Designer to edit the template.

   See "Working in the Report Designer" on page 527.

4. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

❖ To create a new report template

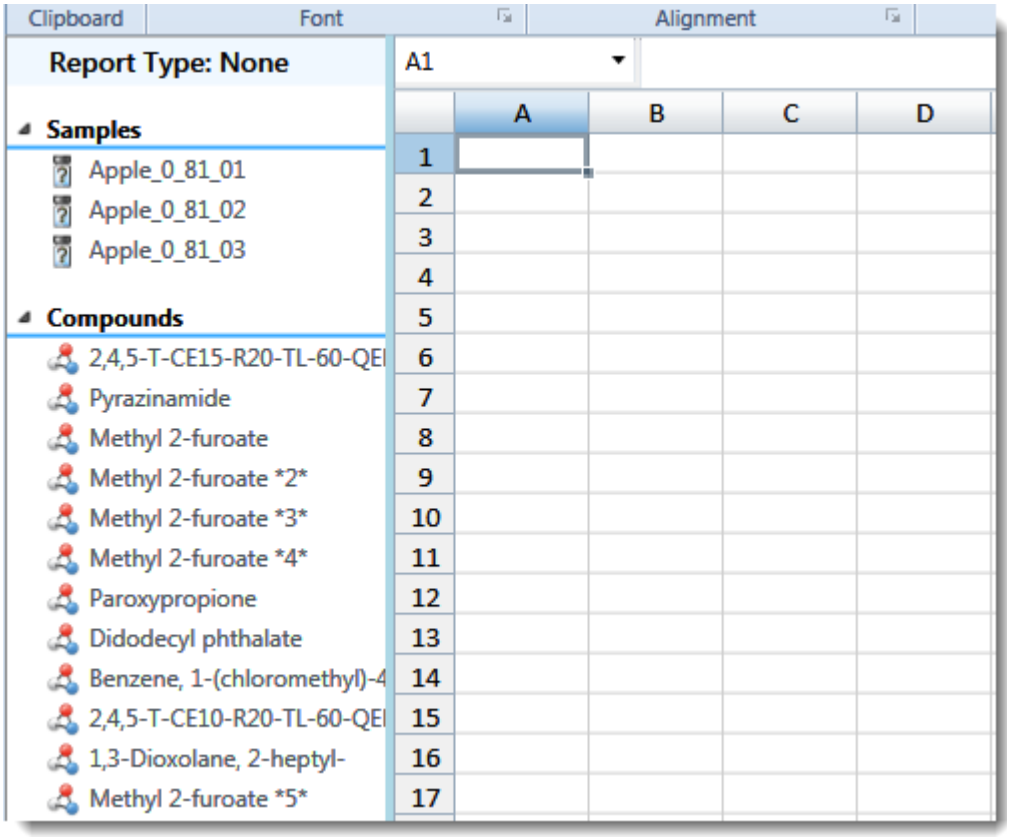
1. Click **New**, New.

   The application opens the Report Designer showing an empty template in an Excel spreadsheet.

   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 161. Report Designer showing a new, empty template



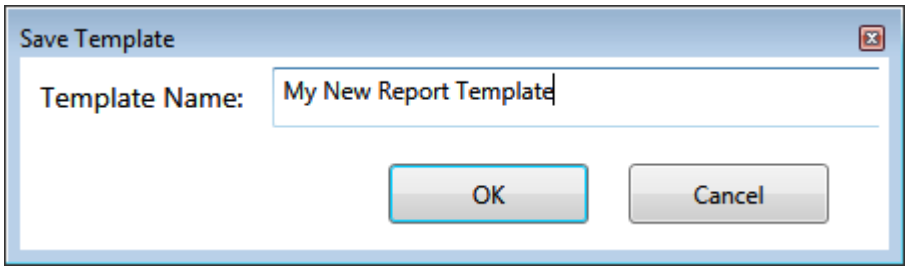
2. Use the features in the Report Designer to create the report template.

   See "Working in the Report Designer" on page 527.

3. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

   The Save Template dialog box opens.

   Figure 162. Save Template dialog box



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 163. Report View

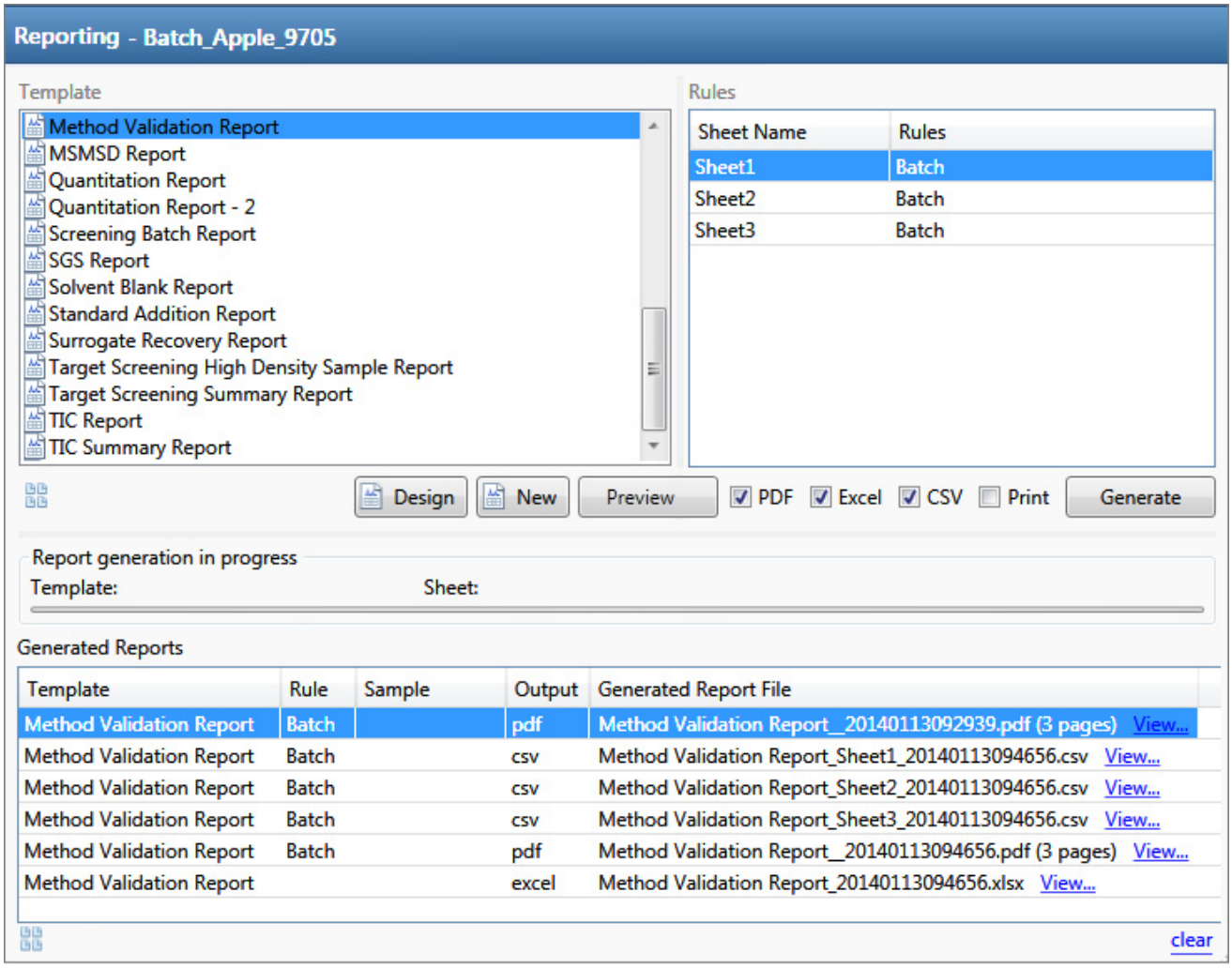


Table 109. Report View parameters (Sheet 1 of 2)

Parameter	Description
Template	
	Displays all report templates.
Rules	
Sheet Name	Specifies each sheet in the report.

Table 109. Report View parameters (Sheet 2 of 2)

Parameter	Description
Rules	Specifies the type of data used in each sheet in the selected report. • Batch • EachSample • SampleType: *SampleType* • CompoundType: *CompoundType* • SampleCustomFormula:
Buttons	
View Report Templates	Displays the C:\TraceFinderData\32\Templates\ReportTemplates folder that contains all report templates.
Design	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\32\Projects*batch*\ReportOutput folder.
Excel	Writes the generated report to a PDF file in the …\TraceFinderData\32\Projects*batch*\ReportOutput folder.
CSV	Saves the generated report as a PDF file in the …\TraceFinderData\32\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 template list" on page 521.
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\32\Projects folder.
View	Displays the generated output file.
View Generated Reports	Displays the C:\TraceFinderData\32\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\32\Projects folder.

Working in the Report Designer

Use the features in the Report Designer to create or edit report templates.

The Report Designer supports reports from previous versions of the TraceFinder application.

Use one of the Excel template files (in C:\TraceFinderData\32\Templates\ReportTemplates). Each template has an XLS file and a metadata file to support report generation. These templates can support file sizes up to 70 MB that provide the following:

- A live preview of data
- Excel-like features:
  - Formulas
  - Text formatting
  - Rich content, including images, shapes, and charts
  - User interface layout with worksheet tabs and a ribbon

To create a report, combine the output from the Report Data Manager with the template file using the Report Generator. After you have combined the data with the template, you can print, preview your print job, or create a PDF or an Excel file.

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 the Excel application.
- Add or remove graphics.
- Add repeated frames of many types.
- Format fonts, colors, and so forth.
- Add or edit formulas.
- Edit template text, headers, and so forth.

In addition to the procedures in this section, you can view video instructions at http://mytracefinder.com/plugins/reporting/.

This section includes the following topics:

- Editing a Template
- Toolbar Reference
- Quick Tips

Note To edit or create a template, you must have an open batch.

Editing a Template

Choose what type of report you want and which samples to include in the report, and then use the Report View to combine the samples and templates into a report.

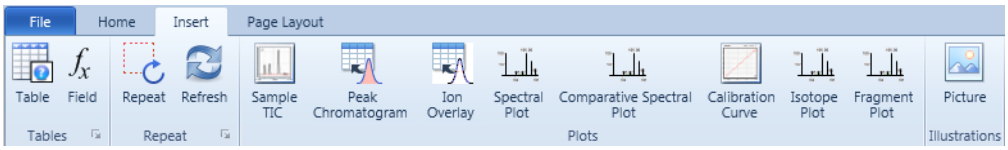
Use the following procedures:

- To insert graphics into a report template
- To insert a 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 frames

❖ To insert graphics into a report template

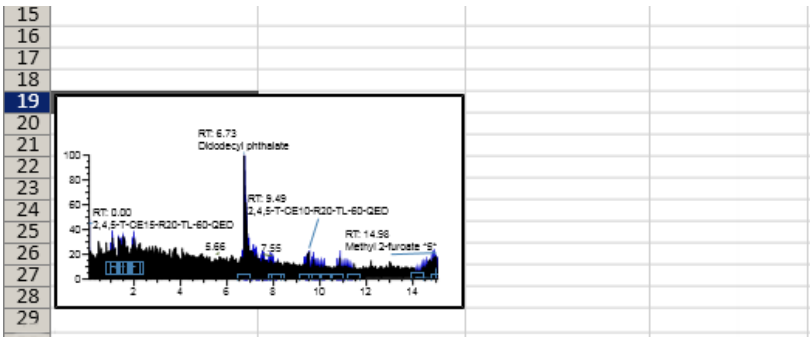
1. Select cells where you want to place the item.
2. Click the **Insert** tab.

   The Insert page displays the available objects for insertion.

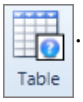


3. Select an item from the toolbar to insert into the cells on the template.
   - When you select a series of cells across rows and columns, the application inserts the item into the selected area.
   - When you select a single row of cells, the application inserts the graphic at a default size.

Figure 164. Example of inserted graphic

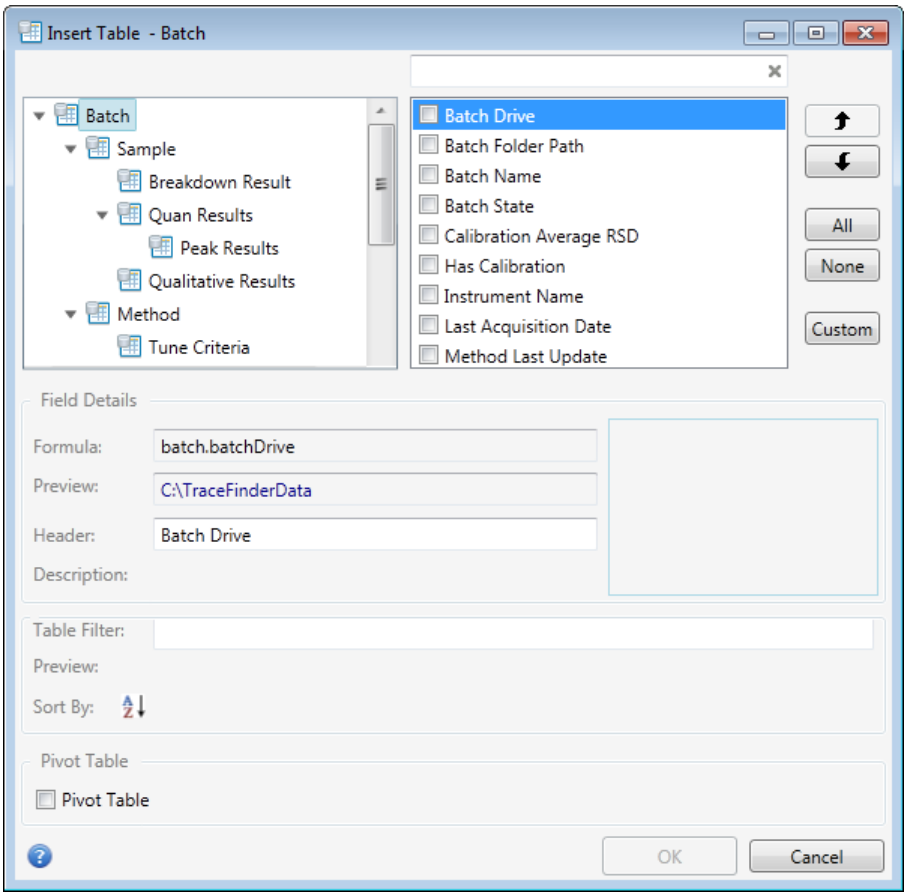


❖ To insert a table

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 Insert Table dialog box opens.



   The left pane lists choices for the type of data that you want to include in the table. You can select only one item from this list.

   The right pane lists the specific parameters that you want to include for that type of data. You can select as many parameters as you want. The table displays each selected parameter as a table column.

   For example, when you select to display data for a Sample**,** you can then select sample parameters to include in the table, such as the raw data file name or sample type.

3. Select a data item in the left pane and then select the parameters for that data type that you want to include in the table.
4. To edit the header for a table column, select the parameter in the parameters 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 parameter name.

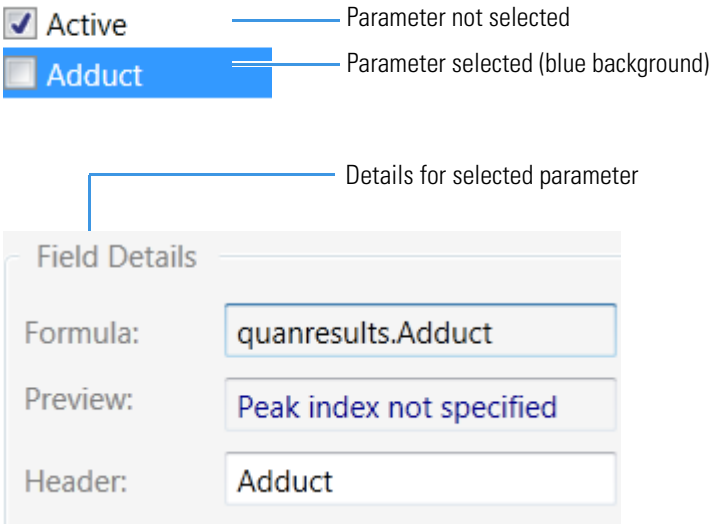
5. To move a column left or right in the table, select the parameter name and click the **Up** or **Down** arrow.

The Up arrow moves the column one position to the left.

The Down arrow moves the column one position to the right.

6. To find the formula for a parameter, select the parameter.

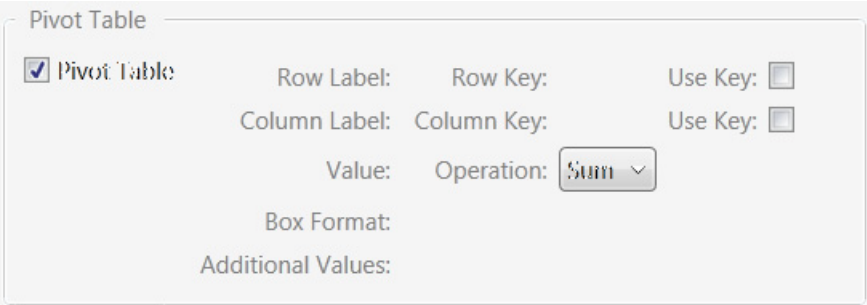
   The application displays the formula in the Formula box.



7. To switch rows to columns for easier access to large amounts of data, create a pivot table as follows:

   a. Select the **Pivot Table** check box.

      The Pivot Table area expands to display the pivot table options.



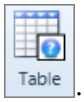
   b. Select the **Use Key** check box for the row label.

   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.

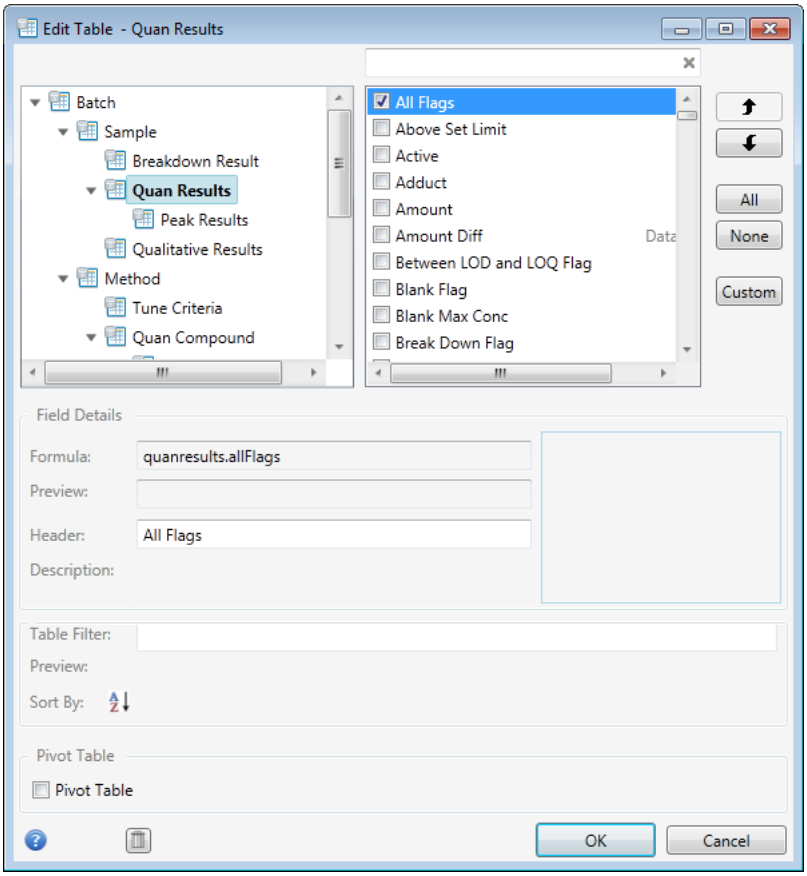
8. When you have made all your table selections, click **OK**.

❖ To make changes to a table

1. Select the table in the report template.
2. Click the **Insert** tab, and then click the **Table** icon, 

.

   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 Insert Table dialog box.



3. Edit the parameters for the table and click **OK**.

   Follow the instructions in "To insert a table" on page 529.

❖ To format header text in the spreadsheet

1. Select the header in the spreadsheet table.

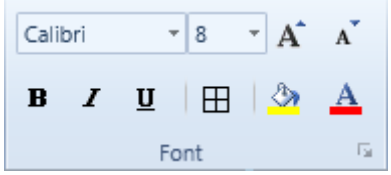
   To change all headers, select an entire header row.

   To change a single header, select only a single 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

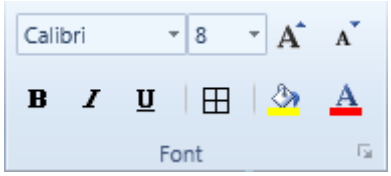
1. Select the data you want to format.

   To format all rows in a column, select only the first cell of data. Do not 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

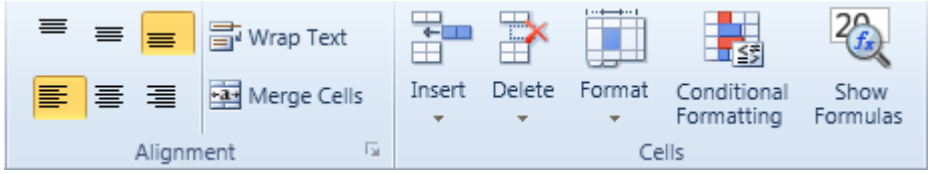
1. Select the cells you want to modify:

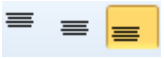
   To change all cells in a row, select the entire row.

   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  .
4. To align the cell text to the left, center, or right of the cell, click .
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**.

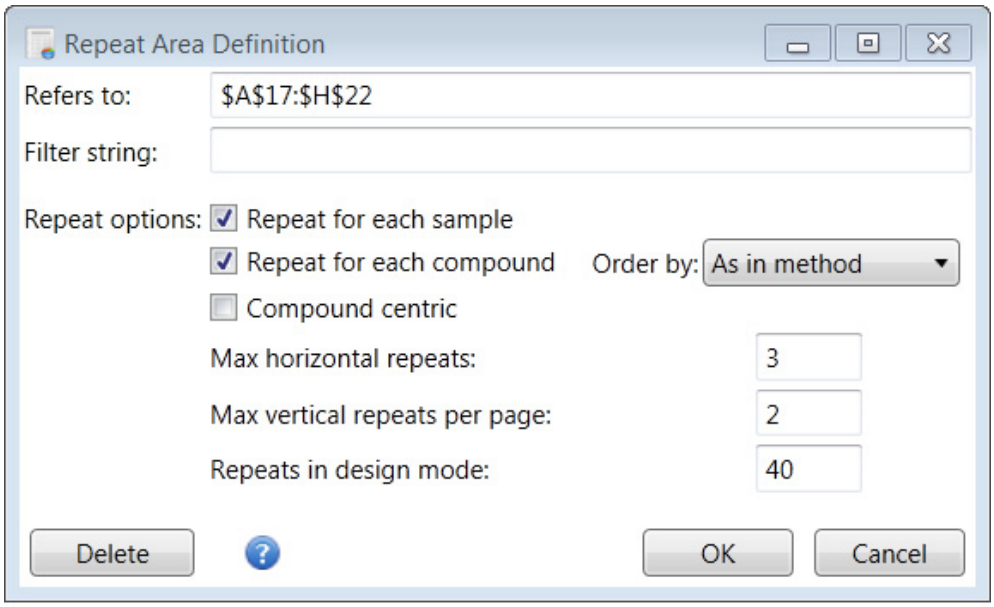
❖ To add repeated frames

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 frames" on page 535.

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 compound, for each sample, 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.

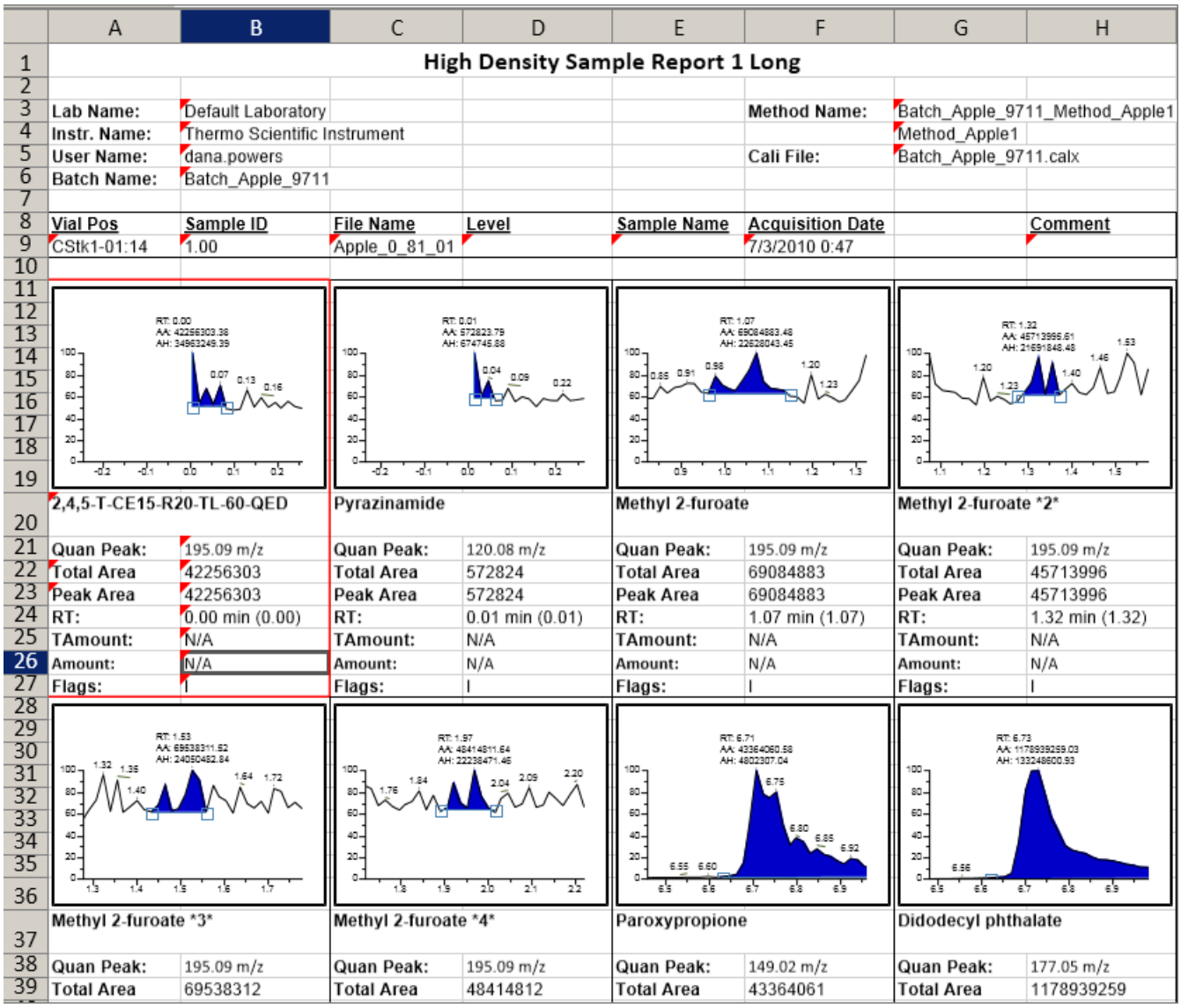
6. To define the number of times to repeat horizontally before wrapping to the next row, type a number in the Max Horizontal Repeats box.

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 increase performance. When generating an actual report, the application does not enforce this limit.

Figure 165. Example of repeated frames



	A	B	C	D	E	F	G	H
1	High Density Sample Report 1 Long							
2								
3	Lab Name:	Default Laboratory				Method Name:	Batch_Apple_9711_Method_Apple1	
4	Instr. Name:	Thermo Scientific Instrument					Method_Apple1	
5	User Name:	dana.powers				Cali File:	Batch_Apple_9711.calx	
6	Batch Name:	Batch_Apple_9711						
7								
8	Vial Pos	Sample ID	File Name	Level	Sample Name	Acquisition Date		Comment
9	CStk1-01:14	1.00	Apple_0_81_01			7/3/2010 0:47		
10								
11–19								
20	2,4,5-T-CE15-R20-TL-60-QED		Pyrazinamide		Methyl 2-furoate		Methyl 2-furoate *2*	
21	Quan Peak:	195.09 m/z	Quan Peak:	120.08 m/z	Quan Peak:	195.09 m/z	Quan Peak:	195.09 m/z
22	Total Area	42256303	Total Area	572824	Total Area	69084883	Total Area	45713996
23	Peak Area	42256303	Peak Area	572824	Peak Area	69084883	Peak Area	45713996
24	RT:	0.00 min (0.00)	RT:	0.01 min (0.01)	RT:	1.07 min (1.07)	RT:	1.32 min (1.32)
25	TAmount:	N/A	TAmount:	N/A	TAmount:	N/A	TAmount:	N/A
26	Amount:	N/A	Amount:	N/A	Amount:	N/A	Amount:	N/A
27	Flags:	I	Flags:	I	Flags:	I	Flags:	I
28–36								
37	Methyl 2-furoate *3*		Methyl 2-furoate *4*		Paroxypropione		Didodecyl phthalate	
38	Quan Peak:	195.09 m/z	Quan Peak:	195.09 m/z	Quan Peak:	149.02 m/z	Quan Peak:	177.05 m/z
39	Total Area	69538312	Total Area	48414812	Total Area	43364061	Total Area	1178939259

Toolbar Reference

The Report Designer includes three tabs that display toolbars.

- Home Toolbar
- Insert Toolbar
- Page Layout Toolbar

Home Toolbar

Use the options on the Home toolbar to modify fonts, align cell data, and format cells.

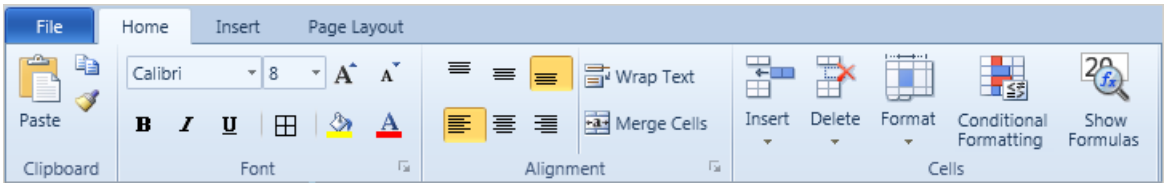


Table 110. Home toolbar options (Sheet 1 of 2)

Parameter	Description
Clipboard	
Paste	Paste the contents of the Clipboard. You can also paste only formating or only a formula.
Copy	Copy text or graphics to use in another place.
Font	
Font and size	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 font size.
Fill color	Apply color to the background for selected cells.
Font color	Change the font color.
Alignment	
	Align the cell text to the top, center, or the bottom of the cell.
	Align the cell text to the left, center, or the right of the cell.
Wrap text	Make all contents visible within a cell.
Merge cells	Join selected cells into one cell.

Table 110. Home toolbar options (Sheet 2 of 2)

Parameter	Description
Cells	
Insert	Insert cells, rows, or columns 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

Use the options on 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.

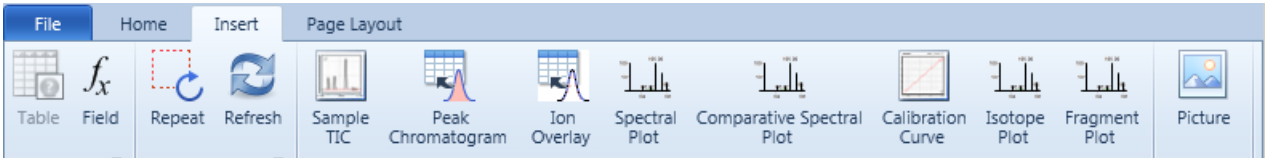


Table 111. Insert toolbar options (Sheet 1 of 2)

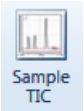
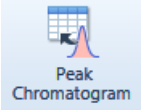
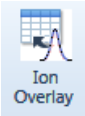
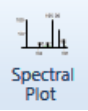
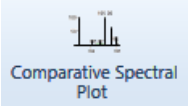
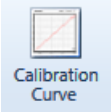
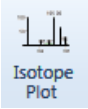
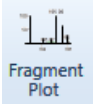
Parameter	Description
Table	
Table	Create a table to manage and analyze data.
Field	Edit the formula for a field by choosing functions and editing arguments.
Repeat	
Repeat	Repeat text, cell, or graphic elements.
Refresh	Update the view to reflect recent changes.
Plots	
	Add a sample TIC.
	Add a peak chromatogram.

Table 111. Insert toolbar options (Sheet 2 of 2)

Parameter	Description
	Add an ion overlay.
	Add a spectral plot.
	Add a comparative spectral plot.
	Add a calibration curve.
	An isotope plot displays the number of isotopes found, the score, a pass/fail flag, and a plot of the isotopes.
	Add a fragment plot.
Illustrations	
Pictures	Insert a picture from a file.

Page Layout Toolbar

Use the options on the Page Layout toolbar to adjust margins, orientation, paper size, and page breaks. To see your changes, click **Print Preview**.

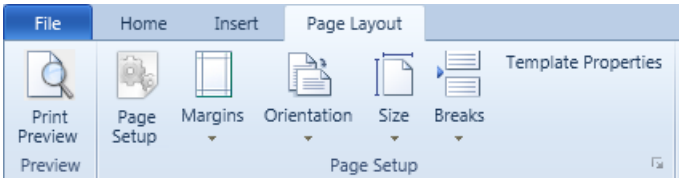


Table 112. Page Layout toolbar options (Sheet 1 of 2)

Command	Description
Print Preview	View your report as the application will print it.
Page Setup	Define page details.
Margins	Select page margins for the current view or the entire document.

Table 112. Page Layout toolbar options (Sheet 2 of 2)

Command	Description
Orientation	Switch the pages from portrait to landscape view.
Size	Choose a page size for the current view or the entire document.
Breaks	Specify where a new page begins in the printed copy.
Template Properties	Opens the SpreadsheetGear Workbook Explorer where you can specify template options.

Quick Tips

❖ To insert items in 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 on the same row as a table.

The Insert toolbar provides these options:

  - Table – insert or edit data table
  - Field – insert or edit data field

- 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, then click **A-Z** to sort on that field.

9

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 550.

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*.

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\3.2\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\32\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\32\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\32\Projects*SubFolder**BatchName*\AuditLog.adb.

The Audit Viewer displays all saved audit log files, and you can filter and sort the audit data.

Use the following 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, .

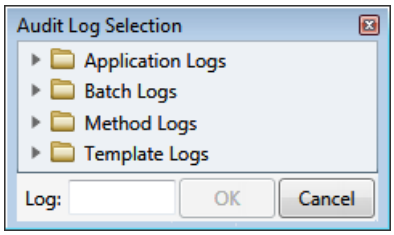
The Audit Viewer opens. For detailed descriptions of parameters in the Audit Viewer, see "Audit Viewer" on page 550.

> **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

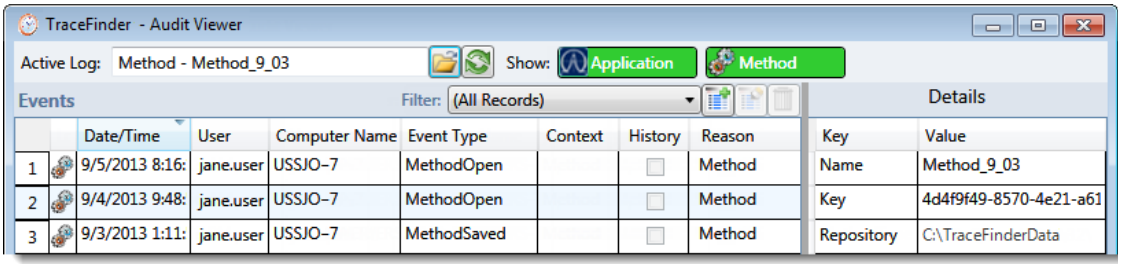
1. Click the **Open Audit Log** icon, .

   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.

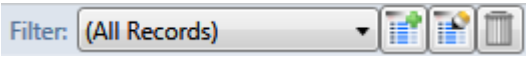
2. Click an icon to turn the display on or off.

   In this example, the Events pane displays Batch and Method events and hides Application events.

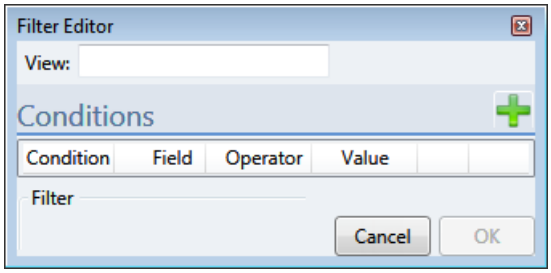
   Note There is no icon for security events in an application log file. You cannot hide the display of security events.

❖ 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.

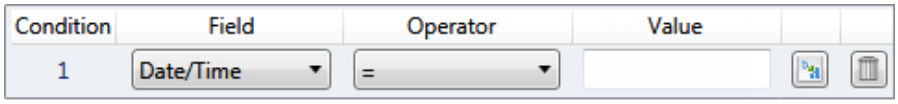
   

2. In the View box, type a name for the new filter.

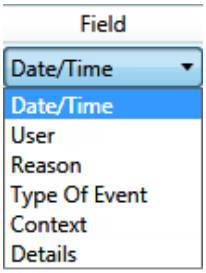
   You can also leave the View box empty when you enter your filter criteria. When you finish adding conditions and click OK (step 8), the application filters the current events list based on the filter criteria you specify, but the filter is not saved. The Filter list in the viewer identifies this filter as (Custom).

3. Click the **Add** icon, .

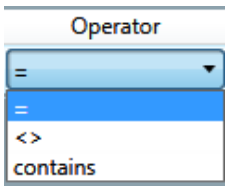
   The application adds a new, undefined condition to the Condition list.

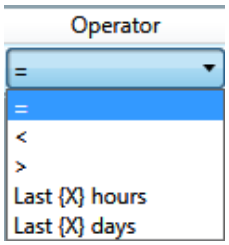
   

4. In the Field list, select one of the following field types.



5. In the Operator list, select one of the available operators.

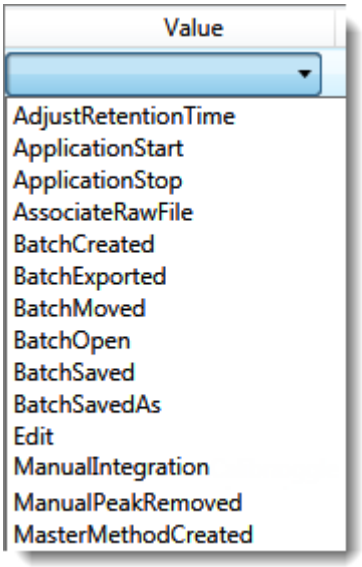


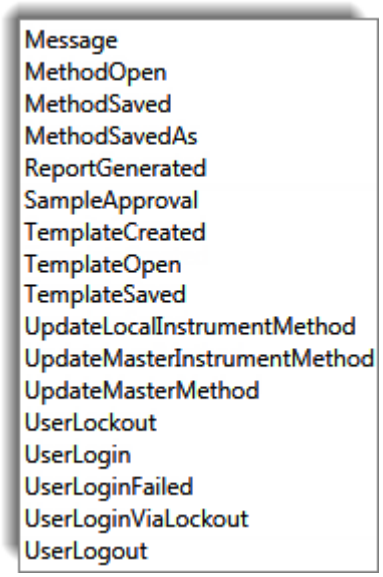


The available operators depend on the field type that you selected.

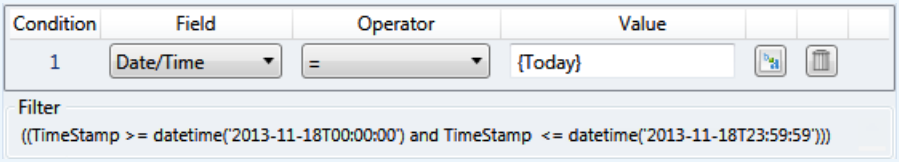
6. In the Value box, type a value or select a value from the list.

- 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.

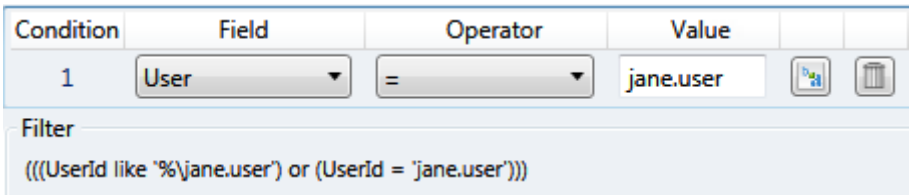




Note You can also click the Tokens icon, , and select a token for the Value. Tokens are predefined values, such as dates and sample or compound identifiers.



The Filter at the bottom of the dialog box displays the complete definition for the filter.



7. Repeat steps 3 through 6 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.

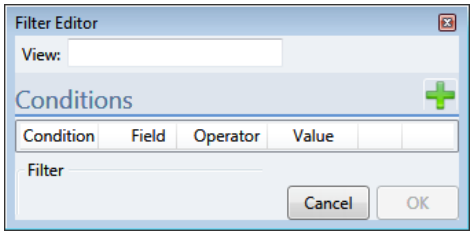
Details for Application log files include whether the events are for a batch or method, the location of the data repository, and, for a batch, the subproject folder where the batch was created.

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.

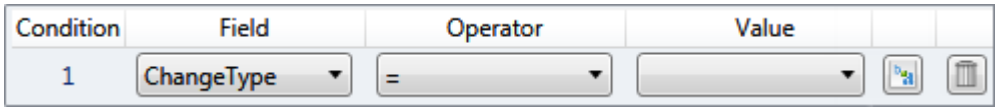


2. In the View box, type a name for the new filter.

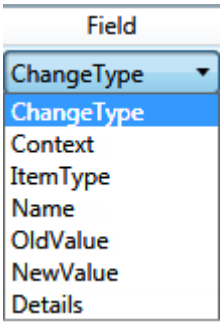
   You can also leave the View box empty when you enter your filter criteria. When you finish adding conditions and click OK (step 8), the application filters the current history list based on the criteria you specify, but the filter is not saved. The Filter list in the viewer identifies this filter as (Custom).

3. Click the **Add** icon, .

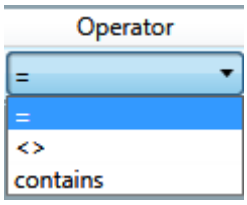
   The application adds a new, undefined condition to the Conditions list.



4. In the Field list, select one of the following field types.

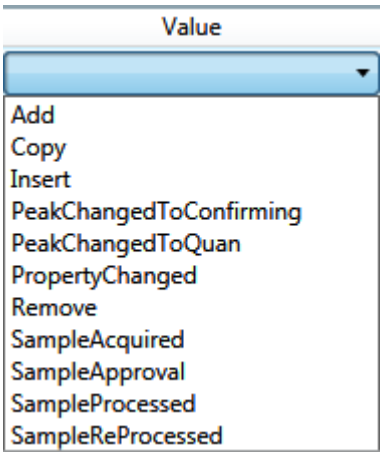


5. In the Operator list, select from ***equals***, ***less than/greater than***, or **contains**.

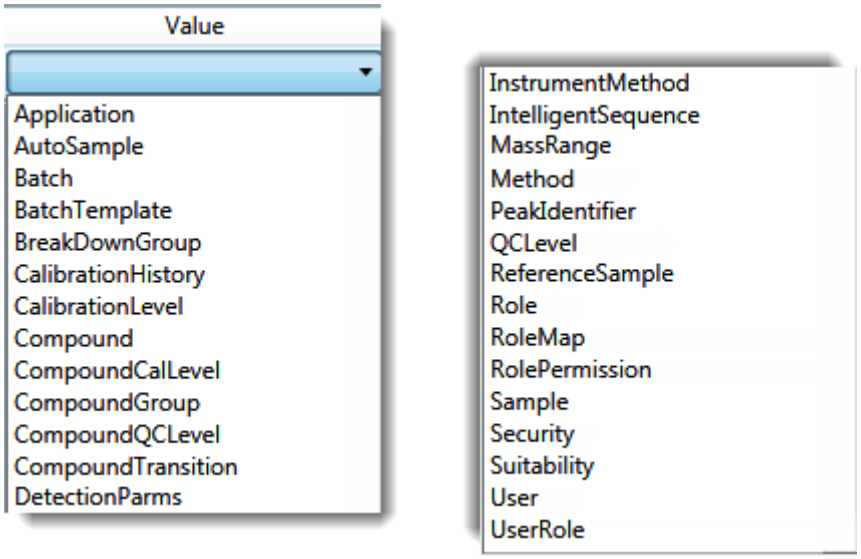


   The available operators depend on the field type that you selected.

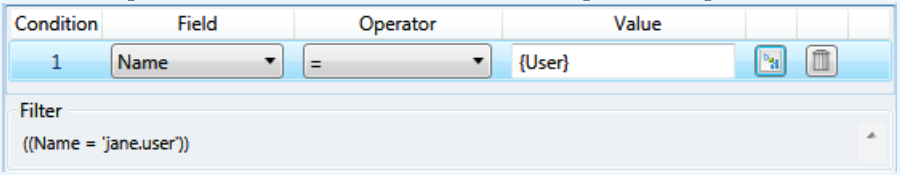
6. In the Value list, type or select a value from the list.
   - For the Name, Context, or Details field, type the appropriate text in the Value box. This value is case sensitive.
   - For the OldValue or NewValue field, type a numerical value in the Value box.
   - For the ChangeType field, select one 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.

Condition	Field	Operator	Value
1	ChangeType	=	PropertyChanged

Filter

((ChangeType = 'PropertyChanged'))

7. Repeat steps 3 through 6 for each condition that you want to include in your filter.
8. 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

1. In the Events pane, select an event that has a selected check box in the History column.

Event Type	Context	History	Reason
BatchOpen		☐	Batch
BatchCreated		☐	Batch
BatchSaved		☑	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)

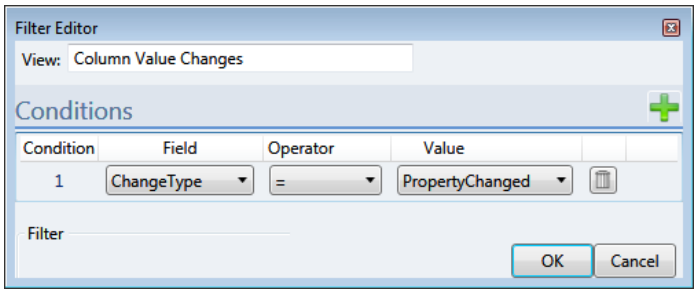
	Order	Change Type	Context	Item Type	Item Name	Old Value	New Value
1	1	Add	Unknown2	Sample	n/a	n/a	1
2	2	Add	Unknown3	Sample	n/a	n/a	2
3	3	Add	Unknown4	Sample	n/a	n/a	3
4	4	PropertyChanged	Apple_0_81	Sample	RawFileName	Unknown1	Apple_0_81_01
5	5	PropertyChanged	Apple_0_81	Sample	SampleID		1
6	6	PropertyChanged	Apple_0_81	Sample	VialPosition		CStk1-01:14
7	7	PropertyChanged	Apple_0_81	Sample	BarcodeExpected		2134

2. 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 546.

Figure 166. 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.

Figure 167. Application log in the Audit Viewer

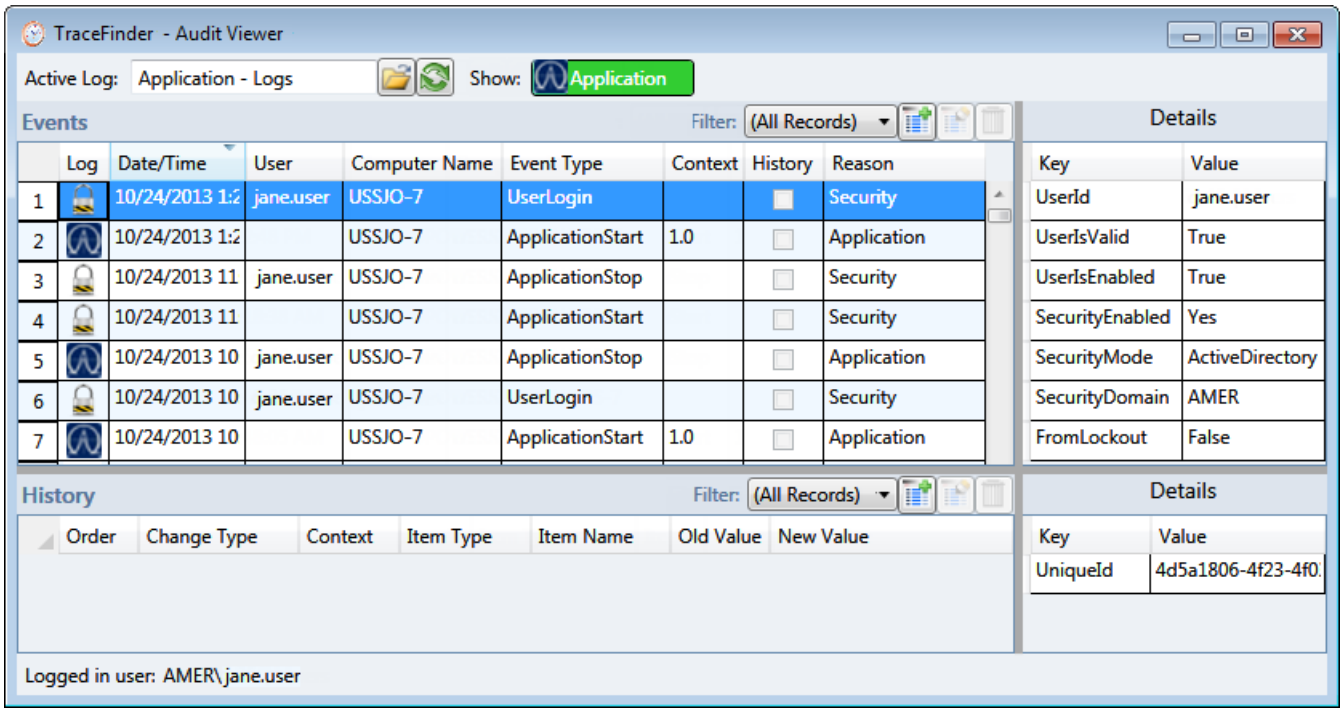


Figure 168. Batch log in the Audit Viewer

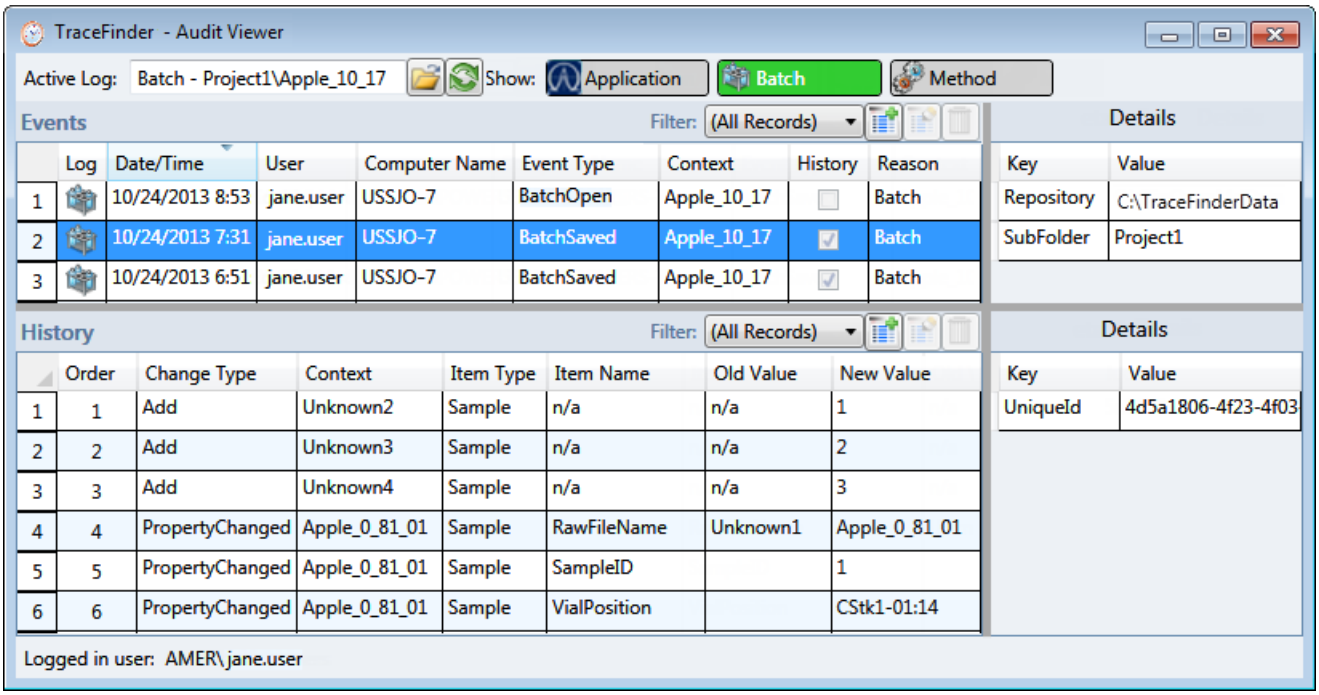


Table 113. Audit Viewer parameters (Sheet 1 of 2)

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. 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	Indicates an event that occurred at the main TraceFinder 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), *User* is the user who confirmed each change to a batch, method, or template. When no confirmation is required, *User* 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 *TraceFinder Administration Console User Guide*.
Context	Name of the sample, batch, method, or application version where the event occurred.

Table 113. 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	Select a filter view to use for displaying the change history. 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 history filter view.
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

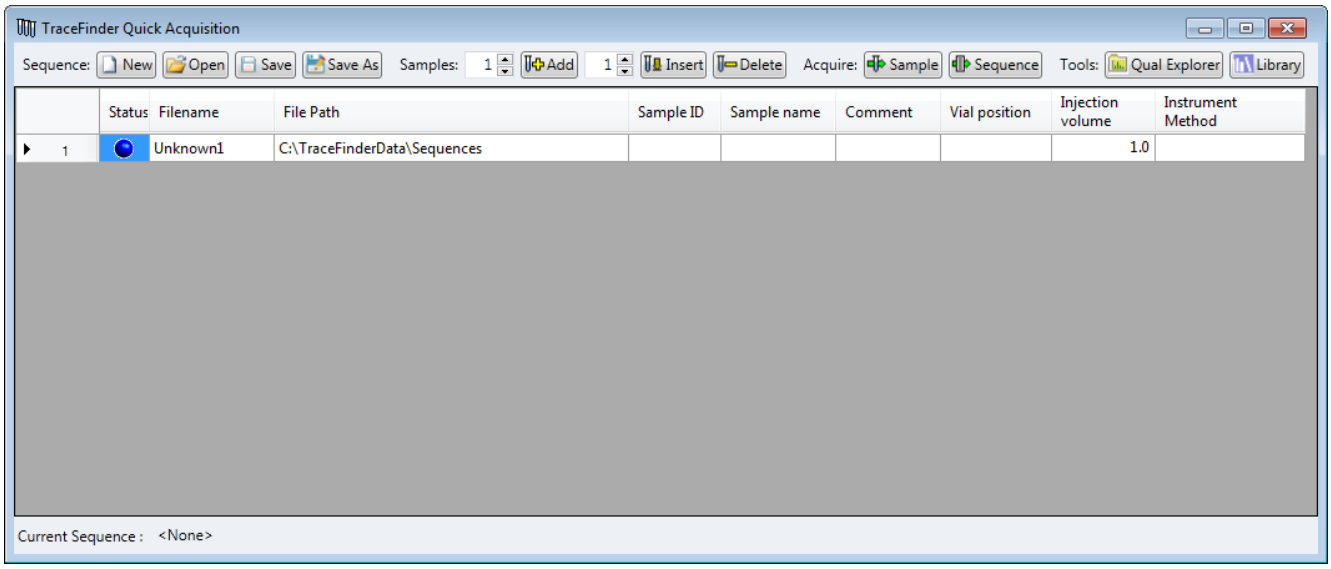
Use the quick acquisition feature to quickly submit samples from any mode in the application.

Note The Quick Acquisition feature is available only when you activate it in the Configuration console. See "Quick Acquisition" on page 56.

❖ To run a quick acquisition

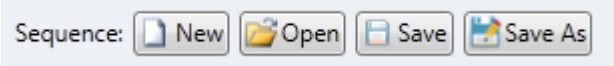
1. Choose **Tools > Quick Acquire Sample** from the main menu or click the **Quick Acquire Sample** icon, .

   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 on the toolbar to open and save Xcalibur sequence (.sld) files.



Icon	Description
New	Replaces the current sequence with a new sequence that contains one Unknown sample.
Open	Opens the Open dialog box where you can open a saved SLD file.
Save	Saves the current sequence as an SLD file in the C:\TraceFinderData\Sequences folder.
Save As	Opens the Save As dialog box where you can save the current sequence to a new file name or location.

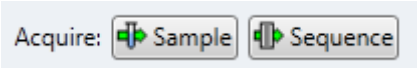
- Use the Samples buttons on the toolbar to create a sequence of samples.

Icon	Description
1 Add	Adds the specified number of new, empty samples to the end of the sample list.
1 Insert	Inserts a new, empty sample or samples above the selected sample.
Delete	Removes the selected samples from the sample list.

- (Optional) Use the Tools buttons on the toolbar to open a qualitative browser or the NIST library browser.

Icon	Description
Qual Explorer	Opens the qualitative explorer that you configured as your default qualitative explorer in the Configuration console. See "Launching a Qualitative Explorer" on page 16.
Library	Opens the NIST library browser. See "Launching the NIST Library Browser" on page 15.

3. When you have completed your sequence of samples, click either of the Acquire buttons.



Icon	Description
Sample	Submits only the selected samples for acquisition, processing, or report generation.
Sequence	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 351.

B

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 114. 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 114. 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: ^{1}H, ^{12}C, ^{14}N, ^{16}O, ^{19}F, ^{31}P, and ^{32}S

- A1 represents the isotope where one atom in the molecule is statistically replaced by another atom approximately 1 amu heavier.

  For example: ^{2}H, ^{13}C, ^{15}N, ^{17}O, and ^{33}S

- 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: ^{18}O and ^{34}S

- 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–

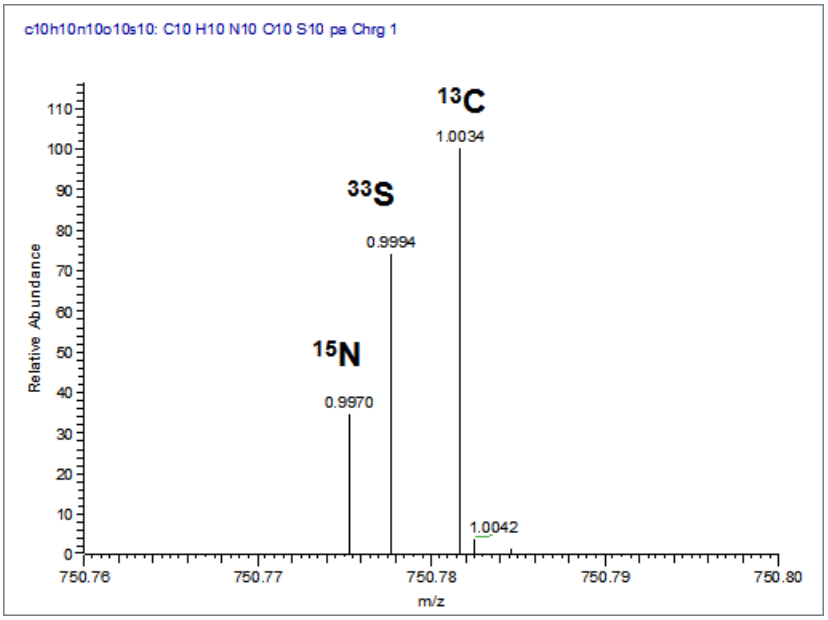
  One atom is replaced by another atom approximately 4 amu heavier.

  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.

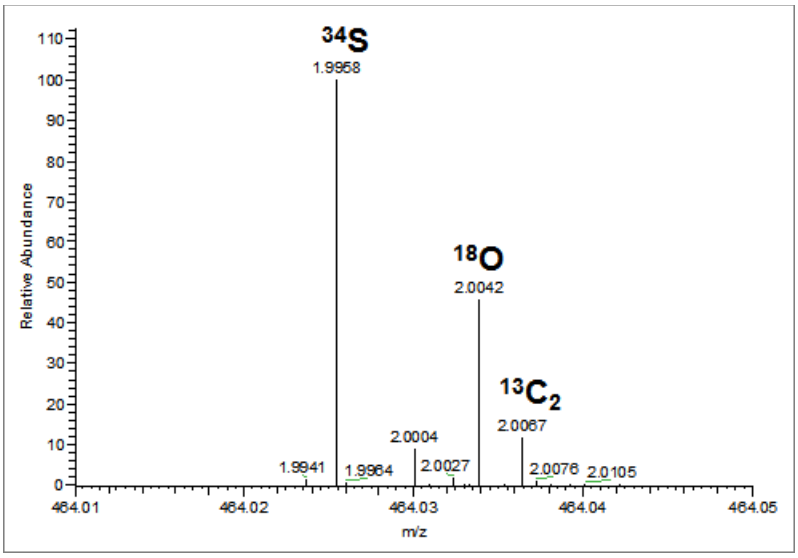
In the following figure, the *x* axis shows the mass difference of A1 relative to the monoisotopic peak (A0) of the ^{13}C, ^{15}N, and ^{33}S isotopes. The *y* axis shows relative abundance in intensity.

Figure 169. Mass difference and abundance of A1 relative to A0



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 $^{13}C2$ isotopes. The *y* axis shows relative abundance in intensity.

Figure 170. 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 557, 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 a 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 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 C8H14N4OS and its adduct is H, so the modeled isotopic pattern is C8H15N4OS.

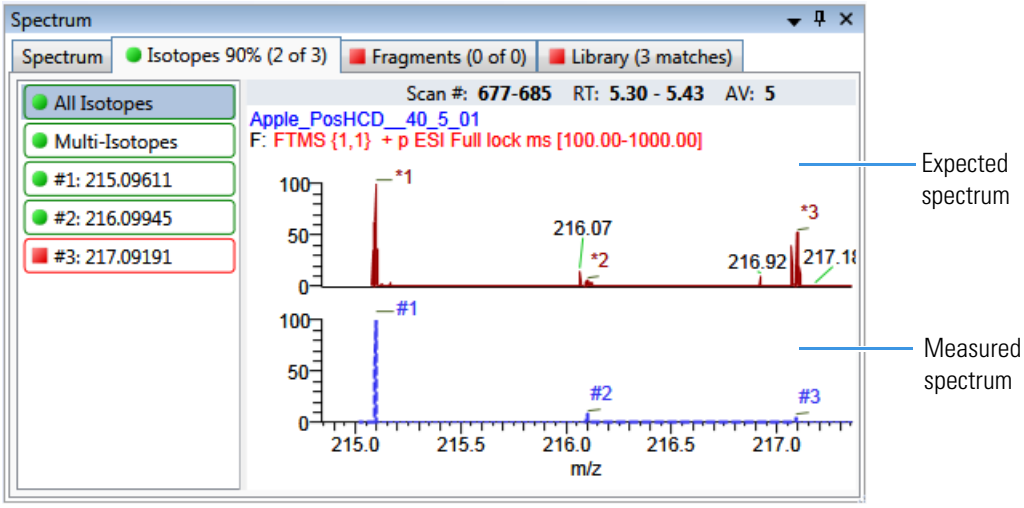
Figure 171. Isotopic data for Metribuzin

Compounds

	Selected	Compound Name	Formula	Isotopic Pattern Score (%)	Num Isotopes Matched
	Aa	Aa	Aa	=	Aa
640		Metribuzin	C8H14N4OS	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 172. 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.

Noise threshold (expected) = *Noise of A0 (measured)* × *Intensity of A0 (expected)* ÷ *Intensity of A0 (measured)*

Following the previous formula, the expected noise threshold is 1482 × 8.55E5 ÷ 4.75E4 = 2.6676E4.

The expected ions in the measured spectrum are those whose intensities are above the expected noise threshold. The following tables lists the ions in the expected spectrum. A "✓" in the Above Threshold column indicates the expected ions.

Table 115. 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 116. Mass deviation data for the expected ions

Isotope order	*m/z* (expected)	*m/z* (measured)	Delta *m/z* (ppm)
A0	215.09611	215.09602	–0.42
A1	216.09945	216.09879	–3.05
A2	217.09191	217.09712	24

where:

Delta *m/z* (ppm) = 1 000 000 × ([*m/z (measured)* – *m/z (expected)*] ÷ *m/z (expected)*)

For example:

1 000 000 × ([216.09879 – 216.09945] ÷ 216.09945)] = –3.05 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 562) 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 562) 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 117. Intensity deviation data for the expected ions

Isotope order	*m/z* (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 562). Each value is a percentage of the isotope's intensity relative to the A0 ion's intensity.

  For example: 7.50E4 ÷ 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 564) 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 565).

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 173. Measured and expected patterns

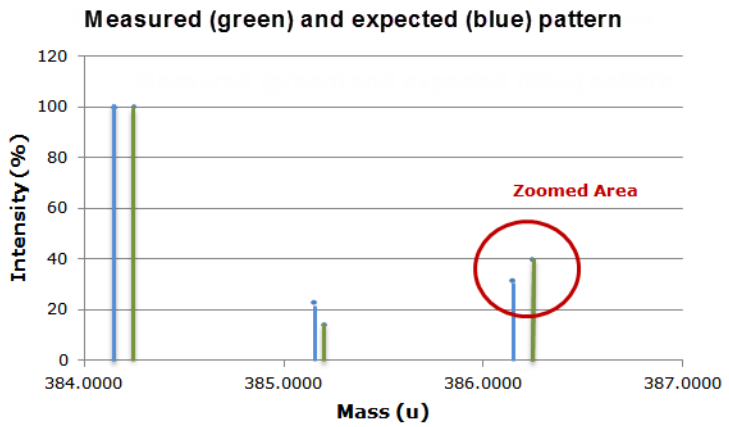
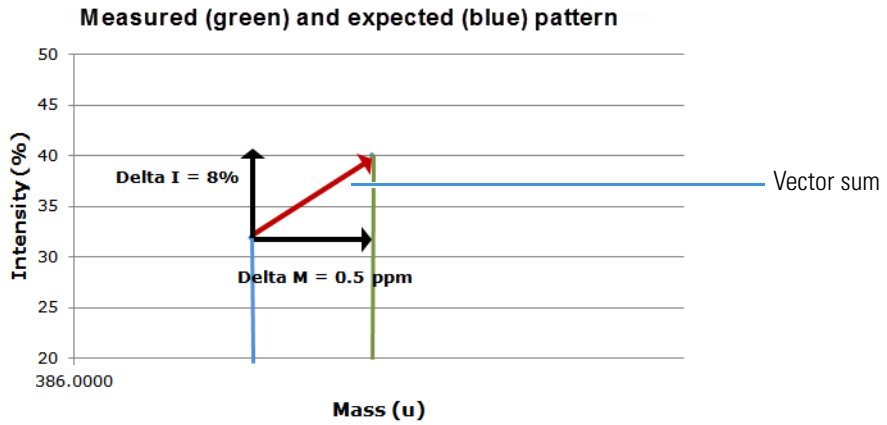


Figure 174. Vector sum of intensity (I) and mass (M) deviations



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 565, 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 118. 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 ÷ 10 = 0.0
A1	216.09945	9.65	10	9.65 ÷ 10 = 0.965
A2	217.09191	68.54	10	68.54 ÷ 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 to 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.

- [absolute value (*Delta m/z*) – 2 ppm] ÷ (5 ppm – 2 ppm) if absolute value (*Delta m/z)* ≥ 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 119. Normalized mass deviation for each of the expected ions

Isotope order	*m/z* (expected)	*m/z* (measured)	Delta *m/z* (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)] ÷ (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 [(*Normalized intensity deviation*)^2 + (*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 120. Calculated vector sum

Isotope order	*m/z* (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 121. 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 ÷ 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 120 on page 568)to be replaced with the penalty value of 1 (in Table 122). 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 122. 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 × 0.0774 = 0.0774

- Isotopic pattern score = 100% × (1.0 – *Sum of all weighted deviation values*)

  For this example, the calculated isotopic pattern score of 100% × (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

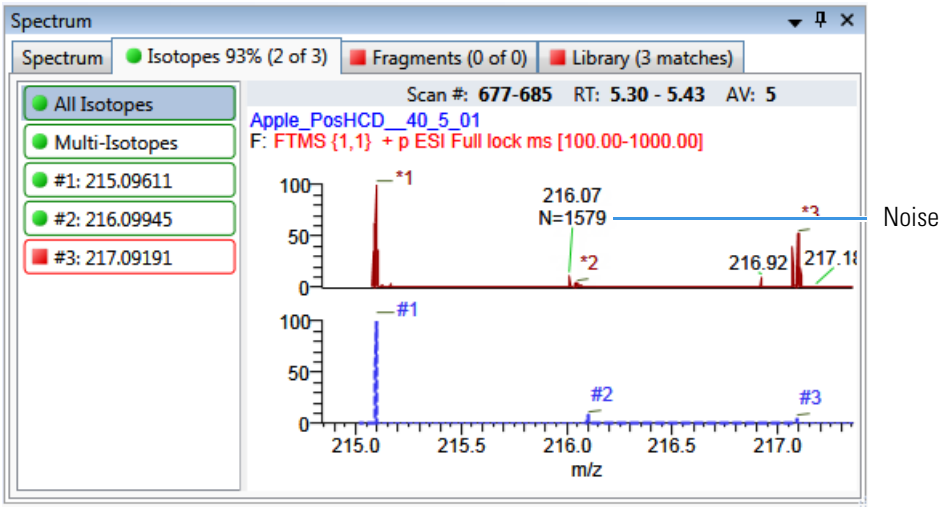
❖ **To find the noise value associated with a mass spectral peak**

1. On the Isotopes page of the Spectrum pane, to view the expected spectrum stacked above the measured spectrum, 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 562 for the compound **Metribuzin**.

3. To view the averaged noise value (N) for a peak in the measured spectrum, right-click the spectrum plot area and choose **Show Noise Label** from the shortcut menu.



In this example, the averaged noise value for the peak is 1579.

C

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.

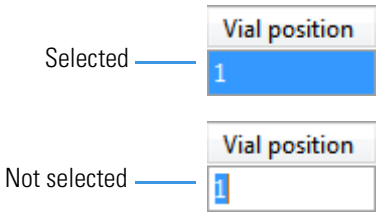
Follow these procedures:

- 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.

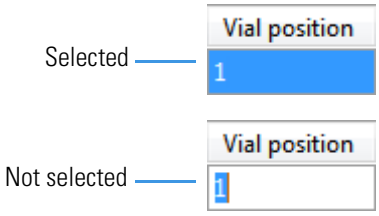
❖ To automatically enter sequential column values

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 TraceFinder application knows the number of vial positions configured in your autosampler and numbers the positions accordingly.

Vial position
A:A1
A:A2
A:A3
A:A4
A:A5
A:A6
A:B1
A:B2
A:B3
A:B4
A:B5
A:B6

❖ To use Copy Down or Fill Down for a range of samples

1. To select a range of sample values, do one of the following:

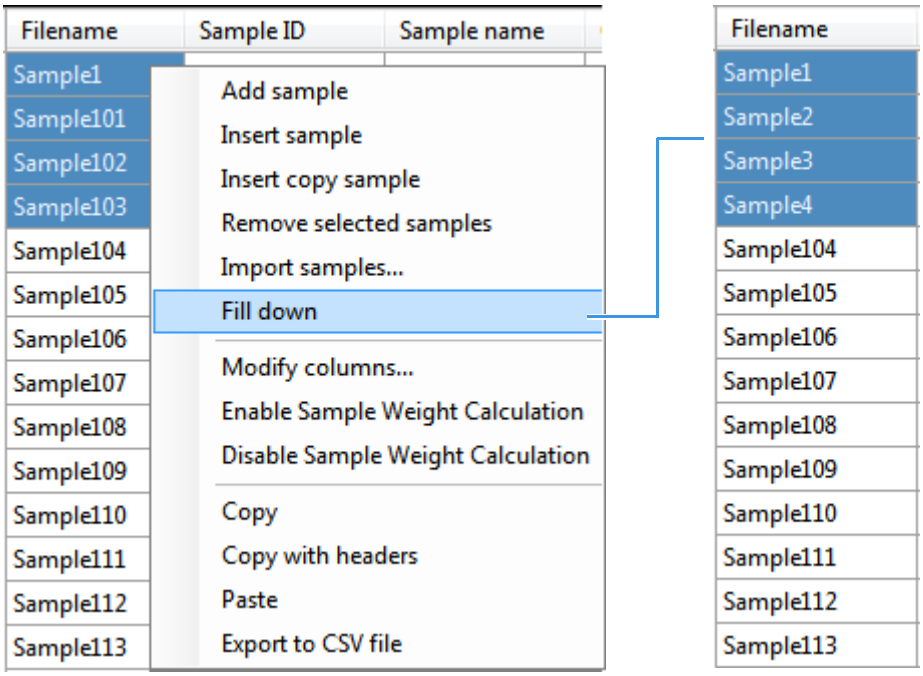
   Drag your cursor to select a contiguous group of sample values.

   –or–

   Hold down the SHIFT key to select a contiguous group of sample values.

2. Right-click and choose the appropriate command from the shortcut menu.

   The column values are copied or entered sequentially starting with the value in the first selected row and ending with the last selected row.



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