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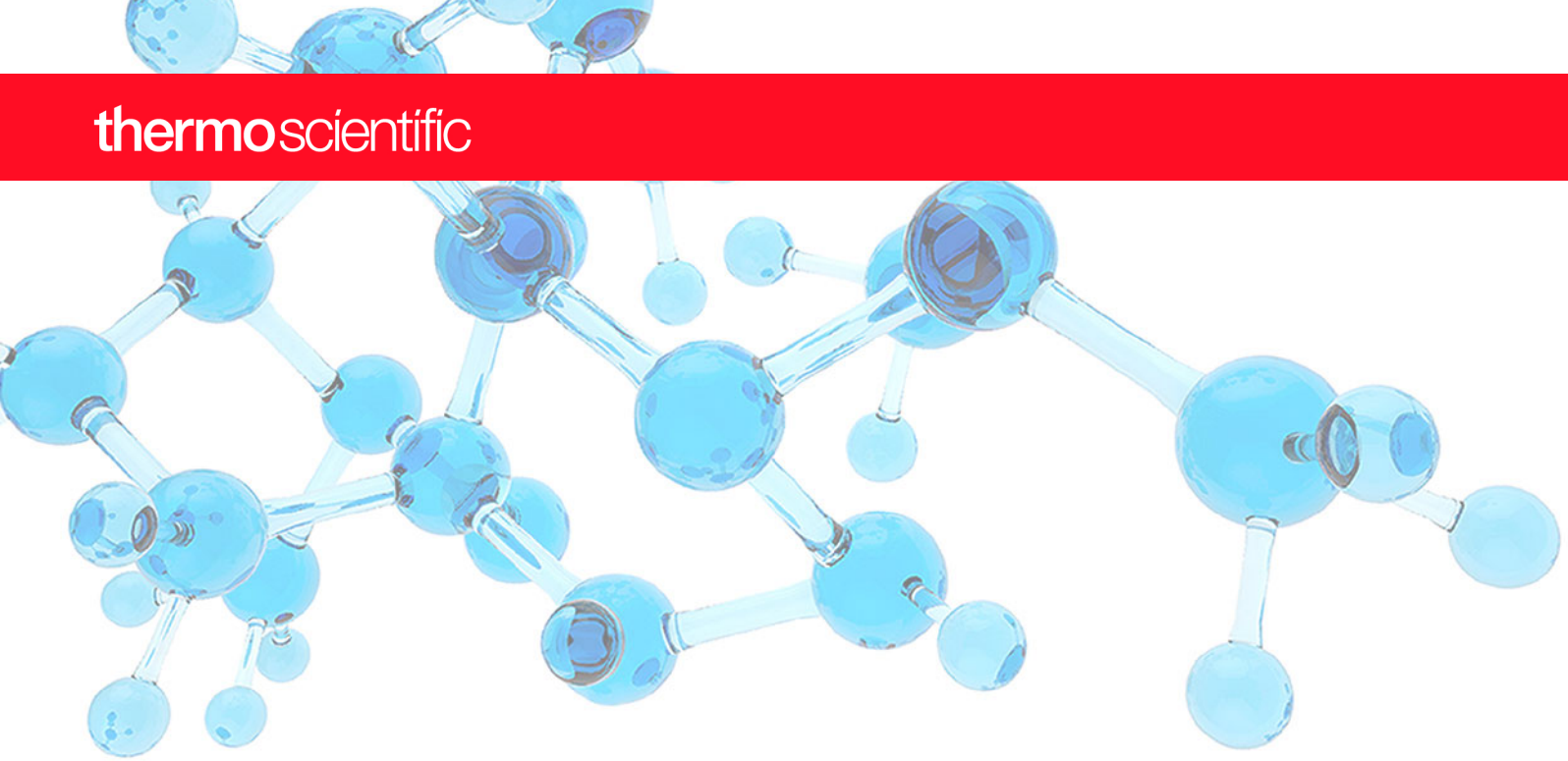

Thermo

TraceFinder

User Guide

Software Version 5.3
Optimized for General Quantitation

B51008907 Revision A • December 2025

ThermoFisher SCIENTIFIC

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Preface

This guide describes how to use the Thermo TraceFinder™ 5.3 application with compatible Thermo Scientific™ GC/MS and LC/MS analytical instruments.

Contents

- Accessing documentation
- Special notices
- Contacting us
- License activation and deactivation
- TraceFinder Help Desk

Accessing documentation

The product software comes with Help files that explain how to navigate the user interface. Full documentation is maintained in the Thermo Scientific Chromatography and Mass Spectrometry portal. This doc portal is regularly updated with the latest content, including video tutorials.

To access the latest help documentation, visit https://docs.thermofisher.com/home.

Tip (Animation) To view "Where are My Manuals?," see **Help > Animations**.

View the TraceFinder documentation

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

–or–

- From the application, choose **Help > Manuals**.

View manuals from the website

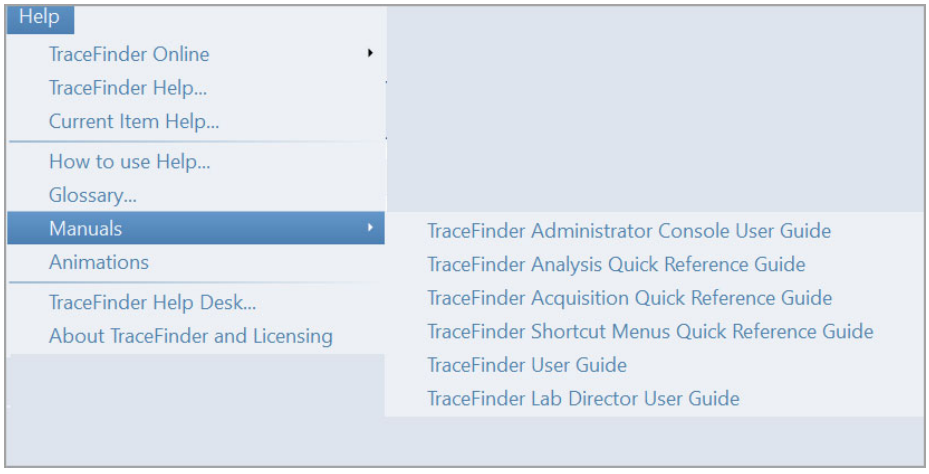
1. Go to thermofisher.com.
2. Point to **Support**.
3. On the left, click **Manuals**.
4. In the Search box, search by the product name.
5. From the results list, click the title to open the document or animation in your web browser.

   To return to the document list, click the browser **Back** button.

Open the TraceFinder Help

1. Open the TraceFinder application and choose **Help > TraceFinder Help**.
   - To find a particular topic, use the Contents or Search panes.
   - To create your own bookmarks, use the Favorites pane.
2. To view the user guides or 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.

View TraceFinder Animations

1. From the Thermo TraceFinder application, choose **Help> Animations**.

   Thermo TraceFinder Animations web browser opens. Select a particular animation topic from the drop drown list.

2. To view the animation select, **click to see the animation**.

Special notices

Make sure you follow the special notices presented in this guide. Special notices appear in boxes; those concerning safety or possible system damage also have corresponding caution symbols.

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

Contact	Email	Telephone	QR Code
U.S. Technical Support	us.techsupport.analyze@thermofisher.com	(U.S.) 1 (800) 532-4752	
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License activation and deactivation

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

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

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

Two types of licenses are available:

- 120-Day Evaluation Version (free of charge)
- Full Version 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 during or after the free evaluation without reinstalling the software.

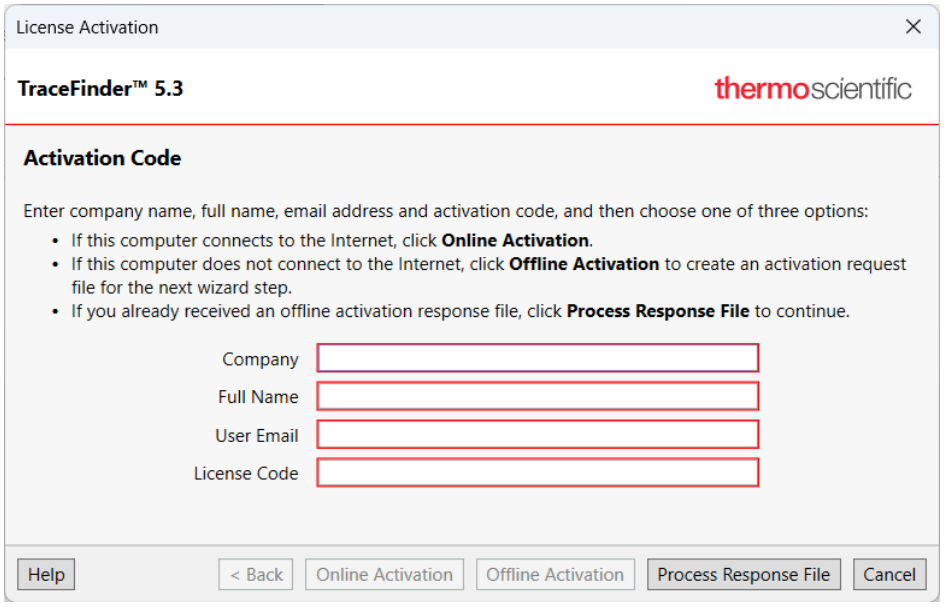
Each activation key is valid for two licenses. Any additional installation generates a different license and requires a different activation key. For software download and licensing questions, contact support at ThermoMSLicensing@thermo.com.

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

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

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

   The License Activation wizard opens.



4. Follow the instructions in the License Activation wizard.

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

TraceFinder Help Desk

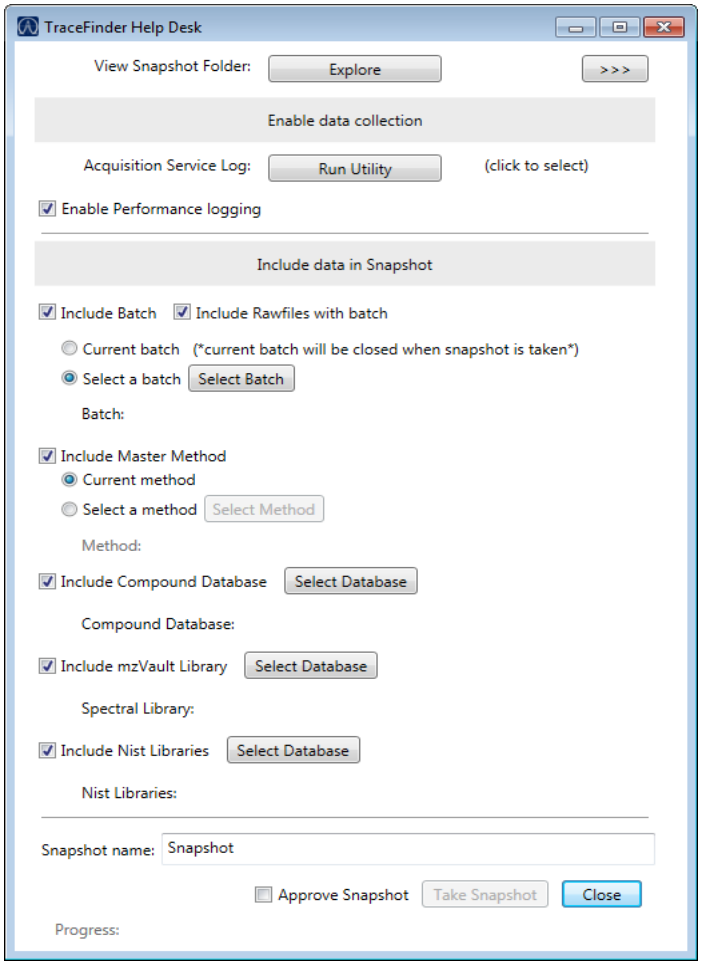
Use the Help Desk to create a snapshot of how the TraceFinder application operates and performs. Then send the resulting zipped data file to the TraceFinder product support team.

Follow these procedures:

- Open the TraceFinder Help
- To view the contents of the Snapshots folder
- To enable data collection
- To log system performance, select the **Enable Performance Logging** check box.
- To capture a snapshot
- To monitor the snapshot status
- To submit a help request

v **To open the TraceFinder Help Desk**

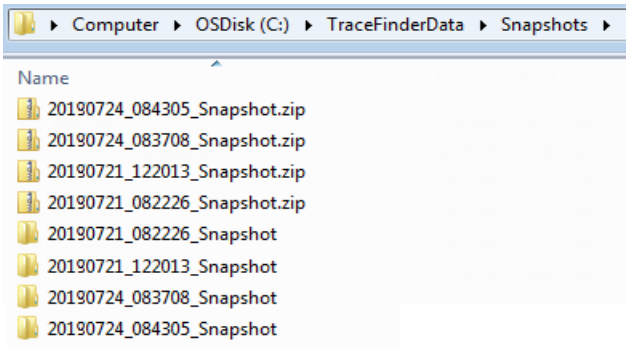
1. Choose **Help > TraceFinder Help Desk.**



v **To view the contents of the Snapshots folder**

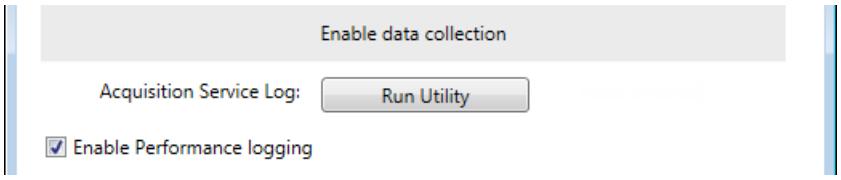
- Click **Explore**.

  The application opens the Snapshots folder. The Snapshots folder includes any snapshot folder that you previously collected and its zipped version.



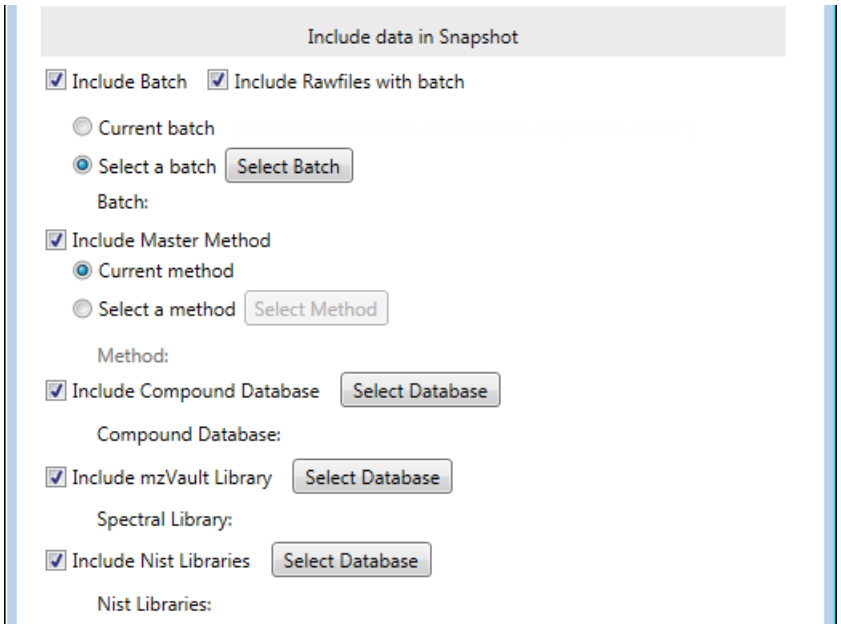
For information about the repository folder where the application creates the Snapshots folder, refer to Chapter 2, "Using the Repository View," in the *TraceFinder Administrator Console User Guide*.

v **To enable data collection**



1. Click **Run Utility**.
2. In the Acquisition Service Tracking dialog box, click **Enable Tracking** and close the dialog box.
3. To log system performance, select the **Enable Performance Logging** check box.

v **To specify data in the snapshot**

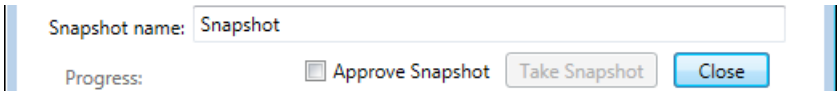


1. To specify the batch data to include in the snapshot, do the following:
   a. Select the **Include Batch** check box.
   b. If you want to include all the raw data files with the snapshot, select the **Include Rawfiles with Batch** check box.
   c. Select to include the current batch, or click **Select Batch** and choose the batch to include.
2. To specify the master method data to include in the snapshot, do the following:
   a. Select the **Include Master Method** check box.

b. Select to include the current method, or click **Select Method** and choose the method to include.

3. To specify the compound database to include in the snapshot, do the following:
   a. Select the **Include Compound Database** check box.
   b. Click **Select Database** and choose the compound database to include.
4. To specify the mzVault™ library to include in the snapshot, do the following:
   a. Select the **Include mzVault Library** check box.
   b. Click **Select Database** and choose the mzVault library to include.
5. To specify the NIST™ library to include in the snapshot, do the following:
   a. Select the **Include NIST Libraries** check box.
   b. Click **Select Database** and choose the NIST libraries to include.

v **To capture a snapshot**



1. Enter the name for the Snapshot folder (*folderName*).

   The application saves the specified data in the Snapshots folder, using the following syntax:

   …\Snapshots*dateStamp_timeStamp_folderName*

   The application also saves the entire folder in zipped format:

   …\Snapshots*dateStamp_timeStamp_folderName*.zip

2. Select the **Approve Snapshot** check box.

   A dialog box informs you that creating a snapshot automatically includes user- and computer-specific information to be used for solving user-reported application issues only.

3. Click **OK**.

   The application makes the Take Snapshot button available.

4. Click **Take Snapshot**.

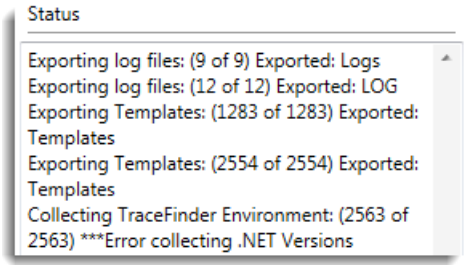
   The Progress section at the bottom of the dialog box reports the progress of the data collection.

Note The Progress section also reports any errors that prevent the application from collecting the data. If there are errors, fix the errors and take the snapshot again.

v To monitor the snapshot status

- Click >>> in the upper right corner of the dialog box.

  The status pane displays details of the collected data files.



v To submit a help request

1. Examine the contents of the collected snapshot folder to verify that it contains all the necessary data.
2. Send the zipped file to the TraceFinder representative.

1

Introduction

This chapter describes general features of the TraceFinder application.

Contents

- About the TraceFinder application
- TraceFinder summary of features
- TraceFinder workflow
- Reporting features

About the TraceFinder application

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

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

The application can import the following file types:

- Sample lists in CSV or XML format

  See Defining a sample list in Chapter 3, "Using the Acquisition mode."

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

  Refer to Chapter 2, "Using Compound Databases in the Method Development Mode," in the *TraceFinder Lab Director User Guide*.

- Batches, methods, or templates from the TraceFinder 3.3, 4.0, 4.1 5.0, 5.1, or 5.2 or 5.3 applications

  See Converting legacy data.

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

  The *TraceFinder Lab Director User Guide* provides detailed information for creating the following methods.

Quantitative processing methods	Chapter 4, "Using the Method Development Mode for Quantitation Methods"
Target screening processing methods	Chapter 5, "Using the Method Development Mode for Target Screening Methods"
Unknown screening processing methods	Chapter 6, "Using the Method Development Mode for Unknown Screening Methods"
Instrument methods	Chapter 3, "Using Instrument Methods in the Method Development Mode"

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

Supported file types

The application supports the following file types:

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

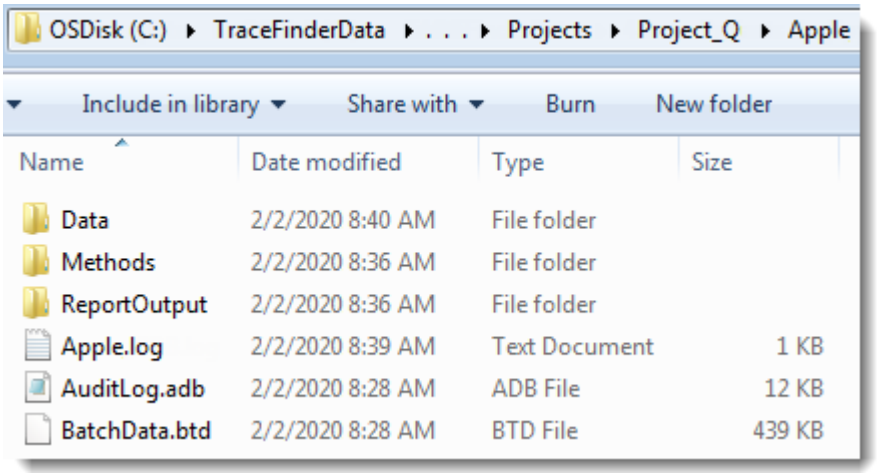
TraceFinder directory structure

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

You can create batches in the Projects folder, or you can create subfolders within the Projects folder for your batches. Create as many subfolders as you want for your batches, but you may not 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 general quantitation applications. The application has a fully automated acquisition mode and a manual data analysis mode. You can use the data acquisition system to create and submit batches and monitor real-time review of results.

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

Key features include the following:

- Role-based authorization for Security, LabDirector, ITAdmin, Supervisor, Technician, and QAQC (quality assurance) roles
- Administrator Console for user security, role-based permissions, and data repositories
- Configuration console for report configuration, detection and acquisition defaults, adduct definitions, screening library selection, and customized columns and flags
- Method Development mode for editing instrument methods, setting processing and error flag parameters, and setting reporting options
- Acquisition mode that guides you in creating batches and running samples
- Analysis mode with batch views, data review, local method views, and reporting views
- Database-capable method development
- Quantification, target screening, and unknown screening workflows
- Spreadsheet-based report designer

Features of the common workflow core include the following:

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

TraceFinder workflow

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

When using the application, follow these basic steps:

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

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

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

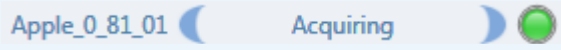
2. Create and submit a batch using the Acquisition wizard.

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

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

   The real-time display is visible from all TraceFinder modes or as a stand-alone window (see Stand-alone Real Time Status window). 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 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:

   A status light might include an exclamation mark.

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

   Click the status light to display details of the error.

4. Evaluate the data in the Analysis mode.

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

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

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

Reporting features

The report engine can generate several different types of reports designed to meet the needs of the laboratory, the laboratory's customers, and key regulatory agencies that might review the results. The following types of reports meet the requirements of various methods and global regulatory agencies, helping to track the performance of LC and GC systems and methods.

Standard report types

- Ad Hoc Tune Report
- Batch Report
- Blank Report
- Breakdown Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- Confirmation Report 2
- High Density Calibration Report
- High Density Internal Standard Report Long
- High Density Sample Report 1 Long
- Intelligent Sequencing
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report

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

Use the features in the Report Designer to create custom report types. See Chapter 7, "Using the Report Designer."

2

Getting started

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

Contents

- Installing TraceFinder
- Installing the NIST and QED libraries
- Launching the NIST Library Browser
- Launching a qualitative explorer application
- Converting legacy data
- Configuring modes and views
- Choosing a mode or console

Installing TraceFinder

To initially install TraceFinder 5.3 software, follow the instructions in the *TraceFinder Installation Guide*. Later, you might need to reinstall the software or other features using the InstallShield Wizard.

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

v **To reinstall TraceFinder**

1. From the Thermo Foundation Instrument Configuration window, remove all instruments.
2. From the Windows Control Panel, uninstall the software and then uninstall all Thermo instrument drivers.
3. Insert the TraceFinder DVD, and install both the TraceFinder 5.3 software and the NIST library as follows:
   a. Open the TraceFinder launcher and click **Next**.

      The InstallShield Wizard opens.

b. Verify that your system meets the requirements list in the Description.

c. Read the End User License Agreement and select the **I agree…** check box.

To open a printable version of the End User License Agreement, click **User Agreement**.

d. Select either the **LC** or **GC** configuration.

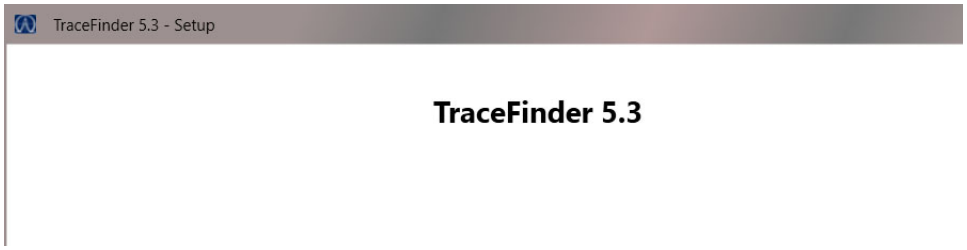
e. Select each version of the TraceFinder application that you want to install.

- TraceFinder General Quan
- TraceFinder EFS
- TraceFinder Clinical Research
- TraceFinder Forensic

f. (Optional) Click **Change** and locate the folder where you want to install the TraceFinder application.

g. Click **Install**.

As the application installs, the Setup dialog box reports the progress.



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

IMPORTANT If prompted to install the Foundation software, click **Yes**, and then when prompted to restart your computer, click **OK**. The wizard continues the installation.

h. When prompted to restart your computer, select the **Yes** option and click **Finish**.

4. (Optional) After your system restarts, open the TraceFinder launcher again, click **Next**, and install any of the following:

a. Click **NIST17** and follow the instructions to install it.

b. Click **mzVault 2.3** and follow the instructions to install the Thermo mzVault application.

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

You can now start the TraceFinder application.

Start the 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 5.3 > TraceFinder 5.3 General Quan**.

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

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

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

1. Enter your user name in the TraceFinder login window.
2. Enter your password and click **Login**.

   The application verifies the user name and password and opens the TraceFinder main window.

   If your user name or password does not match, the system reports Incorrect Credentials.

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

   When you are assigned multiple roles, the application activates the Role list and changes **Authenticate** to **Login**.

3. (Optional) Select which role to use for the session and click **Login**.

   The TraceFinder main window opens.

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

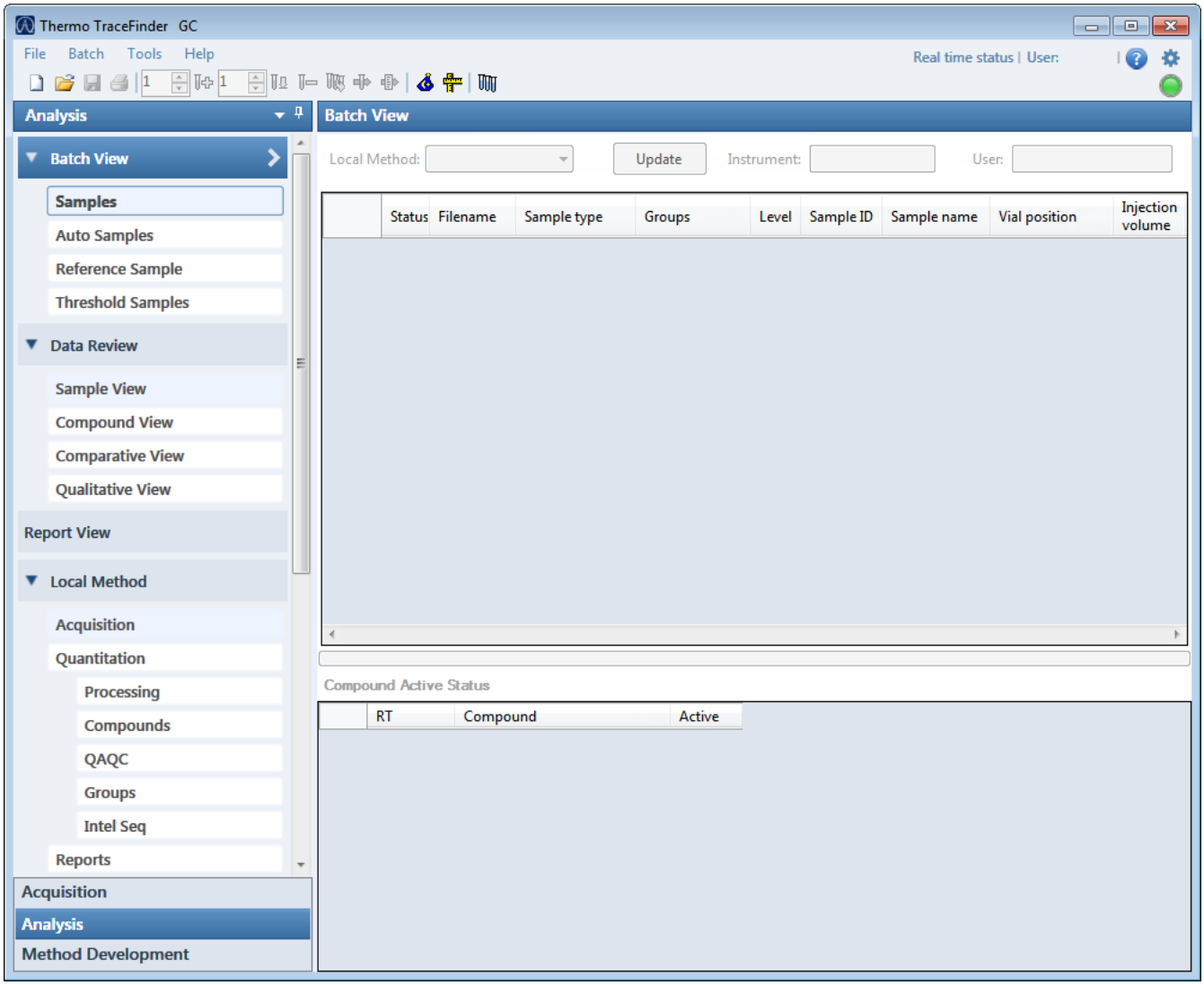


Table 1. TraceFinder main window features (Sheet 1 of 2)

Parameter	Description
Modes	
Acquisition	See Chapter 3, "Using the Acquisition mode."
	Tip (Animation) To view demonstrations of the features of the Acquisition Mode, choose **Help > Animations**.
Analysis	See Chapter 4, "Using the Analysis mode for quantitation batches." See Chapter 5, "Using the Analysis mode for target screening batches." See Chapter 6, "Using the Analysis mode for unknown screening batches."
	Tip (Animation) To view demonstrations of the features of the Analysis Mode, choose **Help > Animations**.

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

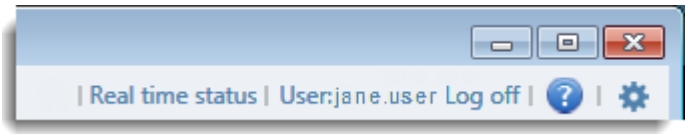
Parameter	Description
Method Development	Refer to the *TraceFinder Lab Director User Guide*.
Additional Features	A TraceFinder window with user security for a user in the default LabDirector role has these functions. 
Real Time Status	Opens the Real Time Status pane for the current acquisition. The acquisition progress is displayed within the current mode window. The Real Time Status is also available as a stand-alone window (see Stand-alone Real Time Status window). **Tip (Animation)** To view a demonstration of "Using the Real Time Status Pane" choose **Help > Animations**.
User	Displays the name of the current user.
Log Off	Logs out the current user and displays the login screen. This function is available only when user security is activated.
Help	Opens the TraceFinder Help. **Tip (Animation)** To view a demonstration showing "Where are My Manuals?," choose **Help > Animations**.
Application Configuration	Opens the Configuration console where you can configure several options for using the application. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*. **Tip (Animation)** To view a demonstration of the features of the "Configuration Console," choose **Help > Animations**.

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.
Role	The application displays links to only the modes, interface areas, and features assigned to this role. Available only when you are assigned to multiple roles.
Login/ Authenticate	**Login** verifies the user name and password, and opens the application. –or– (When the user is assigned multiple roles) **Authenticate** verifies the user name and password, activates the Role list, and changes to Login.
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 (National Institute of Standards and Technology) and QED (Queries on Encrypted Data) libraries.

v **To install the NIST library**

1. Open the TraceFinder launcher, and click **Next**.
2. Click **NIST17**.

   The NIST 17 MS Search and AMDIS 2.7 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 (x86)\NISTMS**.
5. Continue to follow the instructions in the wizard until the setup is complete.

Note The application installs the NIST17 library; however, it also supports the NIST 2008, NIST 2011, and NIST 2014 libraries.

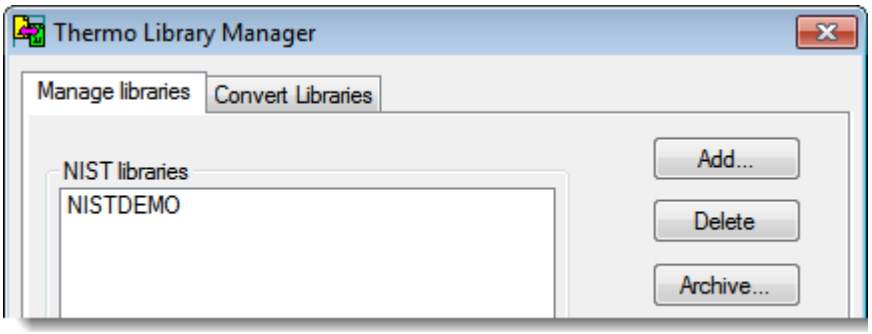
v To install the QED library

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

   The Thermo Xcalibur Roadmap opens.

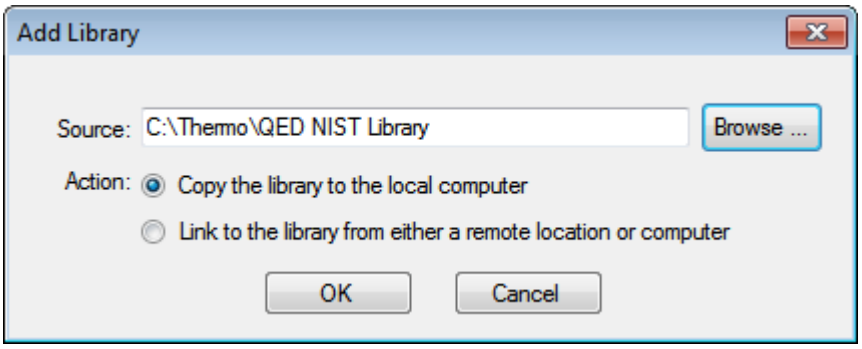
2. Choose **Tools > Library Manager** from the main menu.

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



3. Click **Add**.

   The Add Library dialog box opens.

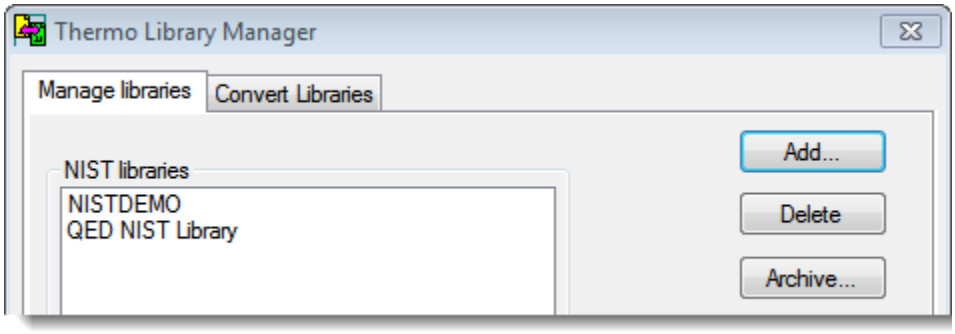


4. Click **Browse**, and locate your QED library in the C:\Thermo folder.
5. Click **OK**.

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

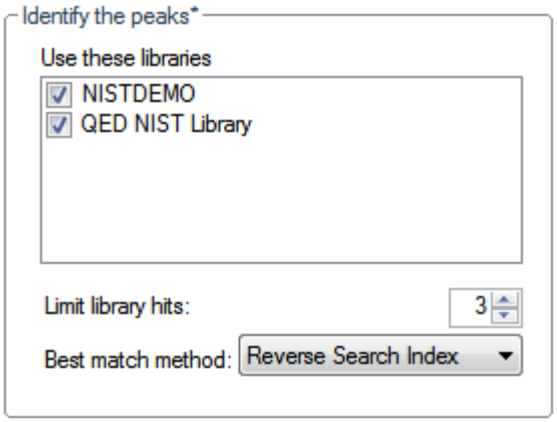
6. Click **Dismiss** to close the message box.

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



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

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

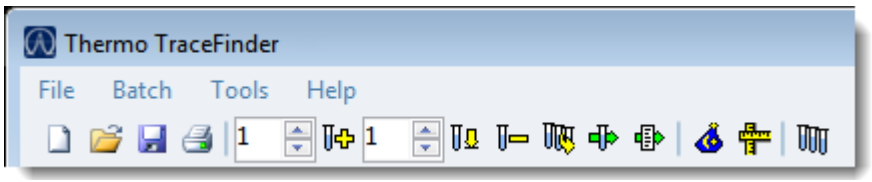


Launching the NIST Library Browser

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

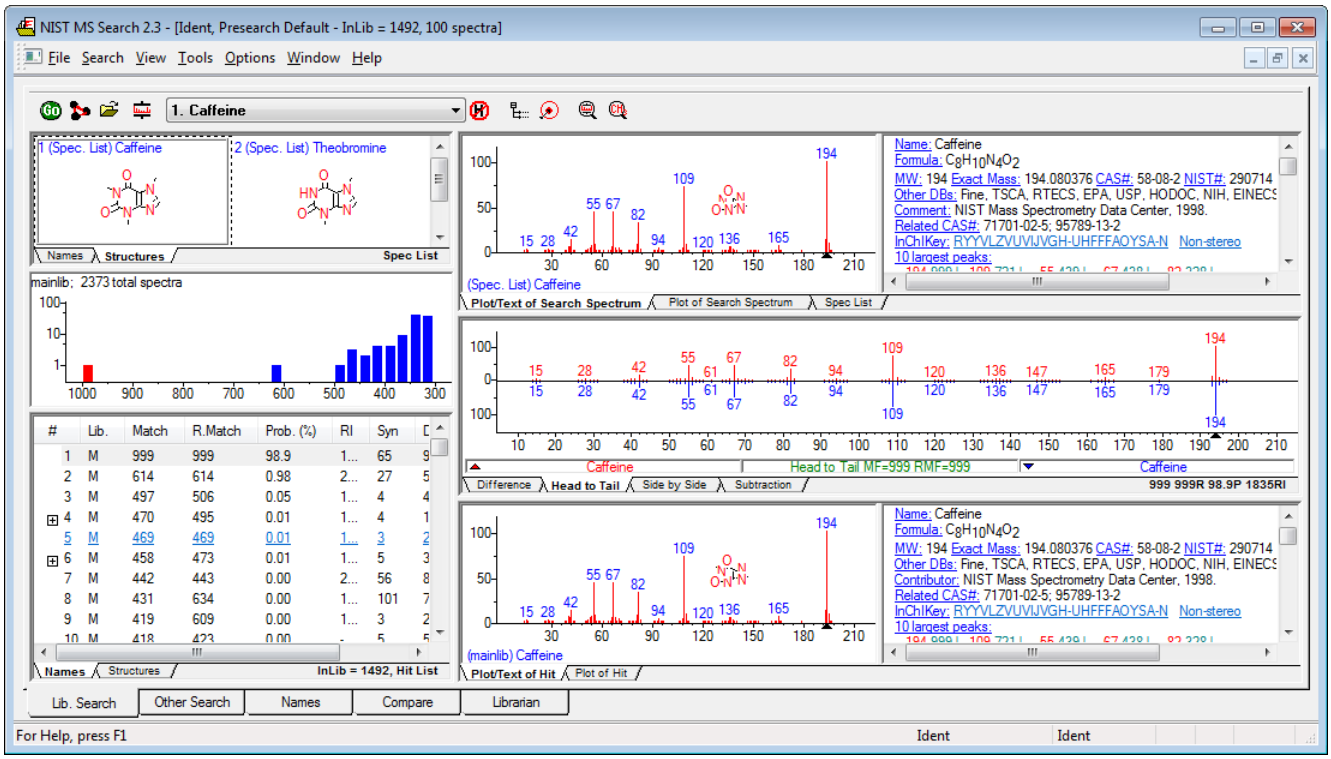
v **To open the NIST library browser**

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



The NIST MS Search window opens.

Figure 5. NIST MS Search window



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

Launching a qualitative explorer application

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
- Converting legacy data

Thermo Scientific FreeStyle

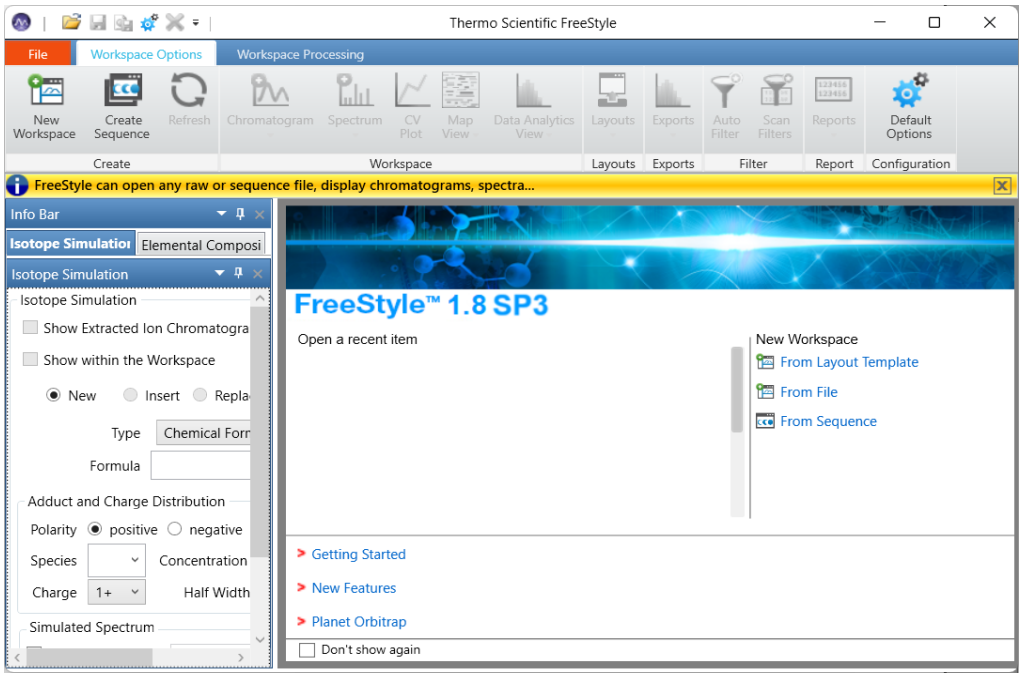
IMPORTANT The Thermo Scientific FreeStyle™ application is available only when you configure it as your default qualitative explorer in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

v **To open the FreeStyle window**

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

  The FreeStyle application opens.

  Figure 6. FreeStyle main window



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

Converting legacy data

Use the TraceFinder Legacy Data Converter to convert methods, batches, method templates, batch templates, or compound databases (CDBs) from the source versions to compatible TraceFinder 5.3 target configurations. You can convert the following:

- Legacy methods, batches, or method templates from TraceFinder versions 3.3, 4.0, 4.1, 5.0, 5.1, or 5.2.
- Legacy batch templates from TraceFinder versions 3.3, 4.0, 4.1, 5.0, 5.1, or 5.2.
- Legacy compound databases from TraceFinder versions 3.3, 4.0, 4.1, 5.0, or 5.1.
- Data from TraceFinder version 5.3 for general quantitation to another installed configuration of TraceFinder 5.3

Note The TraceFinder Legacy Data Conversion Tool in version 5.3 is designed to support legacy data conversion from versions 3.3 and later.

Data created in TraceFinder versions earlier than 3.3 must first be converted using the Legacy Data Conversion Tool included with TraceFinder™ version 4.1. Once converted to the 4.1 format, the data can then be subsequently upgraded to the version 5.3 format.

Version compatibility

This table shows which source versions of methods, batches, method templates, batch templates, or compound databases are compatible with TraceFinder 5.3 target configurations.

Table 3. Version compatibility

Source	TraceFinder 5.3 target			
	General	EFS[a]	Clinical Research	Forensic Toxicology
TraceFinder 5.3 General		3	3	3
TraceFinder 3.3–5.2 General		3	3	3
TraceFinder 3.3–5.2 EFS		3		
TraceFinder 3.3–5.2 Clinical Research			3	3
TraceFinder 3.3–5.2 Forensic Toxicology			3	3

[a] Environmental and Food Safety

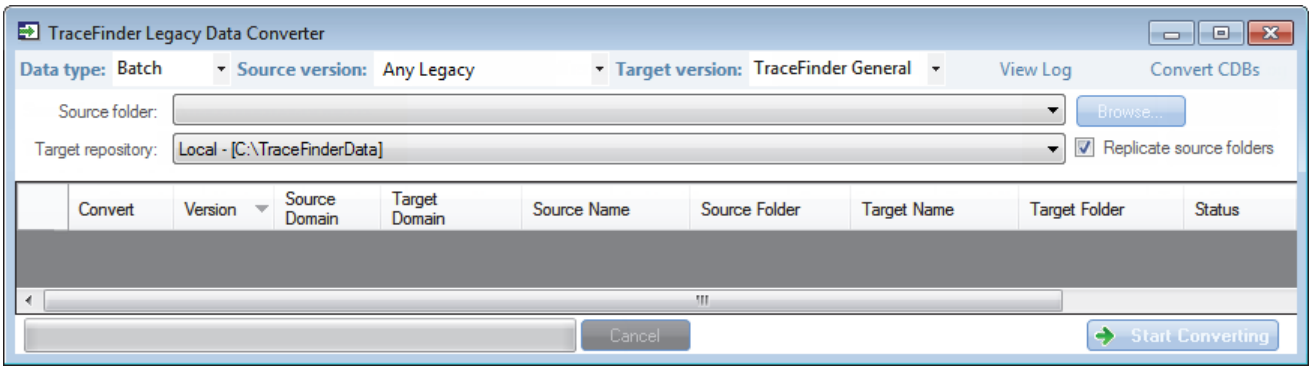
See the following topics:

- Convert methods
- Convert batches
- Convert method templates
- Convert batch templates
- Convert compound databases

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

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

The TraceFinder Legacy Data Converter window opens.



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

Convert methods

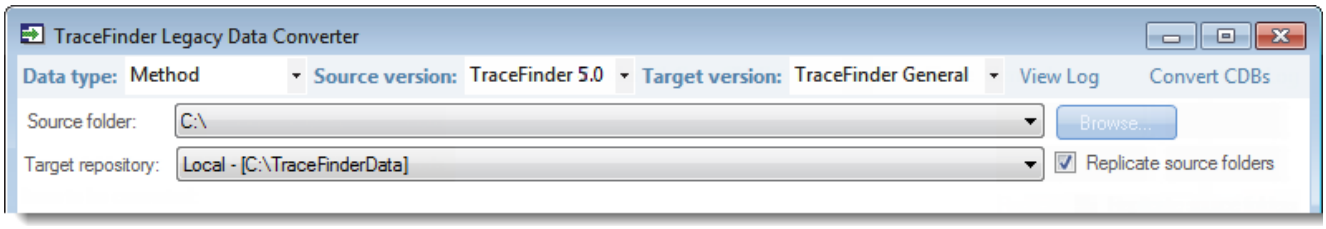
Use the data converter to convert legacy methods to TraceFinder 5.3 methods.

v **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 5.0 General configuration to the current General configuration. For a complete list of version compatibilities, see Version compatibility.



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

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

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

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

   a. Click **Browse** and locate a different source method folder.

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

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

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

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

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

   The list displays only TraceFinder configurations with compatible data. See Version compatibility.

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

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

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

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

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

.

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

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

   When the Status column reports that a method is successfully converted, the application writes the converted file to the specified target repository.

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

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

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

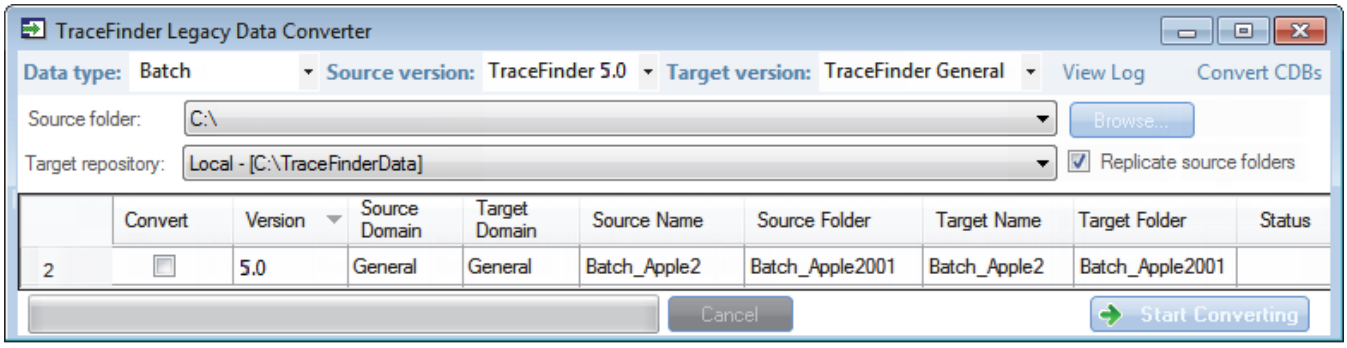
Convert batches

Use the data converter to convert legacy batches to TraceFinder 5.2 batches.

v To convert a batch

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

   The following example shows that you can convert batches from the TraceFinder 5.0 General configuration to the current General configuration. For a complete list of version compatibilities, see Version compatibility.



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

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

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

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

   The list displays only TraceFinder configurations with compatible data. See Version compatibility.

4. In the Target Name and Target Folder columns, type the name of a batch project and subproject folder, or select the **Replicate Source Folders** check box.

   IMPORTANT The conversion cannot overwrite an existing file name. If the new target name is identical to an existing batch folder, the application appends "_001" to the original name.

   IMPORTANT When you select to replicate the source folders, the application recreates only the folder structure within the Projects folder.

5. In the Convert column, select the 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\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.

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

IMPORTANT After you convert a batch, you must reprocess the batch to see the flags in the Samples and Compounds panes in Data Review.

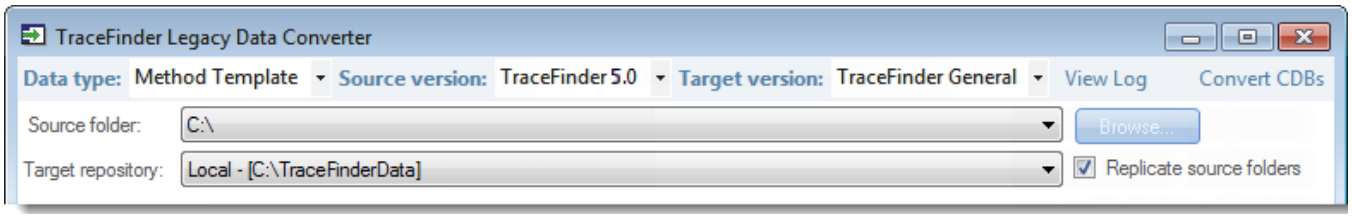
Convert method templates

Use the data converter to convert legacy method templates to TraceFinder 5.3 method templates.

v **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 5.0 General configuration to the current General configuration. For a complete list of version compatibilities, see Version compatibility.



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

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

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

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

   a. Click **Browse** and locate a template folder.

      You can select a specific template folder or a folder that contains multiple templates.

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

   The application displays the selected folder in the conversion table.

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

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

   The list displays only TraceFinder configurations with compatible data. See Version compatibility.

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.

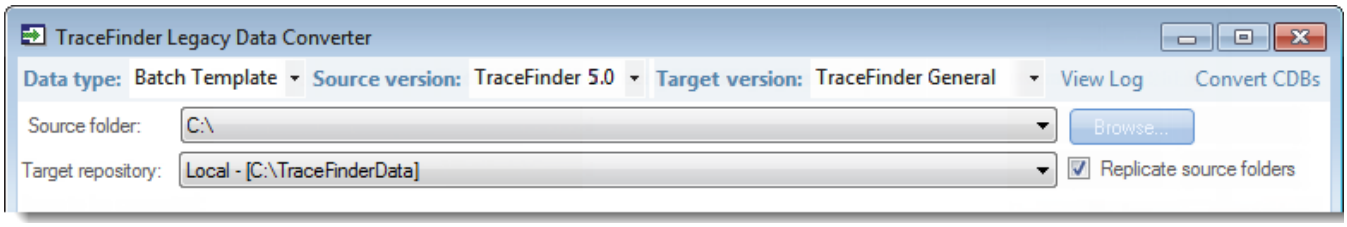
Convert batch templates

Use the data converter to convert legacy batch templates to TraceFinder 5.3 batch templates.

v To convert a batch template

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

   The following example shows that you can convert batch templates from the TraceFinder 5.0 General configuration to the current General configuration. For a complete list of version compatibilities, see Version compatibility.



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

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

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

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

   a. Click **Browse** and locate a template folder.

      You can select a specific batch template folder or a folder that contains multiple batch templates.

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

   The application displays the selected folder in the conversion table.

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

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

   The list displays only TraceFinder configurations with compatible data. See Version compatibility.

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

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

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

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

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

.

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

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

   When the Status column reports that the template is successfully converted, the application writes the converted template folder to the …\TraceFinderData\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**.

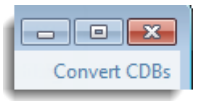
   The application opens a cumulative log file for the session in a Notepad text editor window.

Convert compound databases

Use the data converter to convert legacy compound databases to TraceFinder 5.3 compound databases.

v **To convert compound databases**

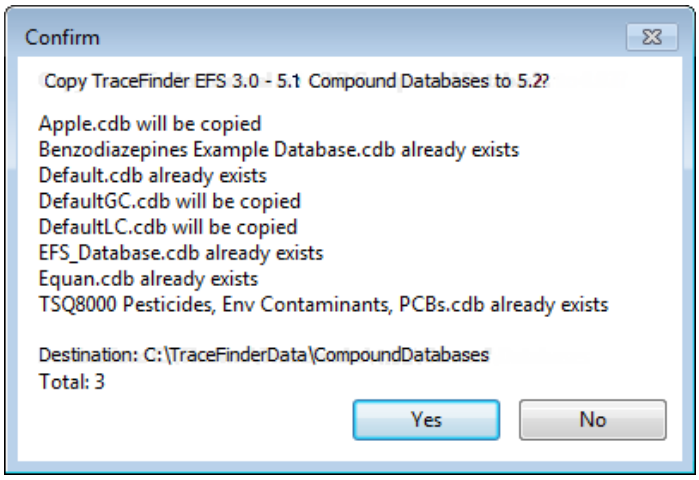
1. Click **Convert CDBs** (in the upper right corner of the window).



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

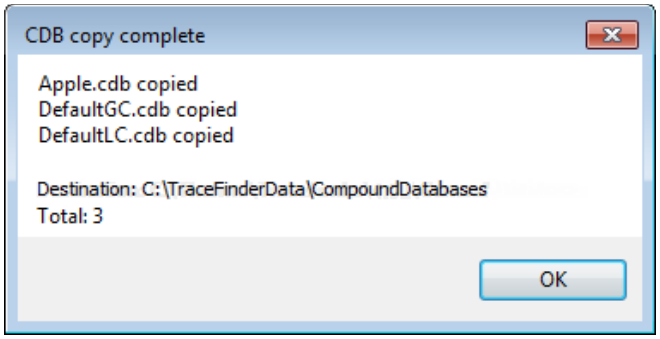
   The Confirm dialog box lists all databases that will be converted to TraceFinder 5.2.

Figure 7. Confirm dialog box



2. Click **Yes**.

   The Confirm dialog box lists all databases that are converted to TraceFinder 5.3.



3. Click **OK**.

   The converted compound databases are now available in the TraceFinder 5.3 application.

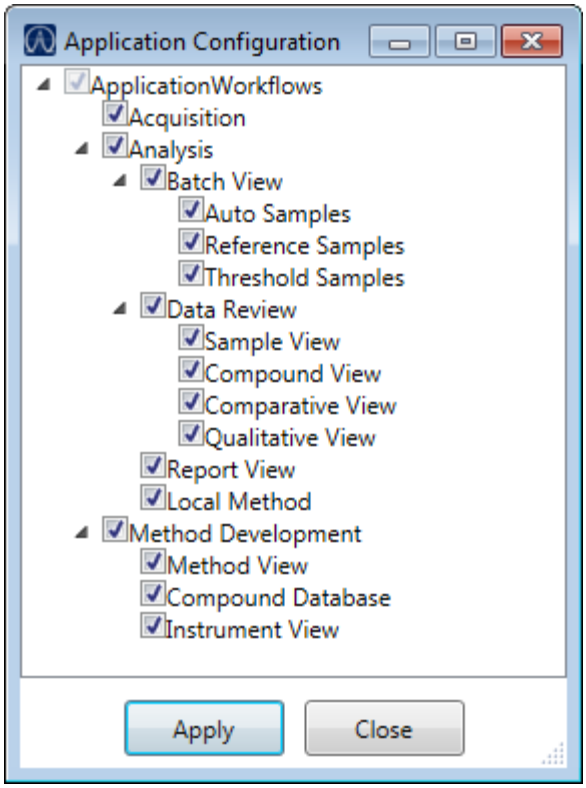
Configuring modes and views

When Configurability Access is enabled, you can choose which modes (Acquisition, Analysis, or Method Development) or views within the modes are displayed in the TraceFinder application.

v **To configure views**

1. From the main menu, choose **Tools > Configure Application Views**.

   The Application Configuration dialog box opens.



2. Select the check box for each mode or view within a mode that you want to display.
3. Click **Apply**.

   The application immediately applies the view configurations you specified.
4. When you have finished specifying the views that you want to display, click **Close**.

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	3	3	3	3	3
ITAdmin					3
Supervisor	3	3	3	3	3
Technician		3	3		
QAQC			3		

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 Administrator console
- To open the Configuration console
- To display a log of instrument errors
- To monitor instrument states
- To watch acquisition and processing

v 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.

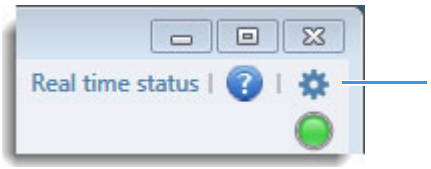
Mode	Description
Acquisition	Opens the Acquisition mode where you can create and review batches, batch data, reports, and local methods. See Chapter 3, "Using the Acquisition mode."
Analysis	Opens the Analysis mode where you can review batches, batch data, reports, and local methods. See Chapter 4, "Using the Analysis mode for quantitation batches." See Chapter 5, "Using the Analysis mode for target screening batches." See Chapter 6, "Using the Analysis mode for unknown screening batches."
Method Development	Opens the Method Development mode where you can create a master method or an instrument method. Refer to the *TraceFinder Lab Director User Guide*.

v **To open the Administrator console**

- From the main menu, choose **Tools > Administrator Console**.

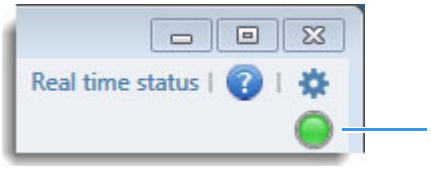
v **To open the Configuration console**

- Click the **Application Configuration** icon.

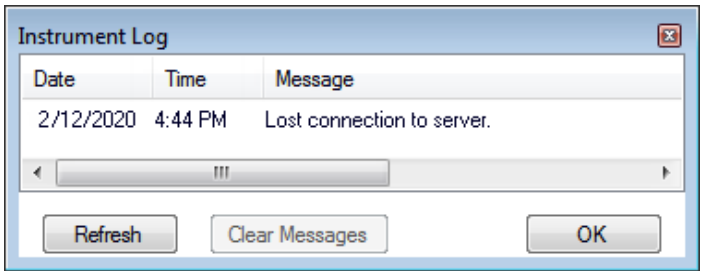


v **To display a log of instrument errors**

1. Click the status light.



The Instrument Log dialog box opens.



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

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

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

     C:\Thermo\TraceFinder\5.2\General\Logs\TraceFinder.log
   - Click **OK** to dismiss the Instrument Log dialog box.

v **To monitor instrument states**

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

  Green indicates that the instrument is ready.

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

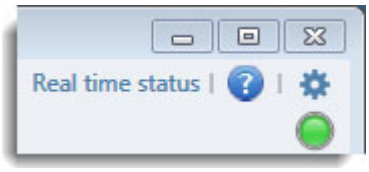
  Red indicates that the instrument is not ready because it is turned off, not configured or connected, currently initializing, or otherwise busy.

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

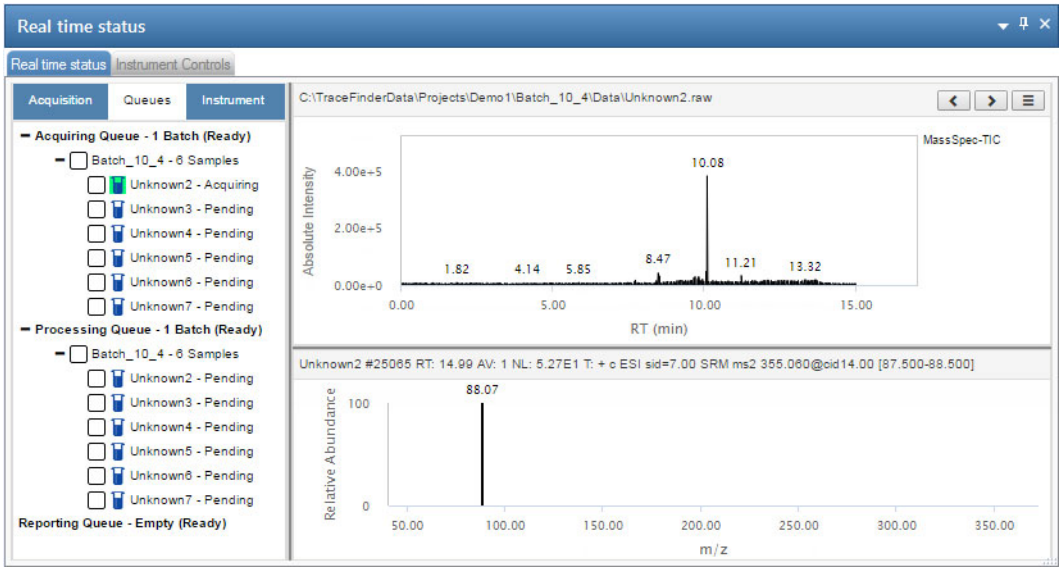
  Click the status light to display details of the error.

v **To watch acquisition and processing**

- Click **Real Time Status**.



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 in Chapter 3, "Using the Acquisition mode."

Note The Real Time Status is also available as a stand-alone window (see Stand-alone Real Time Status window).

3

Using the Acquisition mode

This chapter describes the tasks associated with the Acquisition mode.

Contents

- Working with batches
- Real Time Status pane
- Stand-alone Real Time Status window
- 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.

Using a master method, you can create a batch and run the samples. A batch can represent a single sample or multiple samples that are to be acquired, processed, reviewed, and reported as a set. After you create a batch of samples, you can submit the batch and review the results in Data Review or you can go directly to viewing and printing reports.

You can set up a calibration batch with known concentrations of the target compounds and compare the calibration values against samples in future batches.

You can also use the Quick Acquisition feature to quickly submit samples from any page in the Acquisition mode. See Appendix A, "Using quick acquisition."

Working with batches

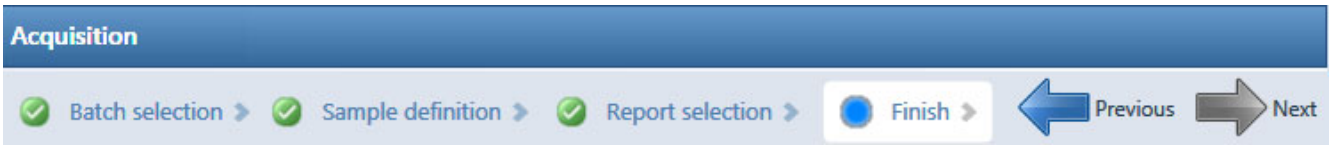
See the instructions for the following tasks:

- Open and navigate the Acquisition mode
- Create and submit batches

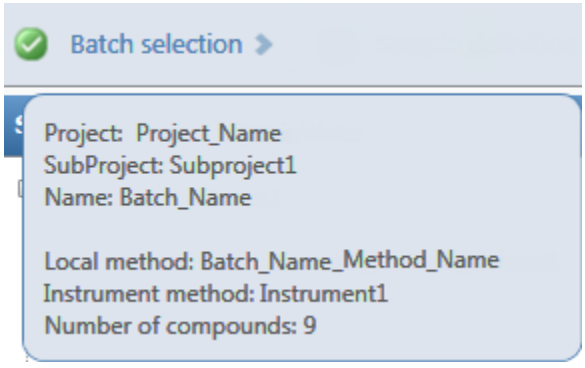
Open and navigate the Acquisition mode

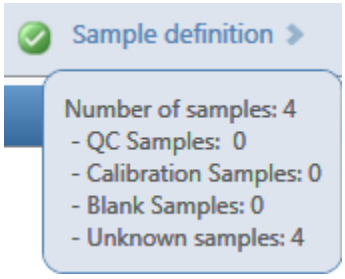
As you progress through the Acquisition mode using any of these methods for creating a batch, the task pane at the top of the view tracks your progress. As you complete each stage, you can point to the view name in the task pane to display the parameters that you specified for the batch. See Example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

Figure 9. Example task pane when you have completed the Acquisition mode



Point to 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: Cal Std

Blank Samples: Matrix Blank

Unknown Samples: All other samples

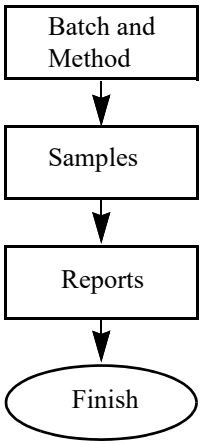
Create and submit batches

To create and submit a batch, the Acquisition mode uses a wizard-style interface to guide you through these major steps:

1. Selecting a batch
2. Defining a sample list
3. Selecting and reviewing reports
4. Submitting a batch in the Acquisition wizard

The Acquisition mode provides multiple techniques for creating either a batch or a batch template. Each batch creation technique has an associated workflow, as shown in the following flowcharts. Each workflow uses a different combination of Acquisition mode pages.

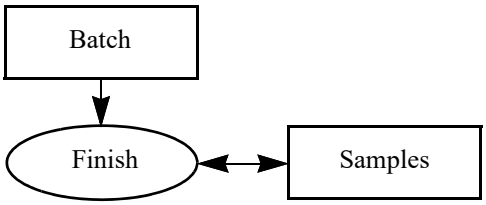
Workflow for creating an original batch



To create an original batch, start with any of these instructions: To start a new quantification batch, or To start a new target screening batch, or To start a new unknown screening batch.

Tip (Animation) To view "Acquiring a New Batch," see **Help > Animations**.

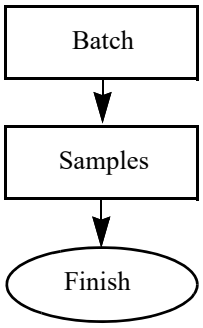
Workflow for acquiring a prepared batch



To acquire a prepared batch, start with the instructions To select a prepared batch.

Tip (Animation) To view "Submitting a Prepared Batch," see **Help > Animations**.

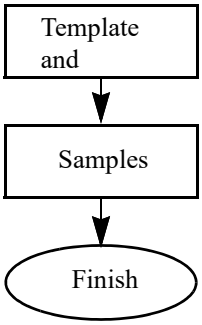
Workflow for reinjecting a previously acquired batch



To process a previously acquired batch, start with the instructions To reinject a sample from a previously acquired batch.

Tip (Animation) To view "Reinjecting Samples," see **Help > Animations**.

Workflow for creating or editing a batch template



To create a batch template, start with any of these instructions: To create a quantitation batch template, To create a target screening batch template, or To create an unknown screening batch template.

Tip (Animation) To view "Creating a Batch Template," see **Help > Animations**.

Selecting a batch

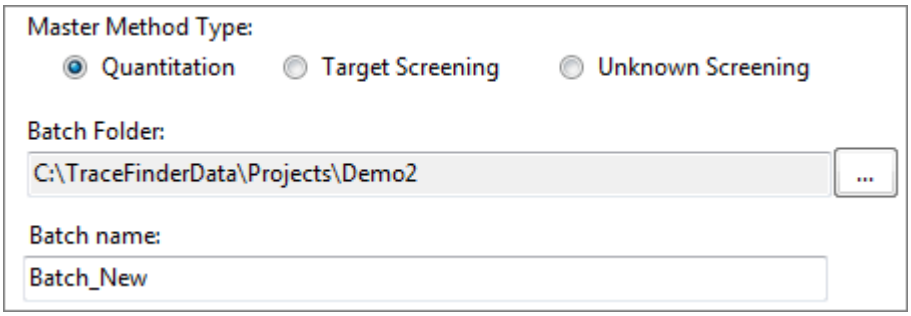
On the Batch Selection page of the Acquisition mode, you can create a new quantitative, target screening, or unknown screening batch in any of your current projects/subprojects. Or, you can submit a batch that you previously prepared and saved, reinject the samples in a batch that you previously acquired,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

Follow these procedures:

- To start a new quantification batch
- To start a new target screening batch
- To start a new unknown screening batch
- To start a new batch from a template
- To select a prepared batch
- To reinject samples
- To create a quantitation batch template
- To create a target screening batch template
- To create an unknown screening batch template

v To start a new quantification batch

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

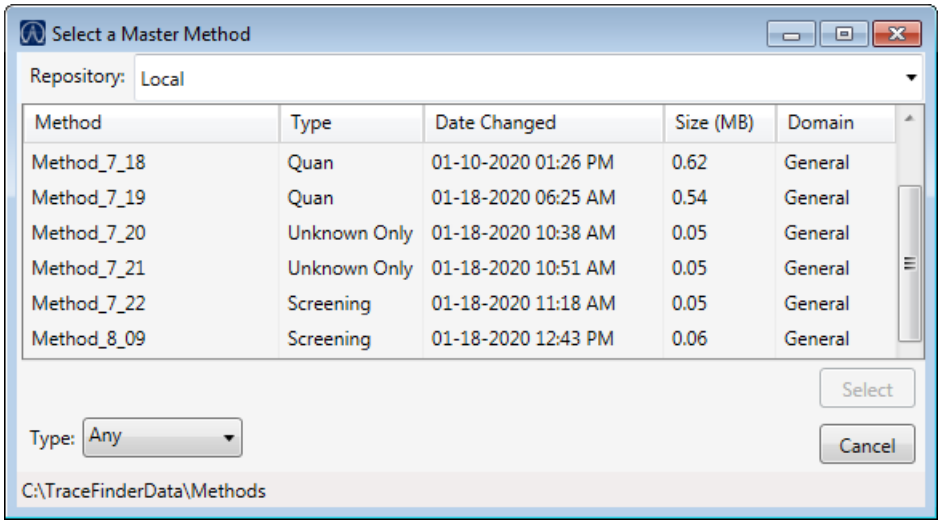


If the name you enter is not unique, a red warning flashes.

5. Click **Select Master Method**.

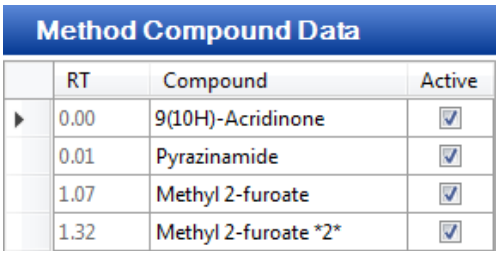
The Select a Master Method dialog box opens.

Figure 10. Select a Master Method dialog box



6. Select a repository and a method from the list, and then click **Select**.

   The Method Compound Data pane displays the compounds in the method. The application uses these databases to identify the compounds in the samples. You cannot edit the compounds list from the Acquisition mode.

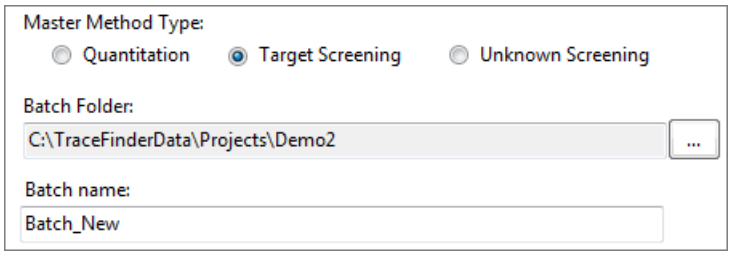


7. To continue to the next page, click **Next**.

   The Sample Definition page opens. See Defining a sample list.

v **To start a new target screening batch**

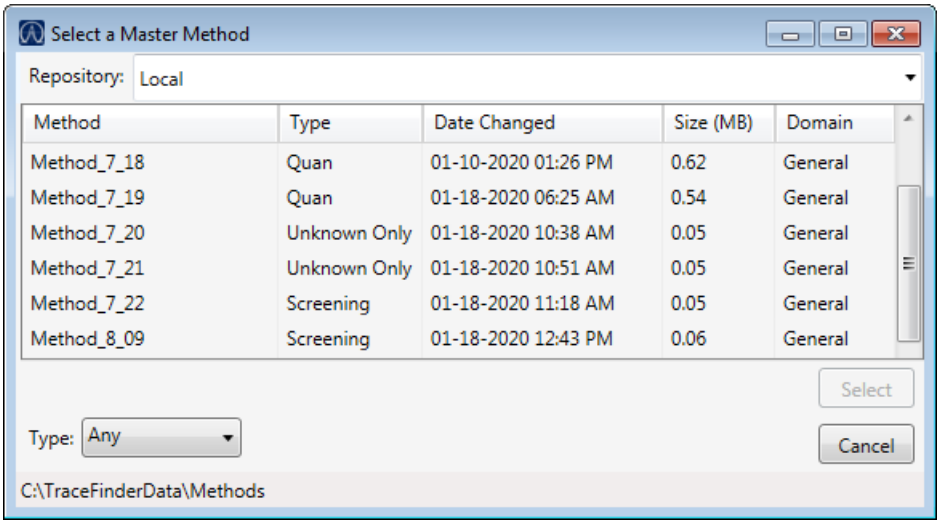
1. Click **Create a New Batch** in the navigation pane.
2. Select the **Target Screening** option.
3. Select the batch folder where you want to create the new batch.
4. Type a name for the new batch in the Batch Name box.



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

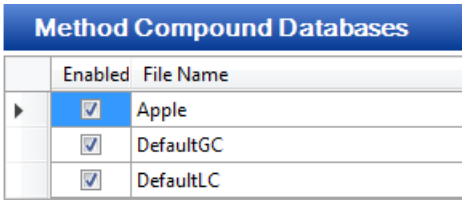
5. Click **Select Master Method**.

   The Select a Master Method dialog box opens.



6. Select a repository and a method from the list, and then click **Select**.

   The Method Compound Databases pane displays the compounds in the method. The application uses these databases to identify the compounds in the samples. You cannot edit the compound databases list from the Acquisition mode.

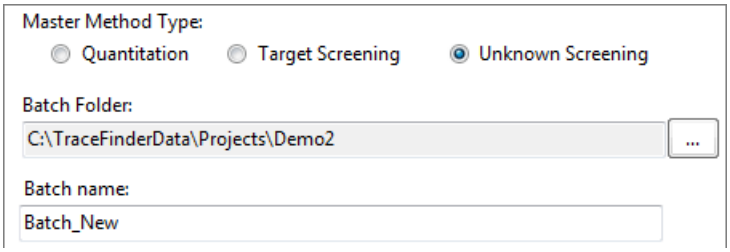


7. To continue to the next page, click **Next**.

   The Sample Definition page opens. See Defining a sample list.

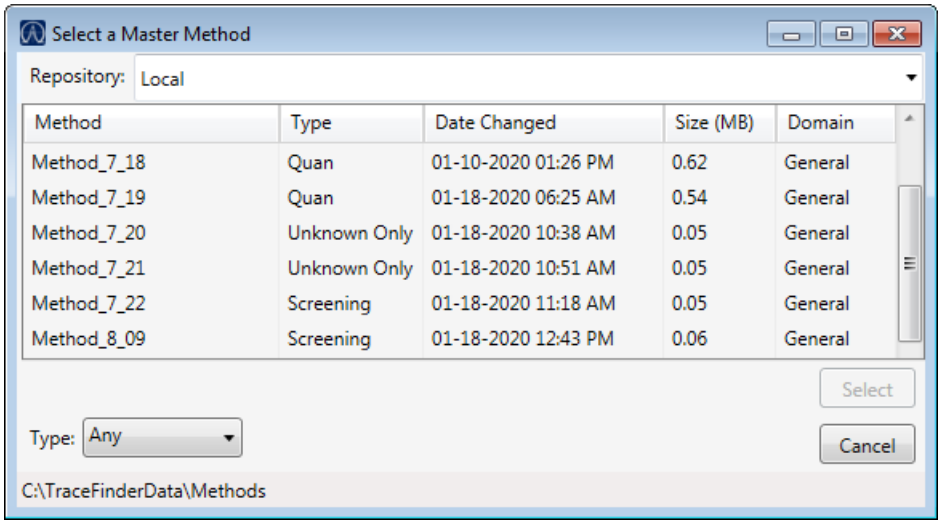
v To start a new unknown screening batch

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



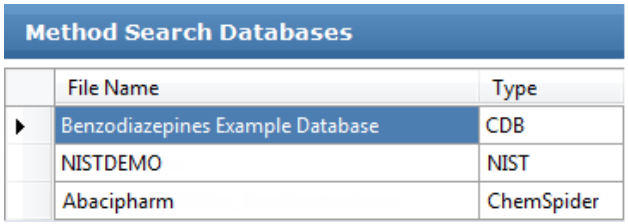
5. Click **Select Master Method**.

   The Select a Master Method dialog box opens.



6. Select a repository and a method from the list, and then click **Select**.

   The Method Search Databases pane displays the databases that you selected in the method. The application uses these databases to identify the compounds in the samples. You cannot edit the database list from the Acquisition mode.



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

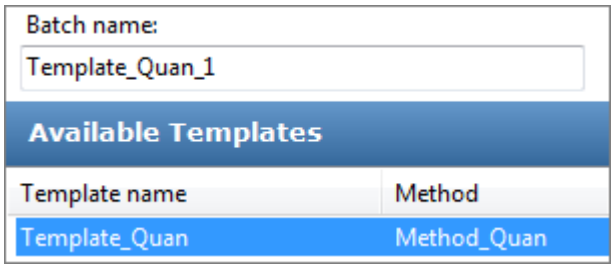
   The Sample Definition page opens. See Defining a sample list.

v **To start a new batch from a template**

1. In the navigation pane, click **Create a New Batch**.
2. Select one of these options: **Quantitation**, **Target Screening**, or **Unknown Screening**.

   The Available Templates pane displays only batch templates for the selected option.

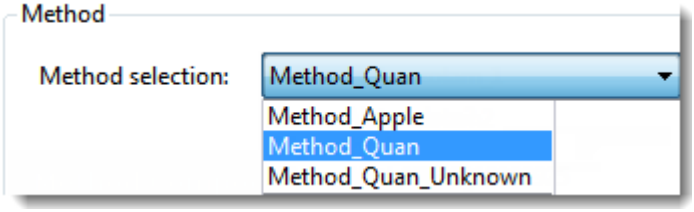
3. In the Available Templates pane, select the template and method combination that you want to use.



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

4. (Optional) Click ... and select a different batch folder where you want to create the new batch.

5. (Optional) Select a different method to use for the new batch.



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

The Sample Definition page of the Acquisition mode opens. See Defining a sample list.

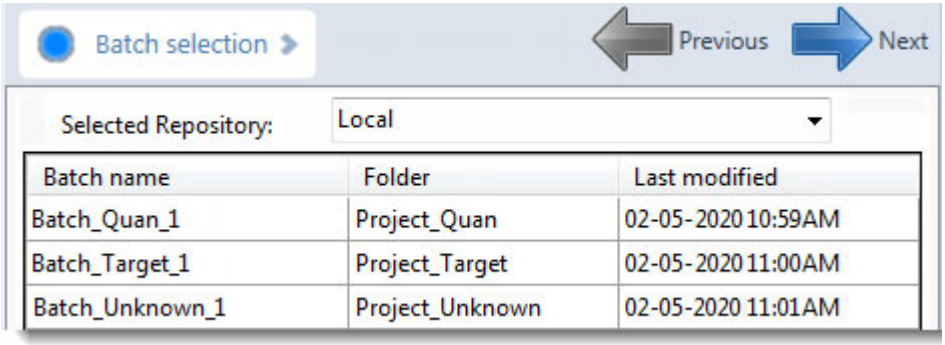
v **To select a prepared batch**

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

2. Select a repository.

The application displays all the unacquired, saved batches in the selected repository.

3. Select the batch that you want to acquire.



4. 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.

5. Do one of the following:

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

     For detailed instructions, see Defining a sample list.

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

.

     For detailed instructions, see Submitting a batch in the Acquisition wizard.

   –or–

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

.

     The application saves your batch in the following folder:

     …\TraceFinderData\Projects\...

     The application closes the Acquisition mode and returns you to the mode you were last using.

v To reinject samples

1. In the navigation pane, click **Reinject Samples**.
2. Browse to and select a batch folder and batch.

   The Select a Batch dialog box displays all previously acquired quantitation, target screening, and unknown screening batches.

3. Select a batch and click **Select**.
4. To continue to the next page, click **Next**.

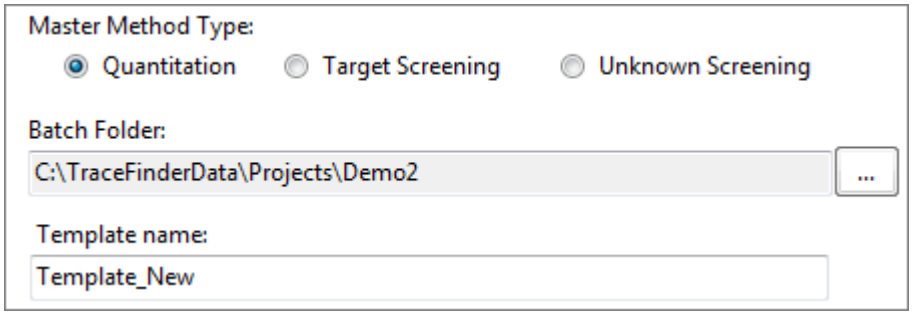
   The Sample Definition page of the Acquisition mode opens. See Defining a sample list.

   - 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.

v To create a quantitation batch template

1. In the navigation pane, click **Create or Edit a Template**.
2. Select the **Quantitation** option.
3. Browse to 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.

Method Compound Data

	RT	Compound	Active
▶	0.00	9(10H)-Acridinone	☑
	0.01	Pyrazinamide	☑
	1.07	Methyl 2-furoate	☑
	1.32	Methyl 2-furoate *2*	☑
	1.53	Methyl 2-furoate *3*	☑

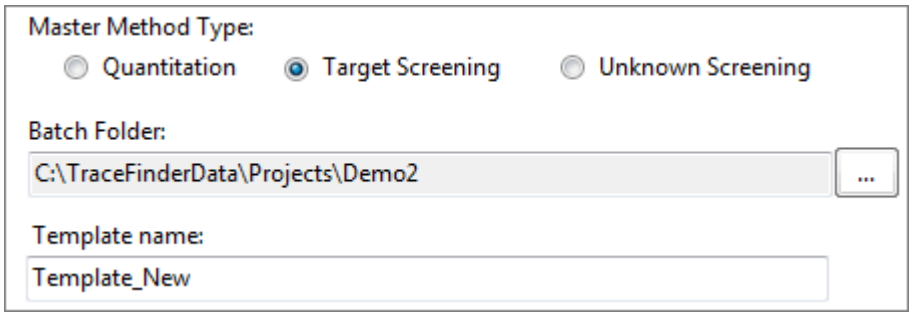
6. To continue to the next page, click **Next**.

   The Sample Definition page of the Acquisition mode opens. See Defining a sample list.

v To create a target screening batch template

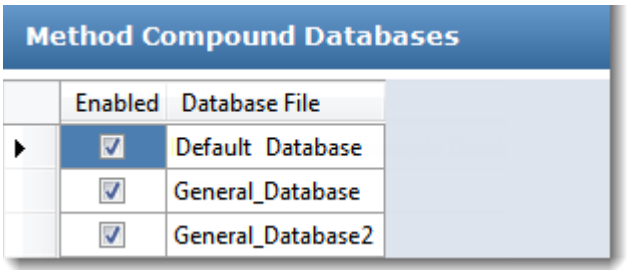
1. In the navigation pane, click **Create or Edit a Template**.
2. Select the **Target Screening** option.
3. Browse to the folder where you want to create the new batch template.

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.

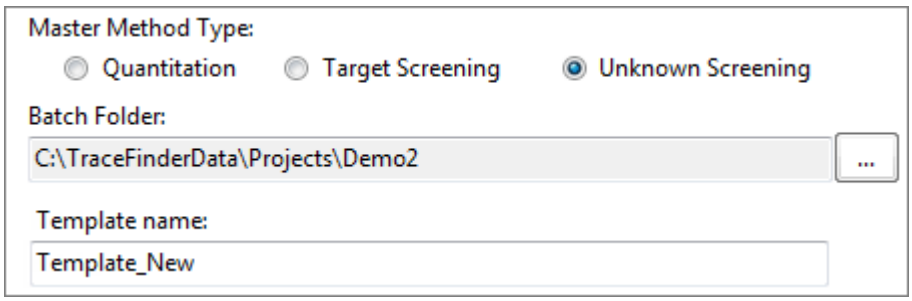


6. Select the check box for each database that you want to use for screening.
7. To continue to the next page, click **Next**.

   The Sample Definition page of the Acquisition mode opens. See Defining a sample list.

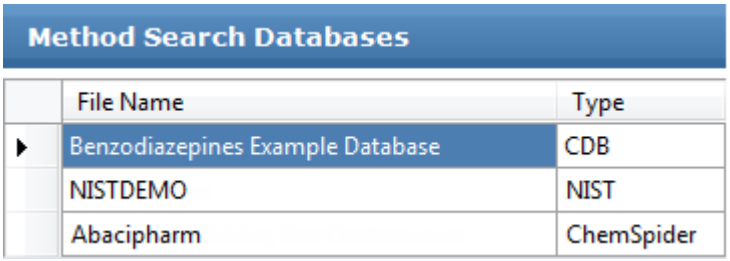
v To create an unknown screening batch template

1. In the navigation pane, click **Create or Edit a Template**.
2. Select the **Unknown Screening** option.
3. Browse to 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 unknown screening databases available for the selected method.



6. Select the check box for each database that you want to use for unknown screening.
7. To continue to the next page, click **Next**.

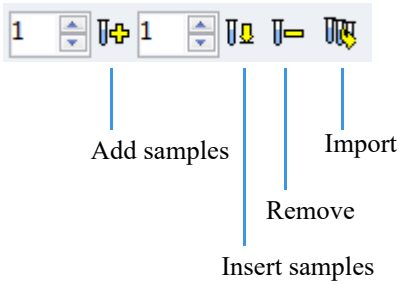
   The Sample Definition page of the Acquisition mode opens. See Defining a sample list.

Defining a sample list

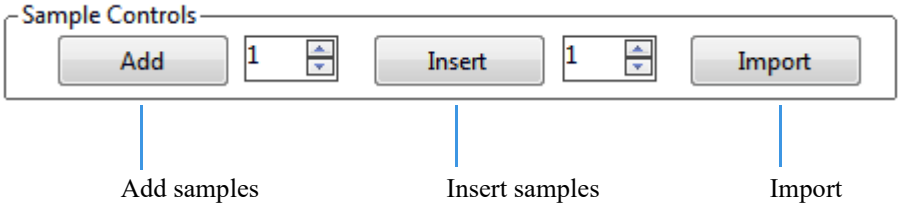
Use the Samples page on the Sample Definition page of the Acquisition mode to create a list of samples for the batch. You can add samples, insert samples, import a sample list, or remove samples from the list. You can use the Reference Sample page to select a reference sample to use as a reference peak in the Data Review.

To create the sample list, you can use either set of function icons or buttons (described in the following graphic) or you can use commands in the shortcut menu (see the Shortcut menu commands area of the Samples page parameters).

Icons in the toolbar



Buttons at the bottom of the sample definition page



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

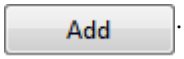
Use any of the following procedures to create a sample list. When you finish defining the list of samples, click **Next.**

- When you create a batch from scratch and click Next, the Report Selection page opens. See Selecting and reviewing reports.
- When you edit a prepared batch, reinject samples, create a batch from a template, or edit a batch template and then click Next, the Finish Selection page opens. See Submitting a batch in the Acquisition wizard.

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

v To add samples to the list

1. Select the number of sample rows to add and then click the **Add** icon, or  .
2. Type a file name in the Filename column for each sample.

   Each file name must be unique.
3. Select a sample type from the Sample Type list for each sample.

Available sample types			
Matrix Blank	Solvent	QC	Unknown
Cal Std			

   For a detailed description of each sample type, see Sample types.
4. For each Cal Std 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, refer to Chapter 4, “Using the Method Development Mode for Quantitation Methods,” in the *TraceFinder Lab Director User Guide*.

5. (Optional) To assign samples to a group, do the following:
   a. For each sample, type a group name in the Groups column.

      Repeat this for each sample that you want to include in a group.

   b. Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
	Benzo26473	groupB, groupA
	Benzo25557	groupB
	Benzo26154	groupB, groupA

The application uses only the first group listed for calculating the Maximum Fold and Group Averages.

For information about Maximum Fold analysis in unknown screening analysis, see Cross Sample Peak List pane.

- For quantitation experiments, after creating groups, you can choose one of the samples as a threshold sample for the group and then compare all of the samples in the Comparative View in Data Review.

  For information about specifying a threshold sample for a group of samples, see Threshold Samples page for quantitation batches. For information about viewing grouped samples in Data Review, see Comparative View for quantitation batches. For information about Group Averages, see Group Averages.

- For unknown screening experiments, you can create a control group (specify the group name as Control) to use for group averages in Data Review. For information about Group Averages, see Group Averages pane.

6. For each sample, type a vial position in the Vial Position column.

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

7. For each sample, type a volume in the Injection Volume column.

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

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

Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name, while the other columns scroll right and left.

To automatically copy or fill values in these columns, see Appendix B, "Using Copy Down and Fill Down."

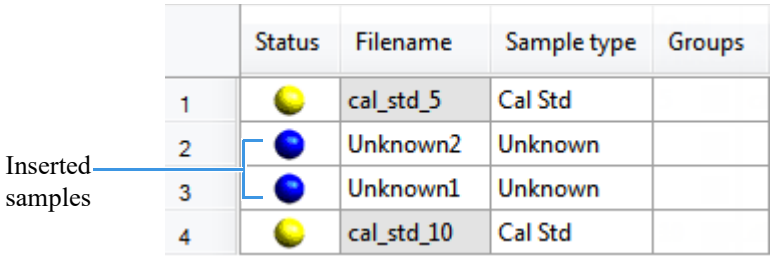
v To insert samples into the list

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

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

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

   The application inserts the Unknown samples above the selected sample.



3. For each sample, type a file name in the Filename column.

   Each file name must be unique.

4. For each sample, select a sample type from the Sample Type list.

Available sample types			
Matrix Blank	Solvent	QC	Unknown
Cal Std			

5. For each Cal Std 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.

6. (Optional) To assign samples to a group, do the following:

   a. For each sample, type the group name in the Groups column.

      Repeat this for each sample that you want to include in a group.

   b. Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
	Benzo26473	groupB, groupA
	Benzo25557	groupB
	Benzo26154	groupB, groupA

The application uses only the first group listed for calculating the Maximum Fold and Group Averages.

For information about Maximum Fold analysis in unknown screening analysis, see Cross Sample Peak List pane.

- For quantitation experiments, after creating groups, you can choose one of the samples as a threshold sample for the group and then compare all of the samples in the Comparative View in the Analysis mode.

  For information about specifying a threshold sample for a group of samples, see Threshold Samples page for quantitation batches. For information about viewing grouped samples in Data Review, see Comparative View for quantitation batches. For information about Group Averages, see Group Averages.

- For unknown screening experiments, you can create a control group (specify the group name as Control) to use for group averages in Data Review. For information about group averages, see Group Averages pane.

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

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

8. For each sample, type a volume in the Injection Volume column.

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

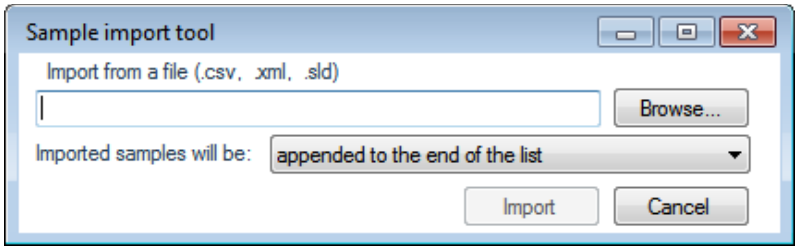
9. (Optional) Type or edit the values for the remaining columns.

Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name, while the other columns scroll right and left.

v 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 data format must match the TraceFinder data format.

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

4. Click **Import**.

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

   When you import samples from an Xcalibur sequence file (.sld), the application makes the following column name substitutions.

Xcalibur column	TraceFinder column
Position	Vial position
Inj Vol	Injection volume
Dil Factor	Conversion Factor

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

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	QC
Std Bracket	Cal Std

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

5. For each Cal Std or QC 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.

   For detailed instructions about defining calibration levels, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

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

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

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

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

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

   Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name, while the other columns scroll right and left.

9. (Optional) When using multiplexing on an LC/MS analytical instrument, select a channel for each imported sample.

   Imported samples default to Auto.

v **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**.

v **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**.

   The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

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

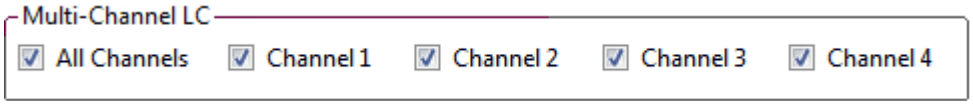
	cal_std_50_INJ001	Cal Std	10
	cal_std_50	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

When you submit this batch, the application acquires only the reinjection samples.

v To select channels for the batch

These features are available only on LC/MS analytical instruments when you have activated the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

- To deactivate a configured channel, clear the check box for the channel in the Multi-Channel LC area at the bottom of the page.



By default, all configured channels are selected. The configured channels are determined by the Multi-Channel LC settings in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

Clearing a channel in the Multi-Channel LC 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.

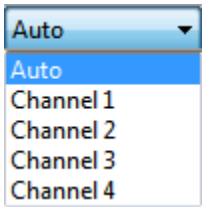
v To assign a specific channel to a sample

1. Scroll to the Channel column.

Note The Channel column is available only on LC/MS analytical instruments when you have activated the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

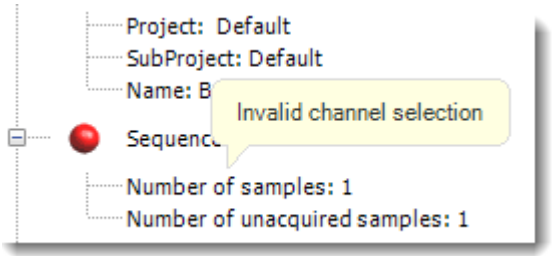
All samples default to Auto.

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.

v **To select a reference sample**

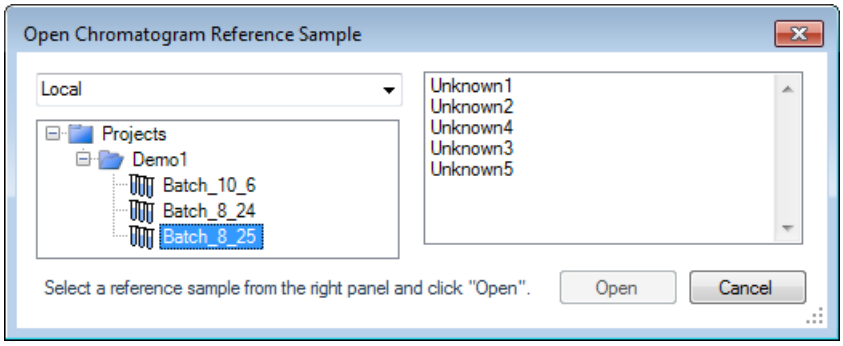
1. Click the **Reference Sample** tab.

   The Reference Sample page on the Sample Definition page opens.

   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**.

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

4. Select a sample from the list of processed samples on the right.

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

5. Click **Open**.

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

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

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

The application uses the peak in this sample as a reference peak in Data Review. See Reference Peak.

v To add an auto sample type

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

   The Auto Samples page opens.

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

   The application adds a Solvent sample to the sample list.

   You can add, insert, or remove samples from this list as you would any sample list.

3. To change the sample type to a Matrix Blank, click the Sample Type column and select **Matrix Blank** from the list.

4. In the Injection Volume column for the sample, type a volume.

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

5. In the Number of Injections column, type the number of injections available in the designated Solvent or Matrix Blank vial.

   After auto sample injections have occurred, you can return to this page to view the number of Injections Used in each vial.

6. In the Vial Position column, type the vial position for the Solvent or Matrix Blank sample.

v To specify different instrument methods for samples

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**.

      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**.

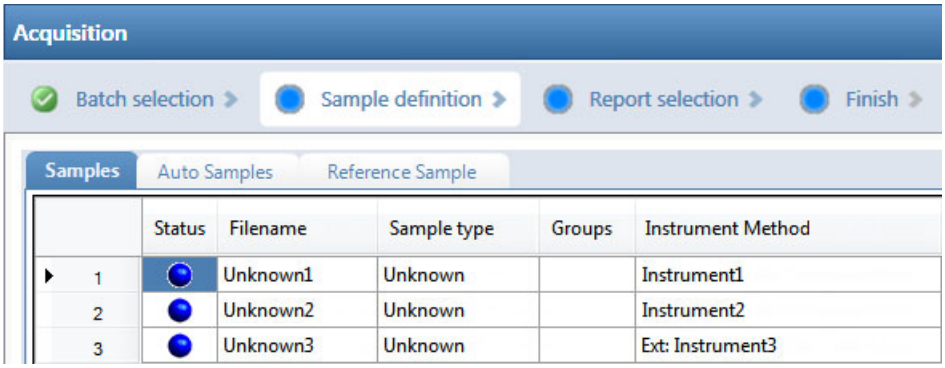
   The application displays the Instrument Method column, defaulting to the instrument method specified in the master method.

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 11. 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\Projects\…*batch*\Methods*method*\Data*ExternalMethods*

Local instrument methods:

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

Samples

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

Figure 12. Samples page on the Sample Definition page

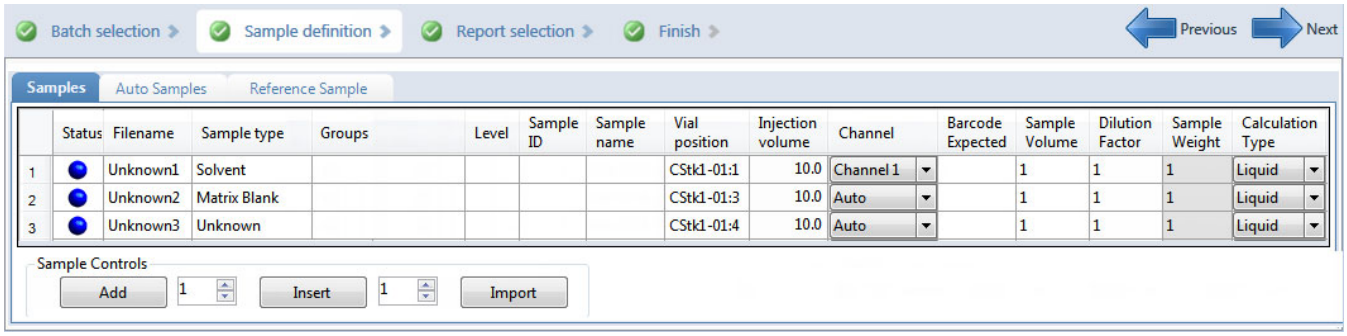


Table 5. Samples page parameters (Sheet 1 of 2)

Parameter	Definition
Previous	Returns you to the previous Acquisition page.
Next	Takes you to the next Acquisition page.
Status	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.
Multi-Channel LC	These features are available only on LC/MS analytical instruments when you have activated the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.
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.
Remove Selected Samples	Removes selected samples from the sample grid.
Import Samples	Opens the Sample Import Tool. Follow the instructions To import samples into the list.

Table 5. Samples page parameters (Sheet 2 of 2)

Parameter	Definition
Browse in Raw File (Move)	Opens the What Raw File Would You Like to Use dialog box where you can select a raw data file to add to the batch. The application moves this raw data file from the original location to the …\TraceFinderData\Projects\…*batch*\Data folder.
Browse in Raw File (Copy)	Opens the What Raw File Would You Like to Use dialog box where you can select a raw data file to add to the batch. The application copies this raw data file to the …\TraceFinderData\Projects\…*batch*\Data folder.
Map Raw Files to Samples	Opens the What Raw File Would You Like to Use 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. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Fill Down	Enters sequential values in the column starting with the value in the selected row and ending with the last row in the column. For detailed instructions about using the Fill Down command, see Appendix B, "Using Copy Down and Fill Down."
Modify Columns	Opens the Modify Columns dialog box. See Column display.
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. For detailed information about editing instrument methods, refer to Chapter 3, "Using Instrument Methods in the Method Development Mode," in the *TraceFinder Lab Director User Guide*.

Column display

The Samples page contains many columns of information. You can scroll to see all the columns, and you can customize which ones to display and their display order. Use the horizontal scroll bar at the bottom of the sample list to view all the information.

Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening) Level, Sample ID, and Sample Name, while the other columns scroll right and left.

1. Right-click the sample list and choose **Modify Columns**.

   The Modify Columns dialog box opens.

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

   These columns appear after the Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

   a. In the Displayed Columns pane, select a column name.

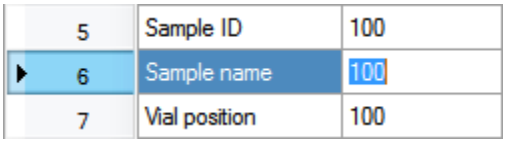
   b. Use **Up** or **Down** to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Samples page sample list, and the last column in the list represents the rightmost column in the Samples page sample list.

      Note The following columns are fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

   a. In the Displayed Columns pane, select the column width.

   b. Type a new value for the width.

5. Repeat step 4 for all columns whose widths you want to change, and click **OK**.

   The columns in the sample list immediately reflect your changes.

Figure 13. Modify Columns dialog box

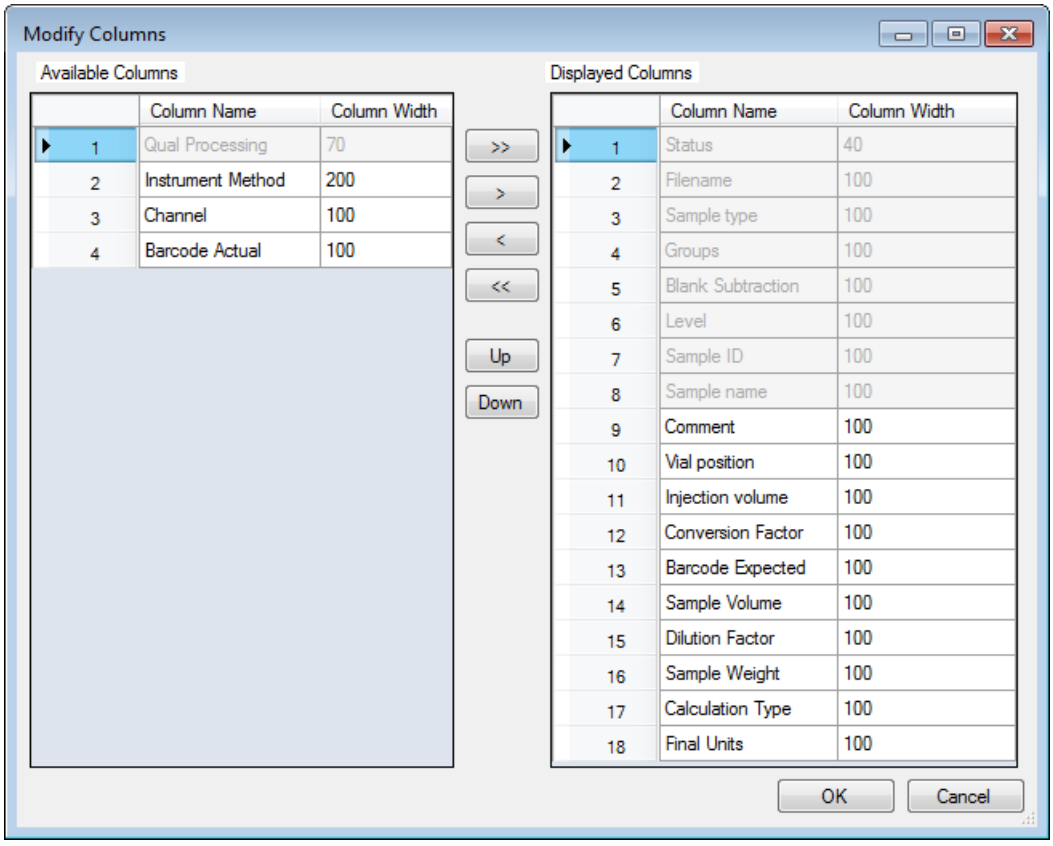


Table 6. Button descriptions for the Modify Columns dialog box

Button	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening), Level, Sample ID, and Sample Name.	
<	Moves the selected column to the Available Columns pane.
<<	Moves all columns except fixed columns.
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.

Auto Samples

Use the features on the Auto Samples page to identify the Solvent or Matrix Blank samples to use for any Auto Sample or Auto Sample and Reinject failure actions as specified on the Intelligent Sequencing page of the method. Refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

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

Figure 14. Auto Samples page on the Sample Definition page

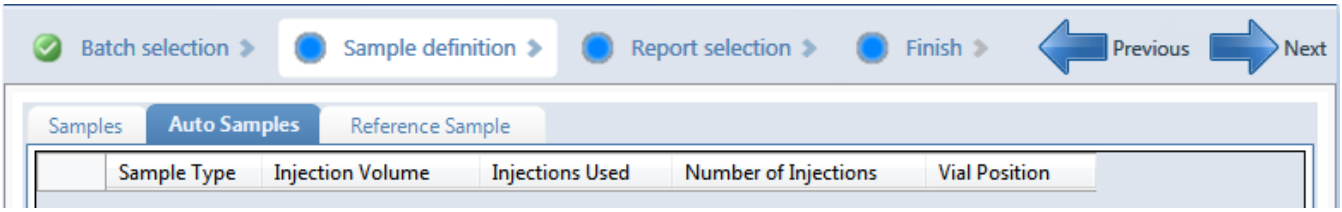


Table 7. Auto Samples page parameters

Column	Description
Sample Type	The sample type for the auto sample injection as specified on the Intelligent Sequencing page of the method—either Solvent or Matrix Blank. Default: Solvent
Injection Volume	The injection volume used for the sample acquisition as specified on the Samples page. Valid range: 0.1 through 5000 µL
Injections Used	The number of times a vial has been used. The count is cumulative across all batches.
Number of Injections	The number of injections available in the designated Solvent or Matrix Blank vial.
Vial Position	Vial position for this sample type as specified on the Samples page.

Reference Sample

Use the features on the Reference Sample page to select a sample to use as a reference peak in Data Review.

Figure 15. Reference Sample page on the Sample Definition page

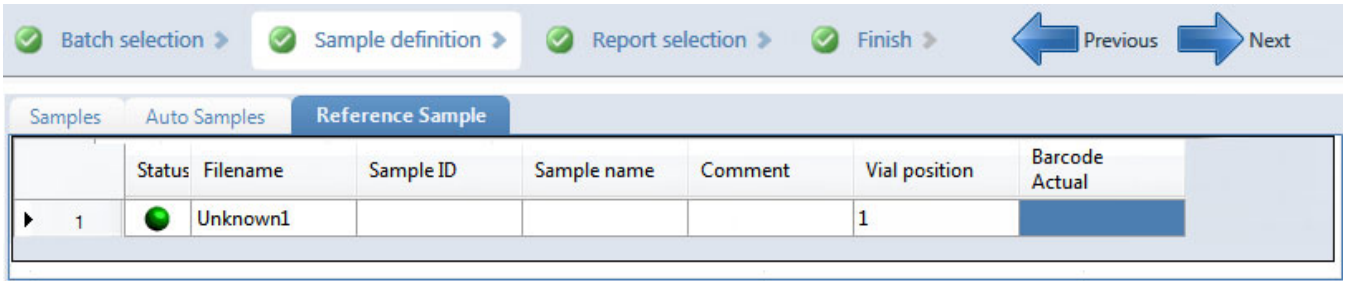


Table 8. Reference Sample page parameters

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

For each report that you generate, you can create a hard-copy printout, a PDF file, a CSV file, or an Excel file.

Use any of the following procedures to create a reports list. When you finish specifying your report options, click **Next** to go to the Finish page and submit your batch. See Submitting a batch in the Acquisition wizard.

The application writes the resulting output files for your reports to the following folder:

…\TraceFinderData\Projects\…*batch*\ReportOutput

Follow these procedures:

- To edit a report title
- To specify a report in print format

v **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.

v **To specify a report in print format**

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**.

   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 16. Report Selection page

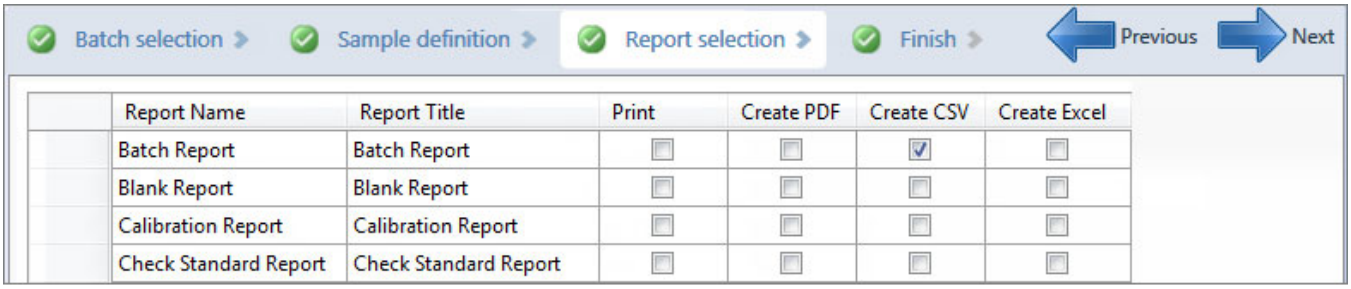


Table 9. Report Selection page parameters (Sheet 1 of 2)

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.

Table 9. Report Selection page parameters (Sheet 2 of 2)

Parameter	Description
Create Excel	Reports to be exported as Excel files.
Shortcut menu: Copy Down	Copies the selected or cleared state to all subsequent reports in the column.

Submitting a batch in the Acquisition wizard

On 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.

Note If you are working with a batch template, the only available function is Save.

Follow these procedures:

- To specify startup or shutdown methods
- To automatically update the timed SRM information
- To specify a calibration batch
- To specify device states
- To save a batch for later acquisition or processing
- To start acquisition or processing
- To view the output files

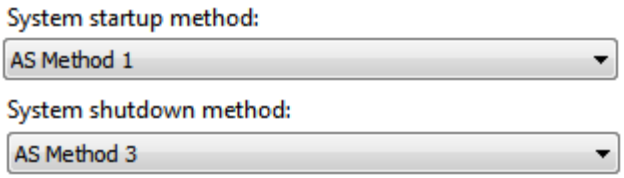
v To specify startup or shutdown methods

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

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

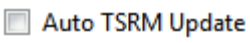
2. Select a method from the System Shutdown Method list.

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



v To automatically update the timed SRM information

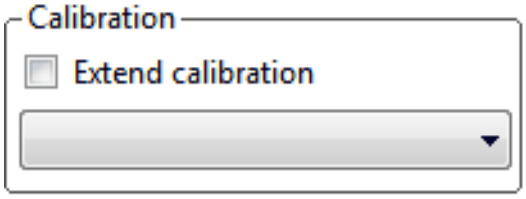
- Select the **Auto TSRM Update** check box.



When you submit the batch, the application updates the TSQ method with mass transitions, collision energy, and other appropriate data for timed selected reaction monitoring (TSRM) functionality.

v 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.

v To specify device states

- In the System Status area, select the name of the device, right-click, and then choose a device state.

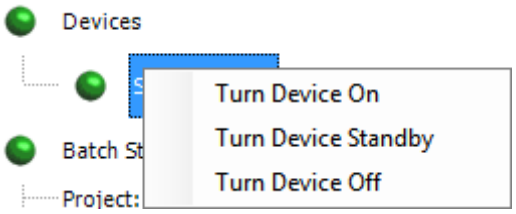


Table 10. Instrument states (Sheet 1 of 2)

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 10. Instrument states (Sheet 2 of 2)

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

v **To save a batch for later acquisition or processing**

- From the Finish page, click Save.

The application saves your batch as a prepared file.

v **To start acquisition or processing**

1. Click Submit.

   The Submit Options dialog box opens.

2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.

   - When all submitted samples have been previously acquired, this option is (by default) not selected.
   - When one or more submitted samples have not been acquired, this option is (by default) selected.

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

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

   The application displays options for each type of method that the batch uses: Quantitation, Target Screening, Unknown Screening, or a combination of methods.

4. For each method type, select the check box for the options that you want to use.

   Peak Detect: Performs peak detection for all method types. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

   Quantitate: Performs quantitation for quantitation methods.

   Identify: Performs identification for unknown screening methods.

   Identify and Confirm: Performs both identification and confirmation for target screening methods.

   With RT Alignment: Performs retention time alignment for unknown screening methods. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.

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

6. (Optional with the Multi-Channel LC feature activated) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.

7. (Optional with the Multi-Channel LC feature activated) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   - **Next Available Batch** places the batch immediately after the currently acquiring batch.
   - **Next Available Sample** places the batch immediately after the currently acquiring sample.

   Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.

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

   b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

      This is usually the autosampler.

   c. Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

      When you clear this check box, individual instruments can start at different times and then must wait for the last instrument to be ready.

   d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.

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

   The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Acquisition mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT When your batch uses unknown screening features, after the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages for the unknown screening features (refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*) and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Figure 17. Submit Options dialog box

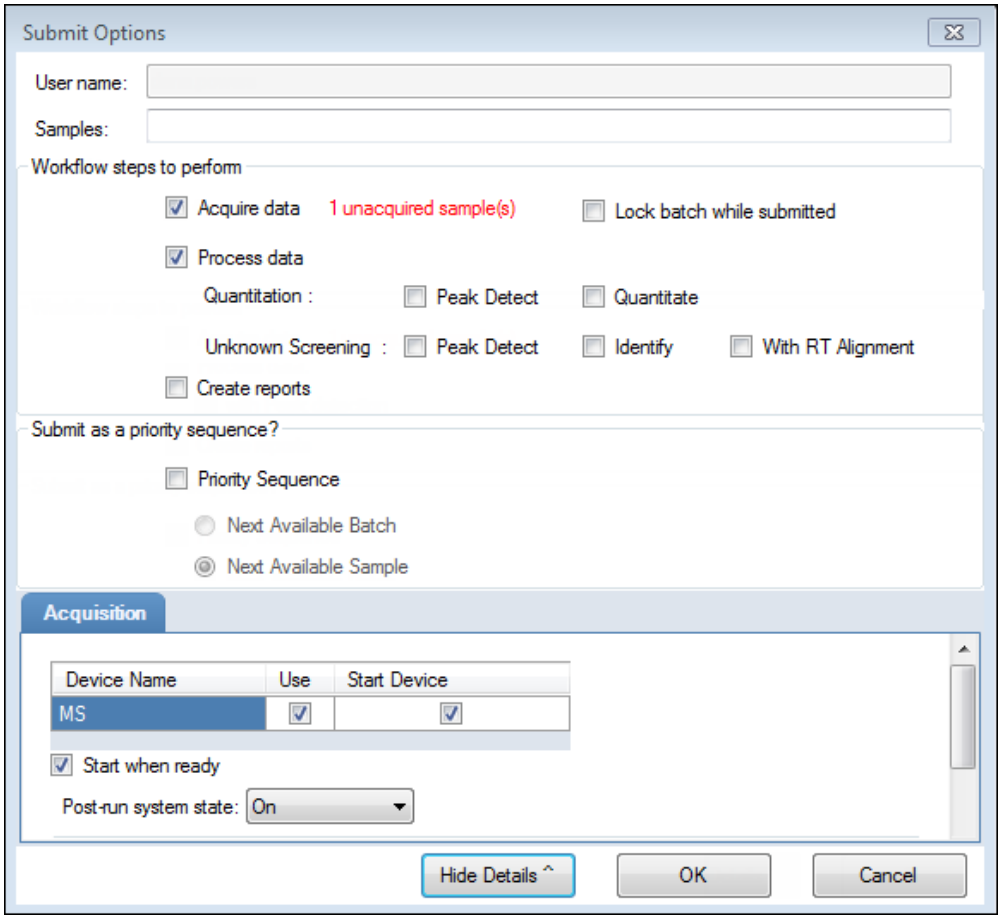


Table 11. Submit Options dialog box parameters (Sheet 1 of 3)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Method Types	Lists the types of methods (quantitation, target screening, or unknown screening) used in the submitted batches.
Workflow Steps to Perform	
Acquire Data	Submits the current batch to acquisition. • When all submitted samples have been previously acquired, this option is (by default) not selected. • When one or more samples in the batch have not been acquired, this option is (by default) selected. • Lock batch while submitted: Prevents users from editing the batch while it is being acquired. Batch View header indicates Read Only.

Table 11. Submit Options dialog box parameters (Sheet 2 of 3)

Parameter	Description
Process Data	Processes the data for the current batch using any of the following options: Peak Detect: Performs peak detection for all method types. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples. Quantitate: Performs quantitation for quantitation methods. Identify: Performs identification for unknown screening methods. Identify and Confirm: Performs both identification and confirmation for target screening methods. With RT Alignment: Performs retention time alignment for unknown screening methods. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.
Create Reports	Creates reports for the current batch.
Submit as a Priority Sequence?	
Priority Sequence	With the Multi-Channel LC feature activated, places the batch immediately after the currently acquiring batch. Without the Multi-Channel LC feature 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 application. You cannot configure an instrument while the TraceFinder application is running. Available only when you select the Acquire Data check box.

Table 11. Submit Options dialog box parameters (Sheet 3 of 3)

Parameter	Description
Use	Specifies the instruments used for this acquisition. Available only when you select the Acquire Data check box.
Start Device	Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler. Available only when you select the Acquire Data check box.
Start When Ready	Starts the specified device when all the instruments are ready to acquire data. When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
Post-run System State	Specifies the system state after it acquires the last batch: On (default), Standby, or Off.
Buttons	
Hide/Show Details	Collapses or expands the acquisition details of the Submit Options dialog box.
OK	Begins the selected processes.
Cancel	Closes the Submit Options dialog box without submitting any tasks.

v **To view the output files**

- Locate the files to view from the following directories:

  The application writes saved batches to the project folder:

  …\TraceFinderData\Projects\…

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

  …\TraceFinderData\Projects\…\Data

  The application saves method information to the batch Methods folder:

  …\TraceFinderData\Projects\…\Methods

  The application writes the reports to the batch ReportOutput folder:

  …\TraceFinderData\Projects\…*batch*\ReportOutput

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 18. Finish page

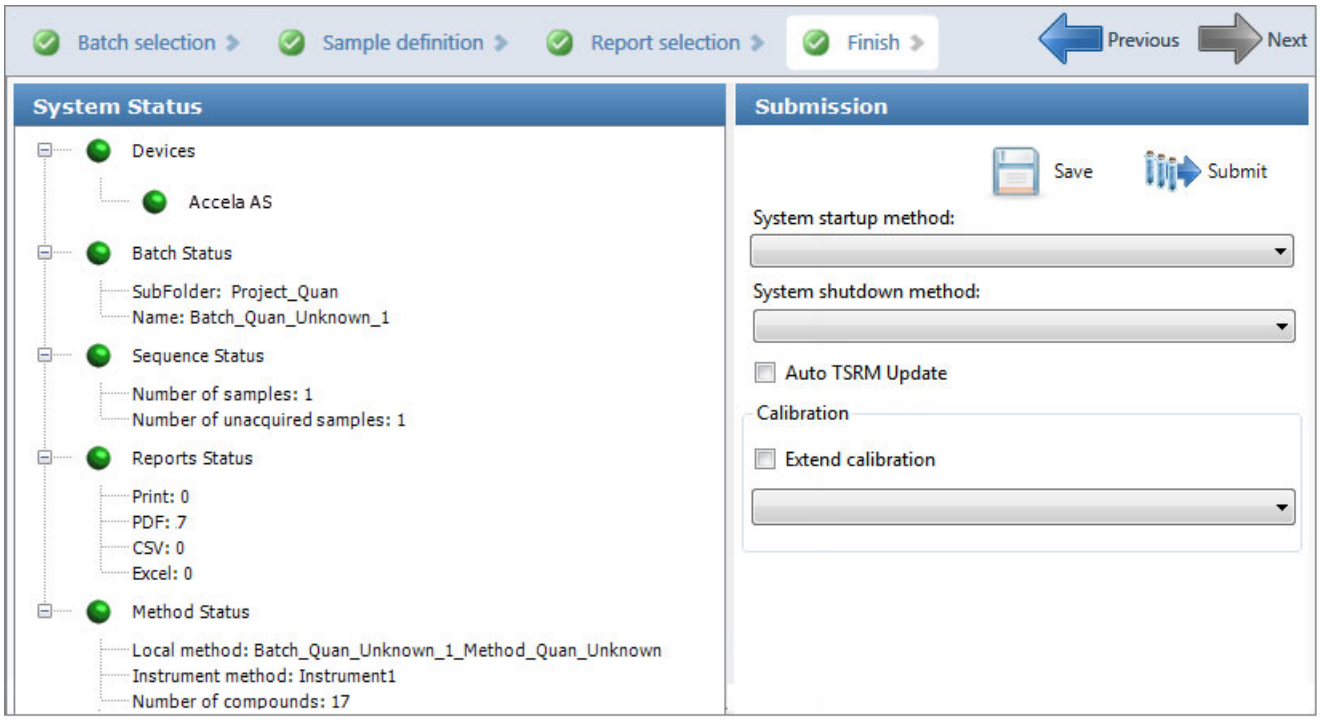


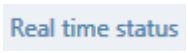
Table 12. Finish page parameters

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.

Real Time Status pane

You can access the Real Time Status pane from any mode in the application. When user security is activated, you must have Real Time Viewer – Edit permission to edit the queues in the Real Time Status pane; otherwise, the Real Time Status pane is read-only.

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

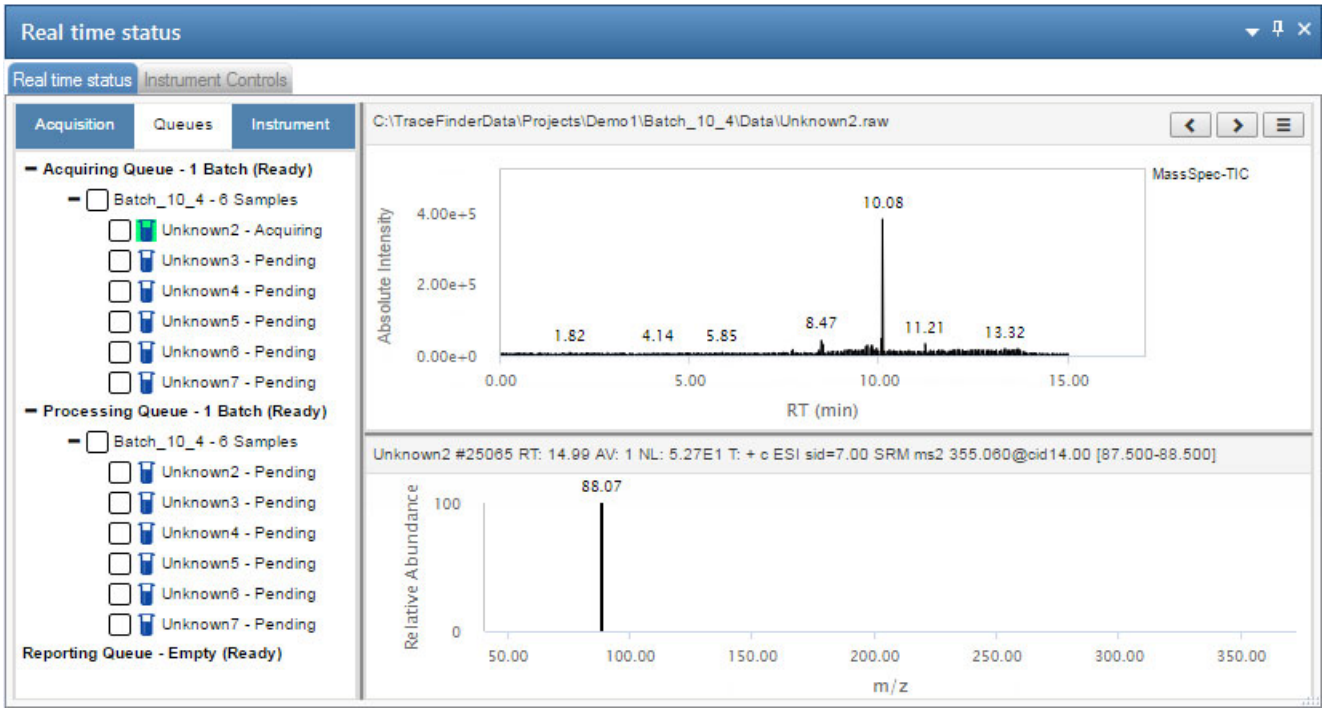
  

  The Real Time Status pane opens at the bottom of the current view.

> **Note** The Real Time Status is also available as a stand-alone window (see Stand-alone Real Time Status window).

Tip (Animation) To view "Using the Real Time Status Pane," see **Help > Animations**.

Figure 19. Real Time Status pane



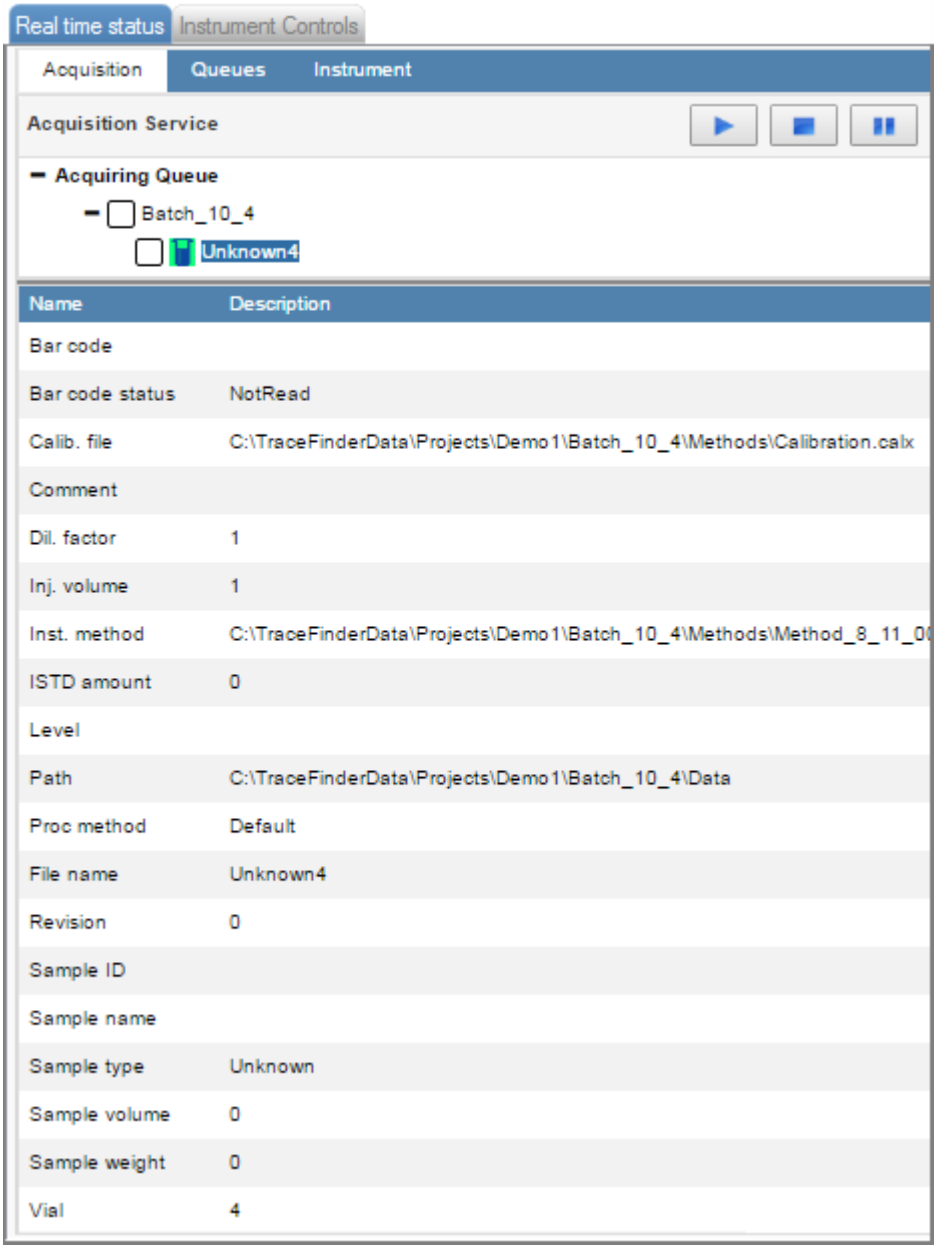
The Real Time Status pane has four pages of information and a real-time trace pane:

- Real Time Status – Acquisition page
- Real Time Status – Queues page
- Real Time Status – Instrument page
- Instrument Controls page
- Real-Time Trace display

Real Time Status – Acquisition page

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

Use the Start, , Stop, , or Pause, , buttons to control batches in the Acquiring



Follow these procedures:

- To remove all pending samples in a batch
- To remove a sample
- To display the last acquired raw data file in a qualitative browser

- To open the Instrument Setup window

v **To remove all pending samples in a batch**

1. Select a batch in the queue.
2. Right-click and choose **Remove Pending Samples.**

   The application removes all pending samples in the batch.

v **To remove a sample**

1. Select a sample.

   Note You cannot remove a sample that is currently acquiring.

2. Right-click and choose **Remove Sample.**

v **To display the last acquired raw data file in a qualitative browser**

- Right-click anywhere on the Acquisition page and choose **View Last Raw File**.

  The last acquired file opens in either the FreeStyle or Qual Browser application.

v **To open the Instrument Setup window**

- Right-click anywhere on the Acquisition page and choose **Open Instrument Method Editor**.

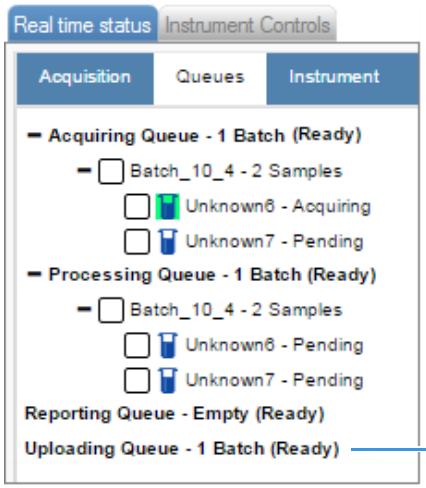
  The Thermo Instrument Setup window opens, displaying the currently running instrument method.

  For detailed information about editing instrument methods, refer to Chapter 3, "Using Instrument Methods in the Method Development Mode," in the *TraceFinder Lab Director User Guide*.

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

Real Time Status – Queues page

Use the Queues page to monitor and control the Acquiring, Processing, Reporting, and optional Uploading queues.



Displayed only when you are uploading to a network repository

- 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.
- Sample-level command: Remove a single sample.

Queue-Level Commands

Use the queue-level commands to pause or remove batches in any of the queues on the Queues page.

Follow these procedures:

- To pause all batches in a queue
- To remove an active batch from a queue
- To remove all batches in a queue
- To remove all pending batches

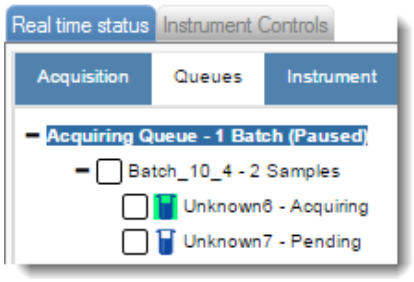
v To pause all batches in a queue

1. Select a queue (Acquiring, Processing, Reporting, or Uploading).

   Note When the Multi-Channel LC feature is activated, you can have as many as four samples acquiring at once. Pausing the Acquiring Queue does not affect any acquiring samples.

2. Right-click and choose **Pause Queue.**

After the current sample is complete, 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.**

v **To remove an active batch from a queue**

1. Select a queue (Acquiring, Processing, or Reporting).
2. Right-click and choose **Stop Active Batch.**

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 is complete, the application removes the batch and all pending samples from the queue. Only the selected queue is affected.

v **To remove all batches in a queue**

1. Select a queue (Acquiring, Processing, or Reporting).
2. Right-click and choose **Stop All Batches.**

The application removes all batches with pending samples from the selected queue. The current sample continues to acquire. Only the selected queue is affected.

v **To remove all pending batches**

1. Select a queue (Acquiring, Processing, or Reporting).
2. Right-click and choose **Remove Pending Batches.**

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.

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.

Follow these procedures:

- To stop a batch
- To remove a pending batch
- To remove all pending samples from a batch
- To remove all selected samples from a batch

v To stop a batch

1. Select an active batch in any of the queues (Acquiring, Processing, or Reporting).

   Note The batch must have at least one active sample and one pending sample.

2. Right-click and choose **Stop Batch.**

   The application confirms that you want to remove the selected batch from the queue. After the current sample is complete, the application removes the batch and all pending samples from the queue.

v To remove a pending batch

1. Select a pending batch in any of the queues (Acquiring, 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.**

   The application confirms that you want to remove the selected batch from the queue and then removes the batch from the queue.

v To remove all pending samples from a batch

- Right-click a batch in any of the queues (Acquiring, Processing, or Reporting) and choose **Remove Pending Samples.**

  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.

v To remove all selected samples from a batch

1. Select the check box for each pending sample that you want to remove.
2. Right-click the batch and choose **Remove Selected Samples.**

The application confirms that you want to remove the selected samples and then removes them from the queue.

Sample-level command

v **To remove a single pending sample from a batch**

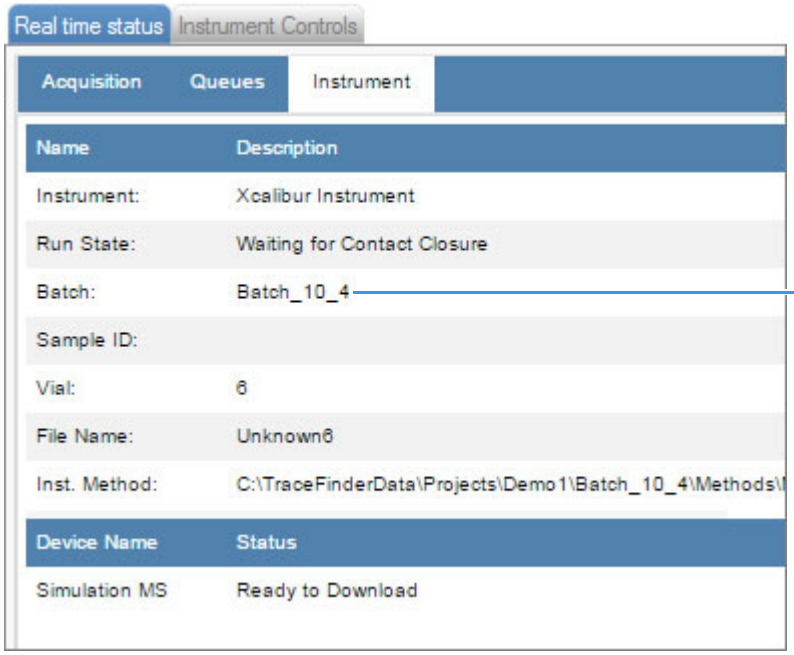
- Right-click the sample and choose **Remove Sample.**

The application confirms that you want to remove the selected sample from the batch and then removes the sample.

Note You cannot remove a sample that is currently acquiring.

Real Time Status – Instrument page

Use the Instrument page to monitor the instrument status for the currently acquiring sample.

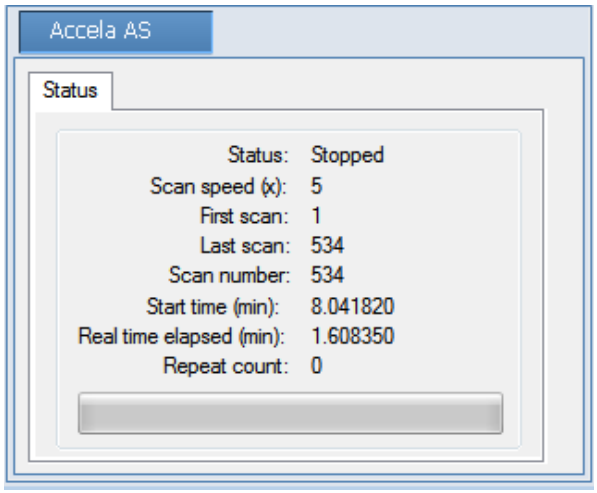


When you run single sample submission, this displays the sample name instead of the batch name.

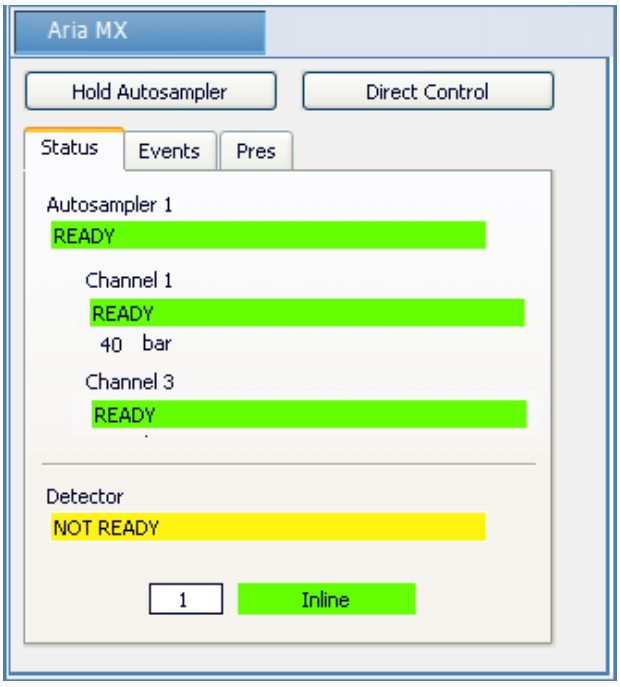
Instrument Controls page

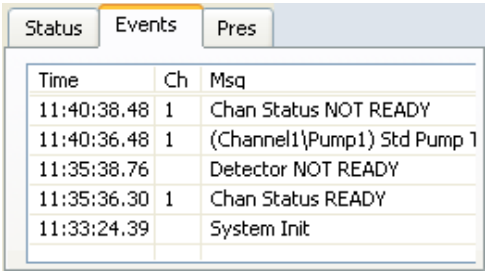
Use the Instrument Controls page to monitor the status of the instrument. The feedback you see on the Instrument Controls page depends on the instrument you are using. The following examples show an Accela™ autosampler and an Aria™ multiplexing device.

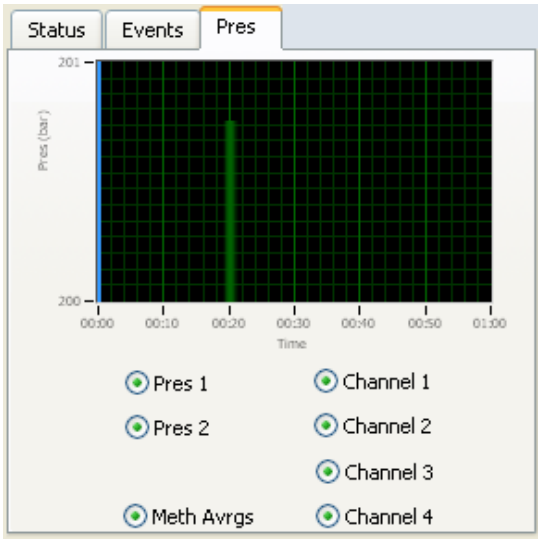
Accela autosampler feedback



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

v 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.

v To control the channels

- Right-click the channel name and choose a command from the shortcut menu.

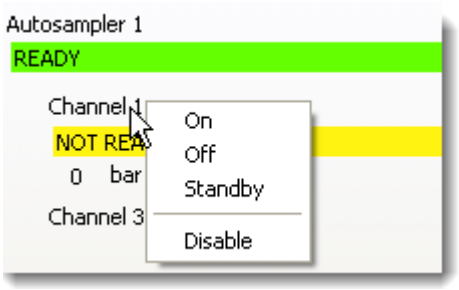


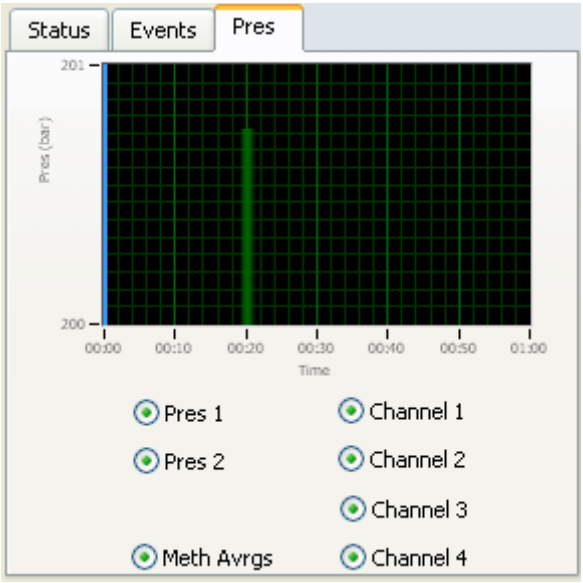
Table 13. Autosampler shortcut menu commands

Command	Description
On	Turns on a stopped pump and continues acquiring the sample list assigned to that channel.
Off	After the current sample is complete, the application stops acquiring and the pump shuts down.
Standby	After the current sample is complete, 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 deactivate 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.

v 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 pressures for all pumps are displayed.

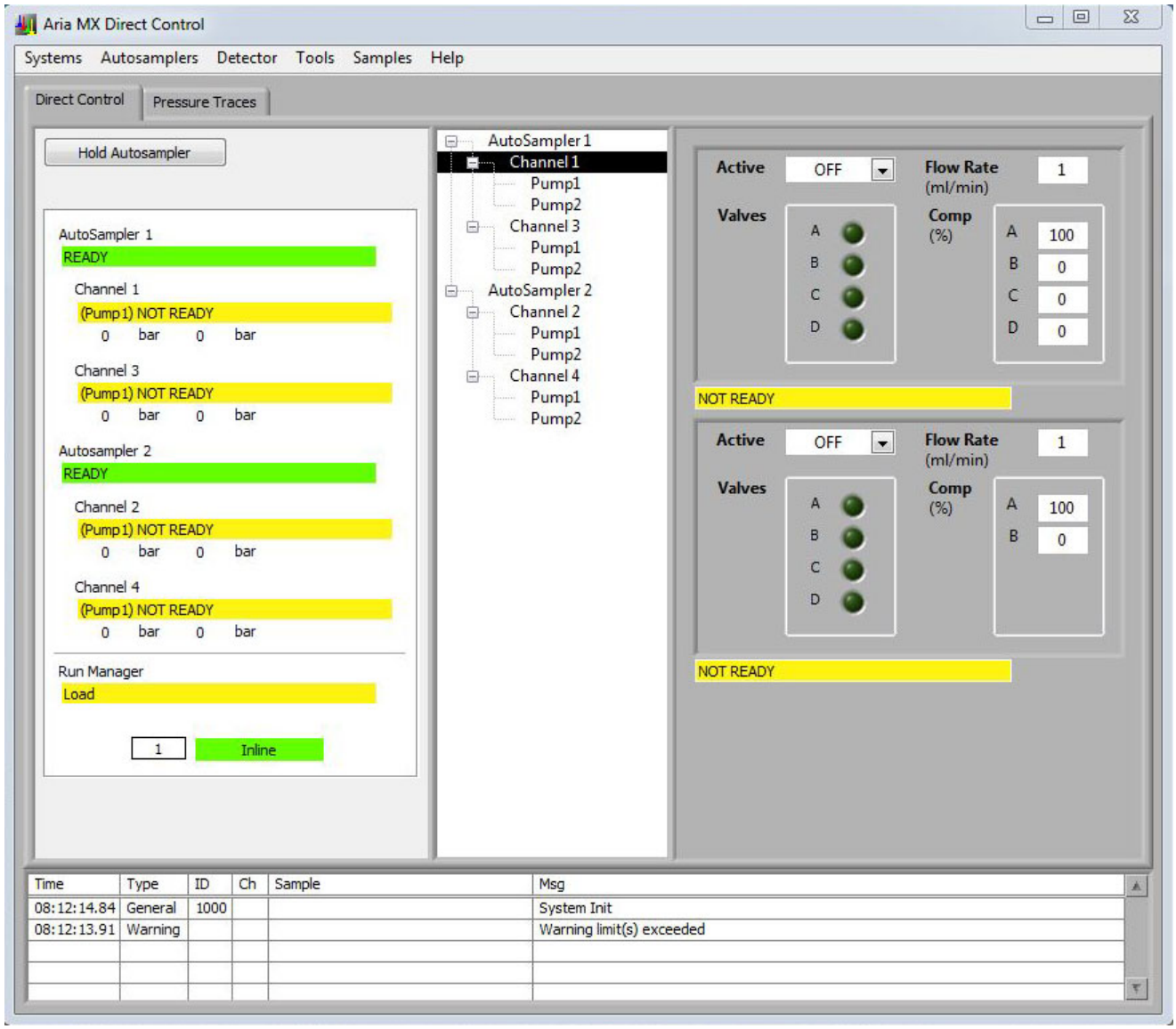
3. To view the pressure for a specific channel, select the corresponding channel number.

   By default, the pressures for all channels are displayed.

v To access the Aria multiplexing controls

- Click **Direct Control**.

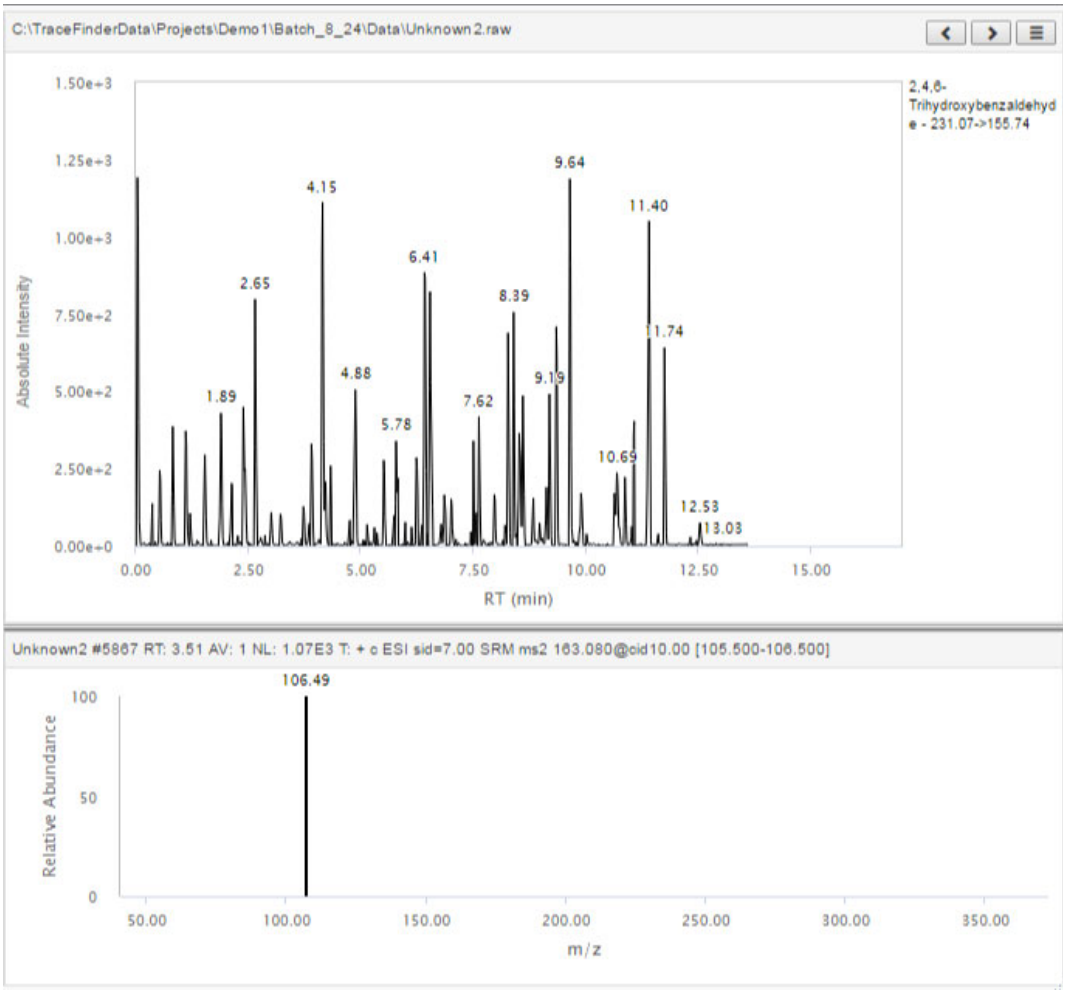
The Aria MX Direct Control window opens.



For detailed descriptions of the features in this window, refer to the *Transcend Systems with Xcalibur Software User Guide*.

Real-Time Trace display

As each sample is acquired, the real-time chromatogram pane shows the retention time, intensity, and relative abundance of the TIC trace.



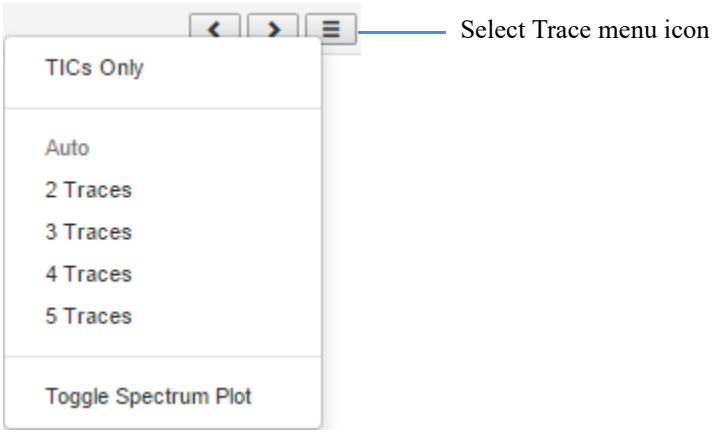
By default, the Real Time Status pane shows only the TIC trace as each sample is acquired. To observe specific traces, such as the internal standard, use the commands in the Select Trace menu to display multiple traces.

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. See Real Time Status pane.

Tip (Animation) To view "Specifying TIC Traces for the Real Time Status Pane," see **Help > Animations**.

Display multiple traces

- Click the **Select Trace** menu icon and choose the number of traces to display.

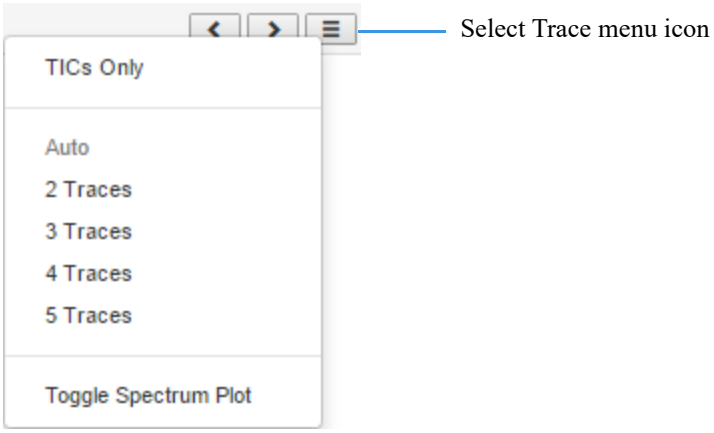


The chromatogram pane displays real-time chromatograms for the selected number of traces.

For each trace, the application displays the mass or precursor mass. See Real-time trace display with multiple traces and a spectrum plot.

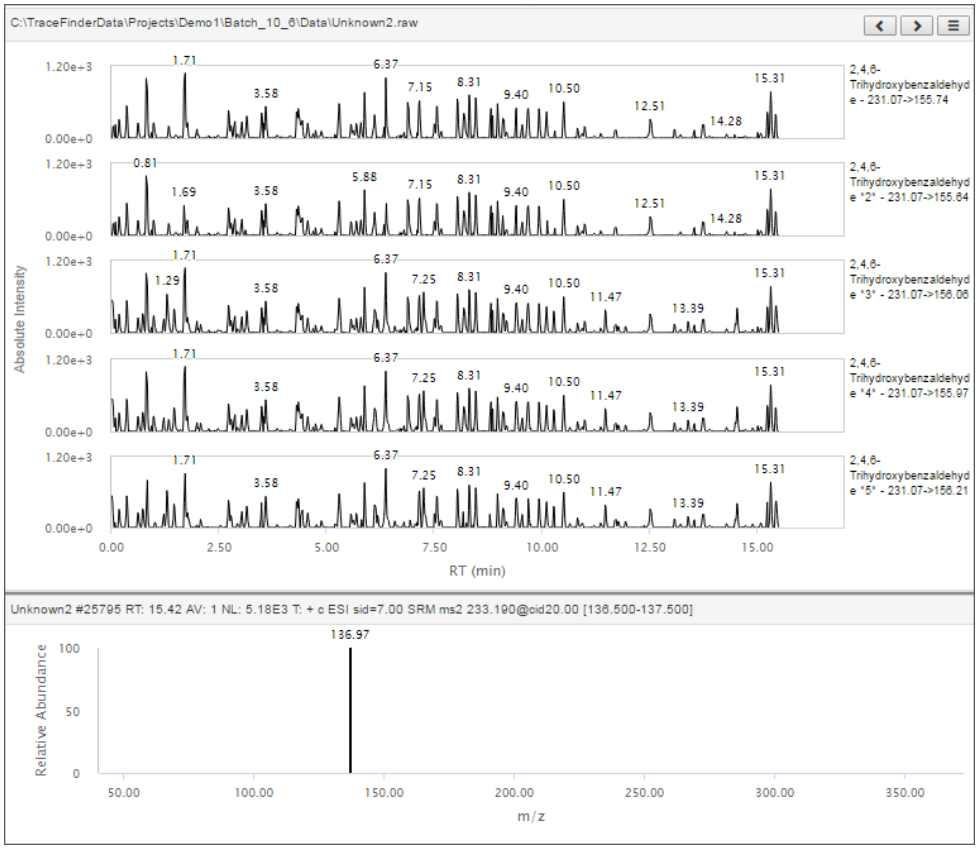
Display the spectrum plot

- Click the **Select Trace** menu icon and choose **Toggle Spectrum Plot**.



The spectrum plot is displayed below the traces in the real-time viewer.

Figure 20. Real-time trace display with multiple traces and a spectrum plot



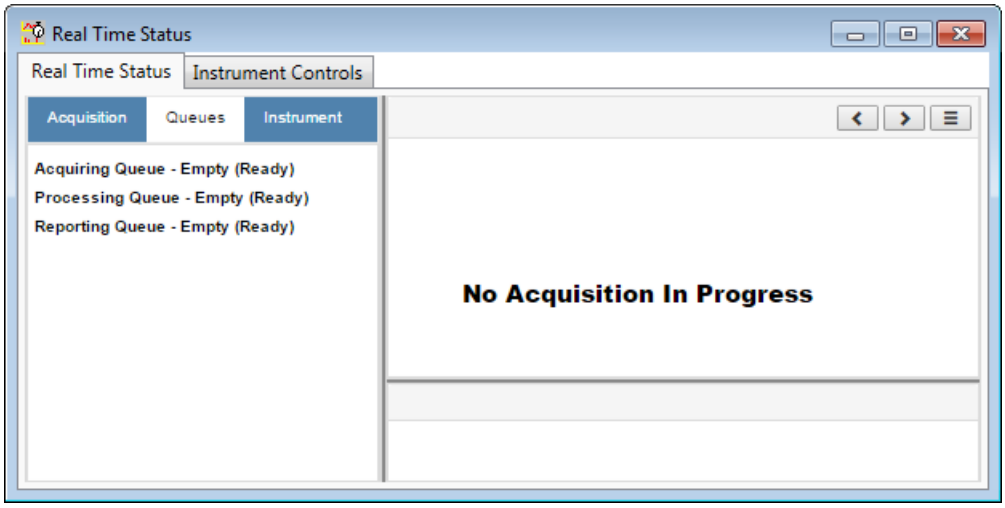
Stand-alone Real Time Status window

Use the Stand-alone Real Time Status window to monitor the Acquiring, Processing, and Reporting queues when the TraceFinder window is closed. You cannot submit samples from this viewer; you can only monitor the status of jobs in the queues.

1. Submit samples from the TraceFinder application.
2. (Optional) Close the TraceFinder application window.
3. From the Microsoft Windows taskbar, choose **Start > All Programs > Thermo TraceFinder 5.2 > TraceFinder Real Time Status**.

   The stand-alone Real Time Status window functions the same as the Real Time Status pane in the main TraceFinder window. See Real Time Status pane.

Figure 21. Stand-alone Real Time Status window



Sample types

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

Table 14. Sample type definitions

Sample type	Definition
Matrix Blank	Contains no target compounds but might contain an ISTD when you use the internal standard quantitative analysis technique. By analyzing a blank sample, you can confirm that there are no residual compounds in the solvent system that can cause erroneous results.
Cal Std	(Calibration standard) Contains known amounts of all target compounds. The purpose of a standard is to measure the response of the instrument to the target compounds so that the processing application can generate a calibration curve for each compound.
QC	(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.
Unknown	Used for quantitative analysis of samples.

4

Using the Analysis mode for quantitation batches

Use the features of the Analysis mode to do the following:

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

Contents

- Working in the Batch View for quantitation batches
- Working in Data Review for quantitation batches
- Working in the Report View for quantitation batches
- Working in the Local Method View for quantitation batches

Working in the Batch View for quantitation batches

In the Batch View, you can manually create and edit a new quantitation batch or open and edit a previously saved batch. When you submit a batch, you can acquire and process data and optionally create reports for the submitted samples.

The Analysis mode includes a toolbar:

Use the Toolbar or the equivalent commands in the Batch View Shortcut Menu to create the sample list and submit samples for acquisition.

See the following topics:

- Samples page for quantitation batches
- Auto Samples page for quantitation batches
- Reference Sample page for quantitation batches
- Threshold Samples page for quantitation batches
- Archiving and importing batches

Samples page for quantitation batches

To open the Samples page, click **Samples** in the Batch View navigation pane.

For details about the Samples page, see the following topics:

- Samples page Features for quantitation batches
- Creating a new quantitation batch
- Editing a quantitation batch
- Submitting a quantitation batch

Samples page Features for quantitation batches

The Samples page is divided into two panes:

- Samples pane

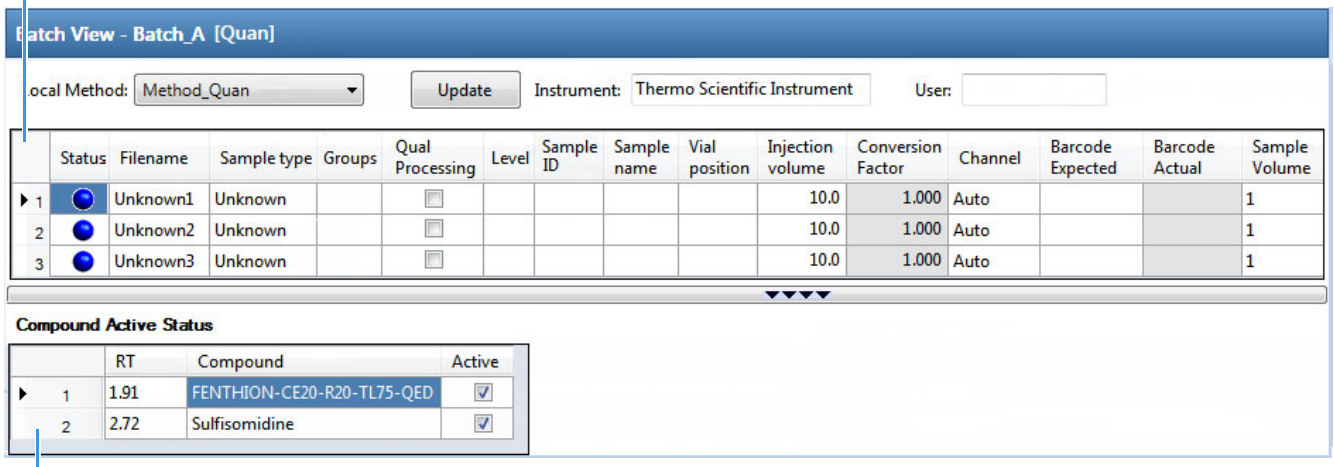
  Use the Samples pane to create a batch.

- Compound Active Status pane

  Use the Compound Active Status pane to make specific compounds active or inactive.

Figure 22. Samples page

Samples pane



Compound Active Status pane

Tip To resize the panes, drag the separator that divides the panes.

Samples pane

The samples pane includes the following features:

- Column display
- Status indicators
- Groups
- Qual Processing
- Sample weight calculation
- Instrument Methods
- Toolbar for quantitation batches
- Batch View sample list
- Batch View shortcut menu for quantitation batches

Column display

The sample list contains many columns of information. You can scroll to see all the columns, and you can customize which ones to display and their display order. Use the horizontal scroll bar at the bottom of the sample list to view all the information.

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

1. Right-click the sample list and choose **Modify Columns**.

   The Modify Columns dialog box opens. For button descriptions, see Table 15.

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

   These columns appear to the right of the sample list's fixed columns: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.

3. To arrange the order of the columns, do the following:

   a. In the Displayed Columns pane, select a column name.

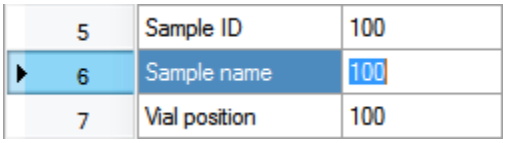
   b. Use **Up** or **Down** to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Batch View sample list, and the last column in the list represents the rightmost column in the Batch View sample list.

      Note The following columns are fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

   a. In the Displayed Columns pane, select the column width.

   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 23. Modify Columns dialog box

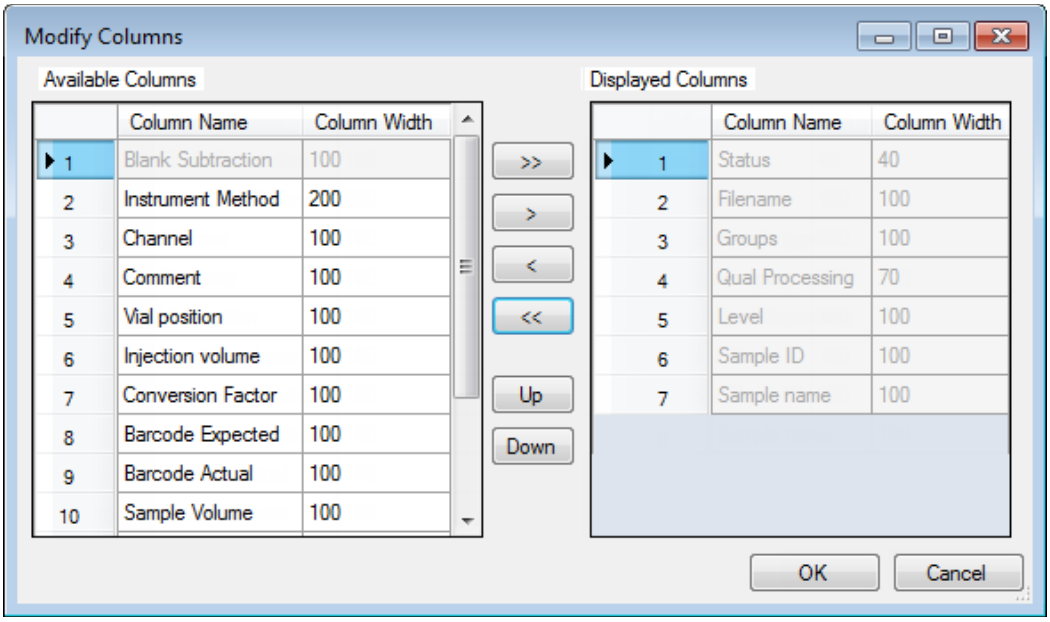


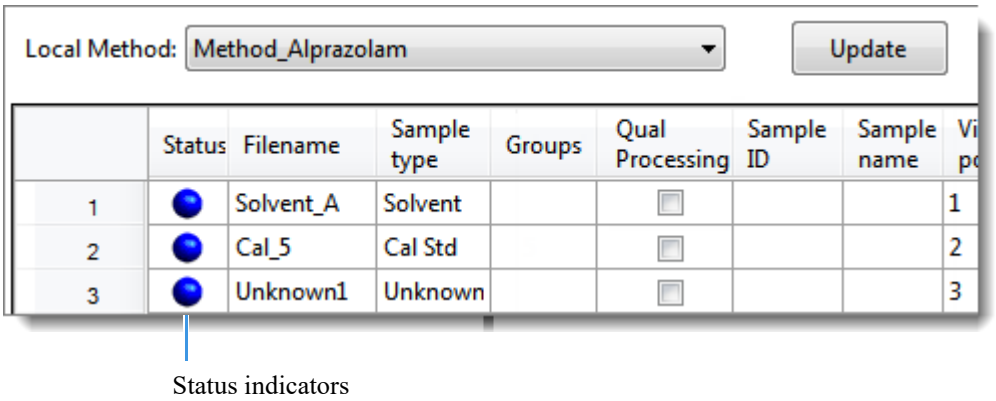
Table 15. Button descriptions for the Modify Columns dialog box

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.

Status indicators

Status indicators show the current status of each sample during acquisition and processing.

- Sample is not acquired.
- Sample is acquired but not processed.
- Sample is acquired and processed.
- Sample is currently acquiring.



Status indicators

Groups

Use the Groups feature to assign samples to a group.

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

   Repeat this for each sample that you want to include in a group.

   Note You must enable custom column in the Application Configuration settings to assign the calibration group to a sample.

   The application supports non-overlapped calibration, which means there can only be one calibration group per sample.

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

Qual Processing

Use the Qual Processing feature to indicate samples to be processed with the qualitative peak processing criteria specified in the method.

Status	Filename	Sample type	Groups	Qual Processing
	VitWaterEquanMaxA001	Unknown		☑
	VitWaterEquanMaxA002	Unknown		☑

The Qualitative View displays processed data for the selected samples. See Qualitative View for quantitation batches.

Note Qual Processing is available only when you have enabled Qualitative Results Display from the Configuration Console. Refer to the instructions in Chapter 1, "Using the Configuration Console" in the *TraceFinder Lab Director User Guide*.

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*

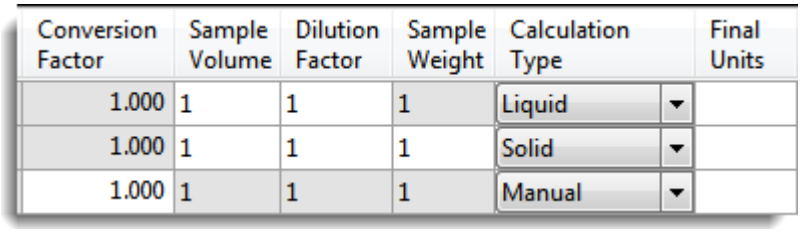
Manual: The application does not calculate the Conversion Factor. Instead, you can enter the Conversion Factor value.

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

v 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**.



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	

v **To calculate the conversion factor for a liquid sample**

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.

Note The application uses the following formula to calculate the Conversion Factor: *SampleVolume* ÷ *DilutionFactor*

v **To calculate the conversion factor for a solid sample**

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.

Note The application uses the following formula to calculate the Conversion Factor: (*SampleVolume* × *DilutionFactor*) ÷ *SampleWeight*

v **To manually specify the conversion factor for a 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.

Note The application uses the specified conversion factor when it calculates the amount for the sample.

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.

1. Display the Instrument Method column in the sample list:
   a. Right-click the sample list and choose **Modify Columns**.

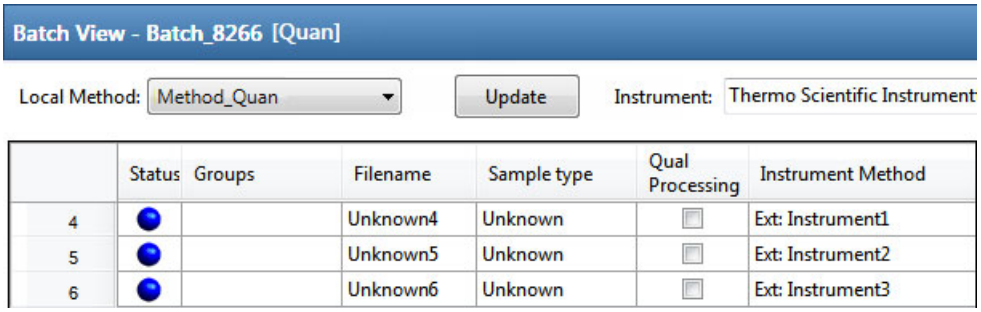
      The Modify Columns dialog box opens.

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

Local instrument methods:

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

Toolbar for quantitation batches

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

Table 16. 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.
	Inserts a new, empty sample or samples above the selected sample. See the instructions To insert samples into the list.
	Removes the selected samples from the sample list. See the instructions To remove samples from the list.
	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.
	Submits only the selected samples for acquisition, processing, or report generation. See the instructions To submit samples in the batch.
	Submits the batch for acquisition, processing, or report generation. See the instructions To submit samples in the batch.
	Submits only the selected peaks for processing. See the instructions To submit selected peaks for processing.
	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 batches.
	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.
	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 8, "Confirming audited changes and using the Audit Viewer." Available only when you enable Auditing in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

Batch View sample list

The sample list, a multi-column table, displays all the quantitative data for the samples of a batch.

Status indicators in the Status column indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The sample list includes the following columns of information:

Figure 24. Batch View sample list

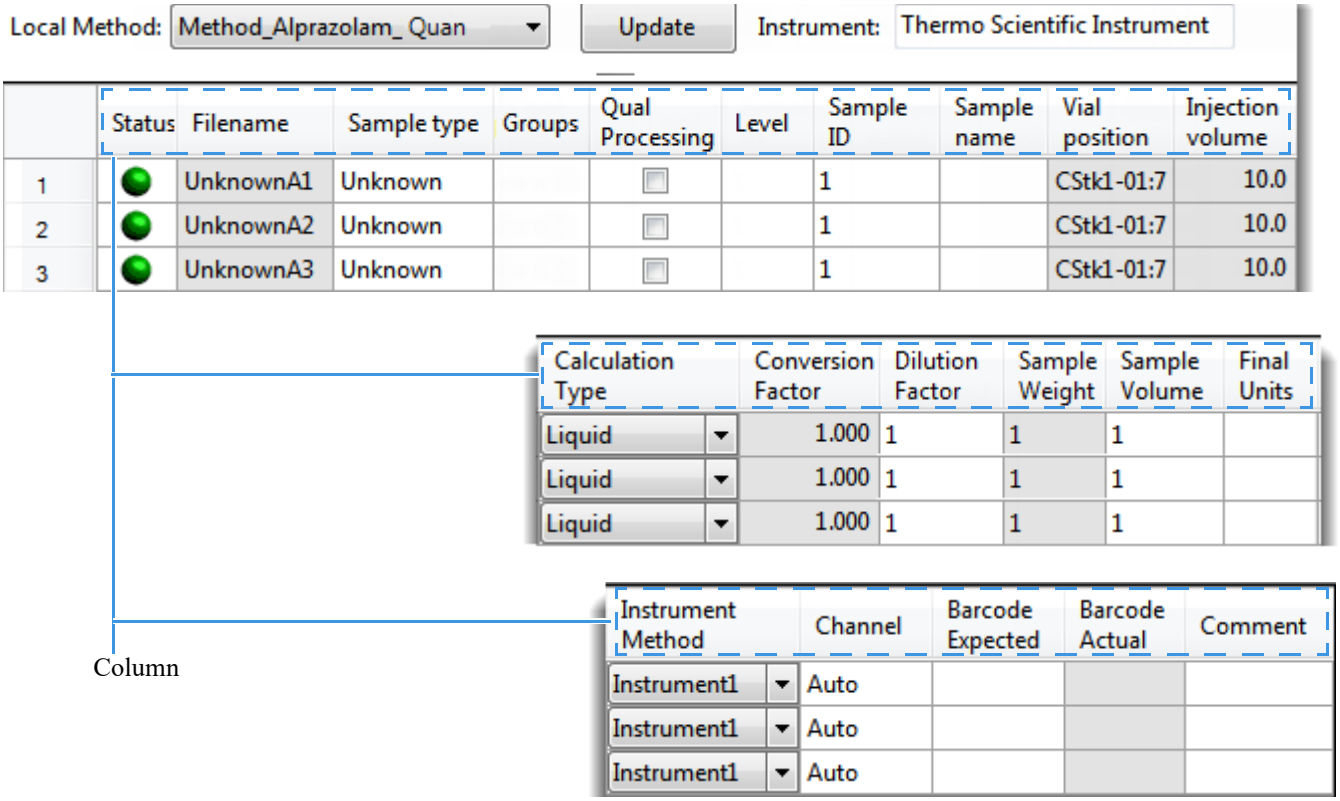


Table 17. Batch View sample list columns (Sheet 1 of 2)

Column	Description
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.
	Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed (), and the Unknown Screening View shows the Status for the samples as acquired but not processed ().
	Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed ().
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 application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC, or Unknown. Default: Unknown
Qual Processing	Indicates samples to be processed with the qualitative peak processing criteria specified in the method. The Qualitative View displays processed data for the selected samples.
Level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined, alphanumeric string that identifies a sample.
Sample Name	A user-defined name that identifies a sample.
Vial Position	The tray vial number used for an autosampler acquisition.
Injection Volume	The injection volume (in microliters) of the injected sample. When you are using an autosampler, you can set the default injection volume in the Autosampler dialog box in the Instrument View. The minimum and maximum injection volumes that you can use depend on the autosampler you configure. The usable range depends on the injection mode and might be smaller than the displayed range. The Injection Volume value set in the master method overwrites the value in the instrument method. Valid range: 0.1 through 5000 µL

Table 17. 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.
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 the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.
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.

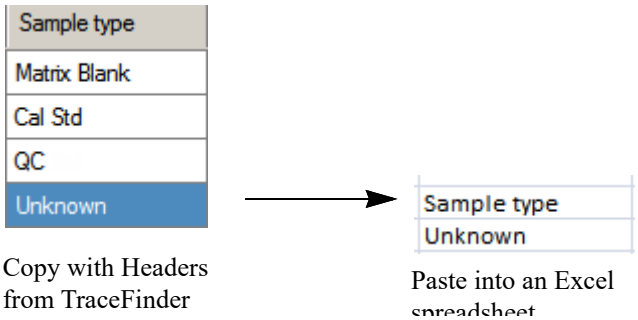
Batch View shortcut menu for quantitation batches

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

Table 18. 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.
Browse in Raw File (Move)	Opens the What Raw File Would You Like to Use dialog box. Select a raw data file to add to the batch. The application moves this raw data file from the original location to the …\TraceFinderData\Projects\…*batch*\Data folder.
Browse in Raw File (Copy)	Opens the What Raw File Would You Like to Use dialog box. Select a raw data file to add to the batch. The application copies this raw data file to the …\TraceFinderData\Projects\…*batch*\Data folder.
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.
Hide Sample Weight Calculation	Displays or hides the Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns.

Table 18. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information into a text editor or spreadsheet application. You cannot paste this data back into the Batch View sample list.
Copy with Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information into another text editor or spreadsheet application, for example,  Copy with Headers from TraceFinder Paste into an Excel spreadsheet You cannot paste this data back into the sample list.
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. For detailed information about editing instrument methods, refer to Chapter 3, “Using Instrument Methods in the Method Development Mode,” in the *TraceFinder Lab Director User Guide*.
View Sample in Qual Explorer	Displays the selected sample in the qualitative explorer application that you configured as your default in the Configuration console. Refer to Chapter 1, “Using the Configuration Console,” in the *TraceFinder Lab Director User Guide*.

Compound Active Status pane

In the Compound Active Status pane, you can choose specific compounds to be 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, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

   - To display compounds alphabetically, right-click and choose **Sort by Compound Name**.
   - To display compounds from shorter to longer retention time, right-click and choose **Sort by Retention Time.**

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

   To change the active/inactive status in the Data Review view, see Inactive and Excluded compounds.

Compound active status

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

Figure 25. Active and inactive compounds in the Local Method View

Local Method View - Batch_2_Method_Vitamin1

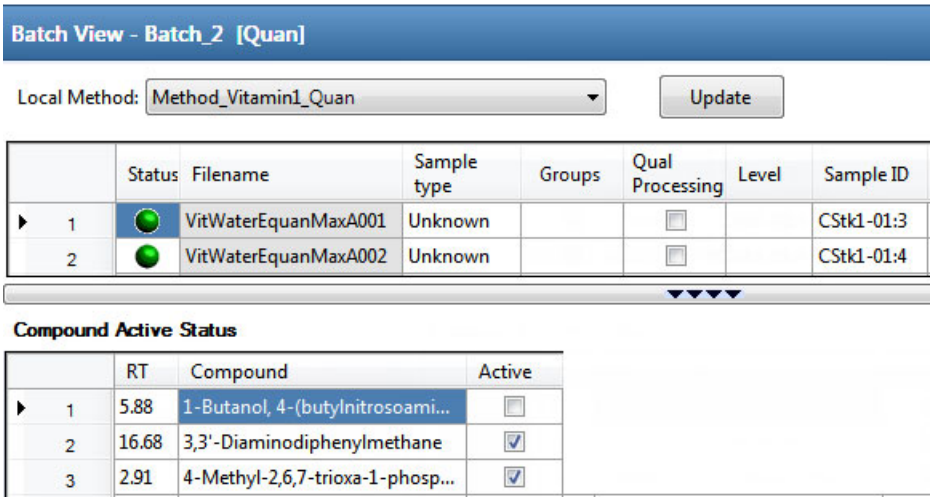
Master method: Method_Vitamin1

Acquisition List | Identification | Detection | Calibration | Calibration levels | Chk Std levels | Real Time View

	RT	Compound	Compound type	Active	CAS No
1	5.88	1-Butanol, 4-(butylnitrosoamino)-	Target Compound	☐	3817116
2	16.68	3,3'-Diaminodiphenylmethane	Target Compound	☑	19471126

For details about setting the status on the Identification page, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

Figure 26. Active and inactive compounds in the Batch View



For details about setting the status in the Batch View, see Compound Active Status pane.

Creating a new quantitation 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

v To create a new batch

1. Choose **File > New > Batch** from the main menu.

   The Create New Batch dialog box opens. See Create New Batch dialog box for quantitation batches.

2. Select a repository from the list.

Tip The application displays all configured and enabled repositories.

The project list displays all projects, subprojects, and batches in the selected repository.

3. Select the folder where you want to store your batch.

   To create a new folder for the storage location, see Editing folders for batches.

4. Type a batch name in the New Batch box.

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.

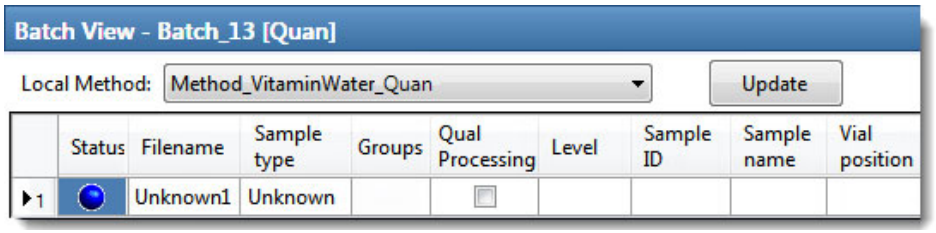
5. To select a master method, do the following:
   a. Select **Quan** from the Type list.
   b. Select a repository from the Repository list.
   c. Select a master method from the Name list.

      The Name list displays all methods for the quantitation type.

6. Click **Create**.

Tip To activate the Create button, you must enter a unique batch name and select a master method. If the Create button is not activated, you have either entered a batch name that is already used or you have not selected a master method.

A new batch opens with one Unknown sample.



The batch name in the title bar indicates that you are creating a quantitation batch.

When you create a batch using a quantitation method that includes unknown screening features, the title bar indicates that the method includes unknown screening.

v To add samples to the list

1. To add a single sample row, right-click the sample list and choose **Add Sample**.
2. To add multiple sample rows, select the number of rows and then click the **Add Sample** icon, .

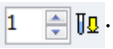
   The application adds the specified number of new, empty samples to the end of the sample list.

v To insert samples into the list

- Select the sample above which you will insert new, Unknown samples, and then do one of the following:

  – To insert a single sample row, right-click and choose **Insert Sample**.

  –or–

  – To insert multiple sample rows, select the number of rows and then click the **Insert Sample** icon  .

  The application inserts the Unknown samples above the selected sample.

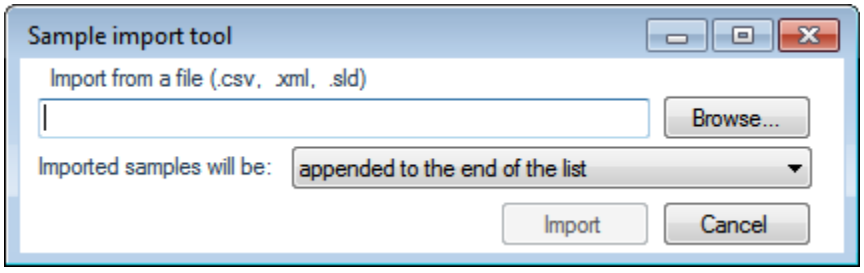
Inserted

	Status	Filename	Sample type	Groups
1		cal_std_5	Cal Std	
2		Unknown2	Unknown	
3		Unknown1	Unknown	
4		cal_std_10	Cal Std	

v To import samples into the list

1. Choose **Batch > Import Samples** from the main menu, or click the **Import Samples** icon, .

   The Sample Import Tool dialog box opens.



   From this dialog box, you can import samples from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file that contains the samples to import.
3. From the Imported Samples Will Be list, select **Appended to the End of the List** or **Inserted at the Selected Row**.

4. Click **Import**.

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

   When you import samples from an Xcalibur sequence file (.sld), the application makes the following column name substitutions.

Xcalibur column	TraceFinder column
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conversion Factor

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

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	QC
Std Bracket	Cal Std

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

   Imported samples default to Auto.

   Note The Channel column is available only when you have activated the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

v **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**.

v **To copy a sample**

1. Select the sample that you want to copy.
2. Right-click and choose **Insert Copy Sample**.

   The application inserts the copy above the selected sample.

v 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**.

   The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

v To edit sample values

1. For each sample, do one of the following:

   - Type a new file name over the current file name.
   - 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**, and then locate a raw data file to use for the sample.

   By default, the application sets the Sample Type to Unknown.

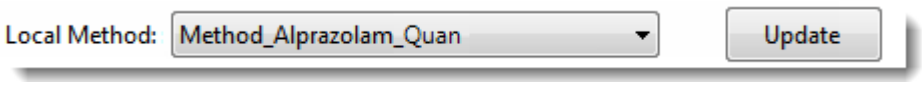
2. For each sample, click the Sample Type column and select a sample type from the list.

Available sample types			
Matrix Blank	Solvent	QC	Unknown
Cal Std			

3. For each Cal Std 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 **Compounds** in the navigation pane.
   d. Click the **Calibration Levels** tab.
   e. Add the levels.
   f. Save the method.
   g. Return to the Batch View in the Analysis mode, and then click **Update**.

   The application updates the local method with the new sample levels.

   For detailed instructions about specifying calibration levels, refer to Chapter 4, “Using the Method Development Mode for Quantitation Methods,” in the *TraceFinder Lab Director User Guide*.

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

5. Type a volume in the Injection Volume column for each sample.

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

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

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

   To automatically copy or fill values in these columns, see Appendix B, "Using Copy Down and Fill Down."

v To browse in raw data files

1. Do one of the following:
   - Double-click the Filename column.
   - Right-click and choose **Browse in Raw File.**

   The What Raw File Would You Like to Use dialog box opens.

2. Select a raw data file to use for the sample or use the CTRL key to select multiple files, and then click **Open**.

   The application overwrites the selected, unacquired sample in the batch with the first "browsed in" file and adds any additional browsed in files below the selected sample.

   For all browsed-in raw data files, the application sets the Status to Acquired, , and sets the Sample Type to Unknown.

   Note You cannot overwrite an acquired sample. When you select a sample that is acquired, the application adds all browsed in files below the selected sample.

v To customize the column display

1. Right-click the Batch View sample list and choose **Modify Columns**.

   The Modify Columns dialog box opens. For button descriptions, see Table 19.

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

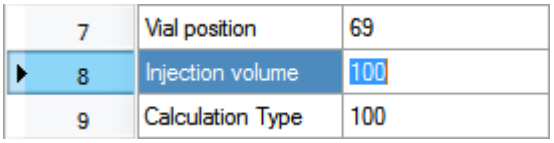
   All the columns you select appear after the Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:
   a. In the Displayed Columns pane, select a column name.
   b. Use **Up** or **Down** to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Batch View sample list, and the last column in the list represents the rightmost column in the Batch View sample list.

      Note The following columns are fixed: Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:
   a. In the Displayed Columns pane, select the column width.



   b. Type a new value for the width.

5. When you have completed your changes, click **OK**.

   The columns in the sample list immediately reflect your changes. The application uses these settings for all sample lists in the Batch View.

Modify Columns dialog box

Use the Modify Columns dialog box to select the columns that you want to display.

Figure 27. Modify Columns dialog box

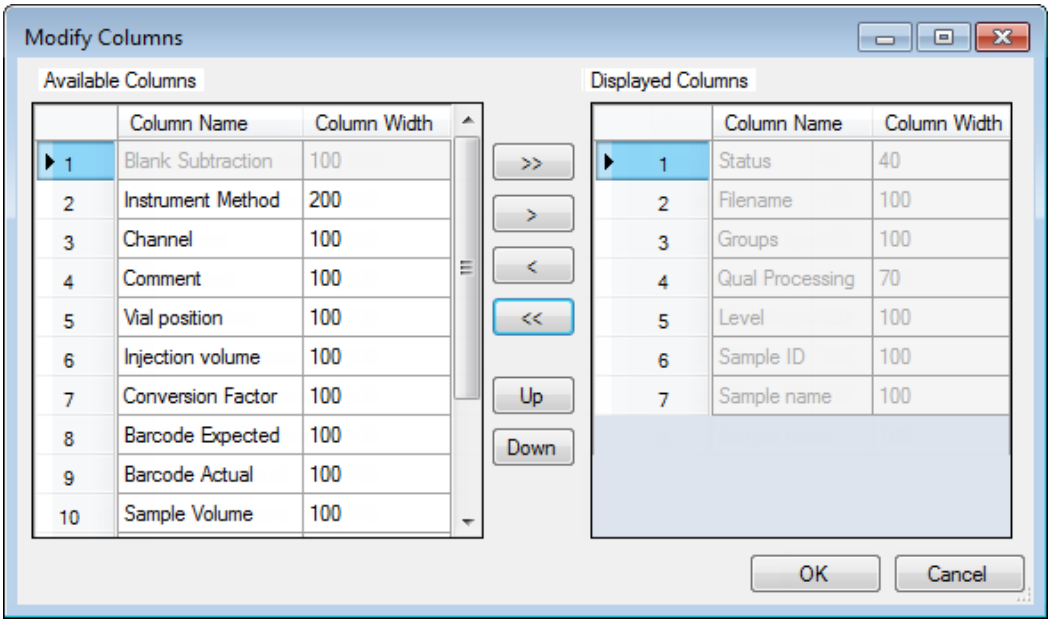


Table 19. Button descriptions for the Modify Columns dialog box

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.

Create New Batch dialog box for quantitation batches

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

Figure 28. Create New Batch dialog box

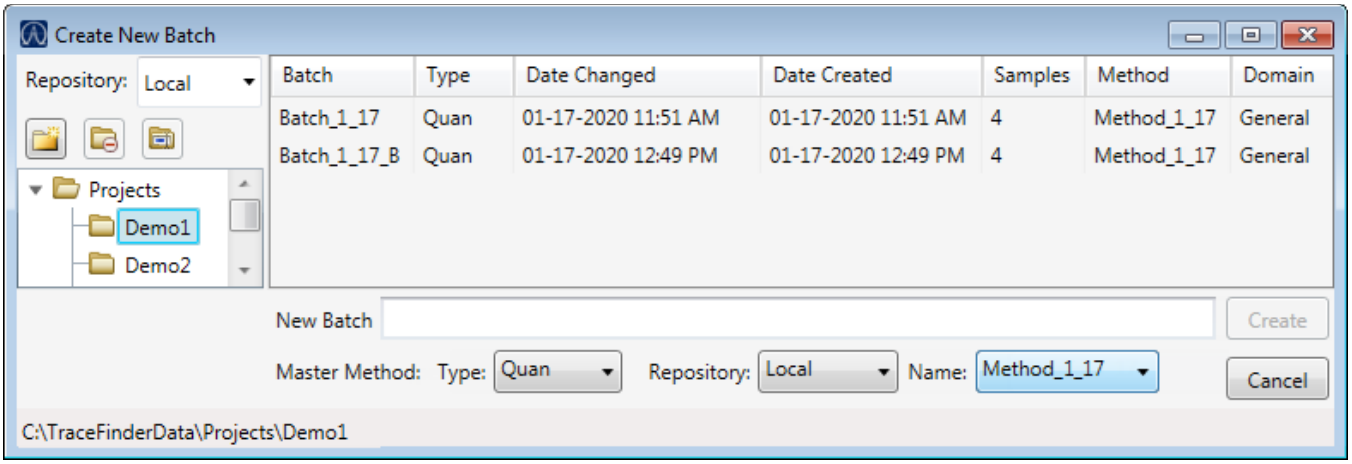


Table 20. Create New Batch dialog box parameters (Sheet 1 of 2)

Parameter	Description
Repository	The default data repository specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

Table 20. Create New Batch dialog box parameters (Sheet 2 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, you can right-click and choose Create Folder.
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, you can right-click and choose Delete.
Rename Folder	Renames the selected folder. Or, you can right-click and choose Rename.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
Batch and Master Method parameters	
New Batch	Name of the new batch to create. **Note** If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Type	Type of batch to create: Quan, Screening, or Unknown Only.
Repository	The repository used to store the new batch.
Name	The method used to create the new batch.
Path	Path to the project in the …\TraceFinderData\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.

Follow these procedures:

- To create new project folders
- To delete project folders
- To rename project folders

v 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\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.

v 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.

v 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 quantitation 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

v To open a saved batch

1. Choose **File > Open > Batch** from the main menu.

   The Open Batch dialog box opens.

2. Select a repository.
3. Select a project and a subproject.
4. Select **Quan** or **Any** from the Type list.

   The batch list displays all batches created with quantitation methods (or all methods of all types when you select Any).

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

   The selected batch opens in the Batch View.

Open Batch dialog box for quantitation batches

Use the Open Batch dialog box to select a batch to open.

Figure 29. Open Batch dialog box

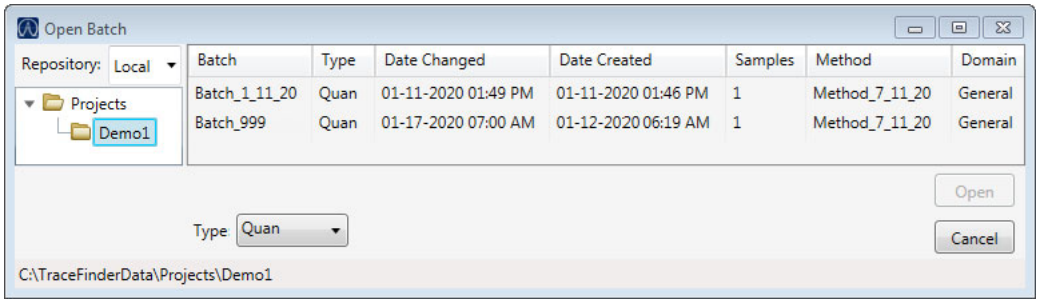
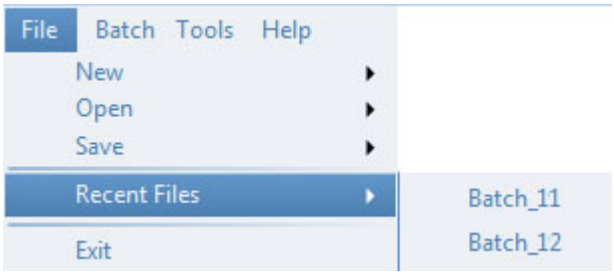


Table 21. Open Batch dialog box parameters

Parameter	Description
Repository	The default data repository specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date the batch was last updated.
Date Created	Date the batch was first created.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Domain	TraceFinder domain in which the batch was created.
Path	Path to the project in the Projects folder where the batch is stored.
Buttons	
Type	Type of batch to display in the Batch list: Quan, Screening, Unknown Only, or Any.
Open	Opens the Batch View for the selected batch.
Cancel	Closes the Open Batch dialog box without opening a batch.

v To open a recent batch

- Choose **File > Recent Files >** ***batch*** from the main menu.



The selected batch opens in the Batch View.

v To edit samples in a batch

- Use the commands described in Working in the Batch View for quantitation batches.

You can add new samples, edit samples, or delete samples.

v **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**.

   The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

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

	cal_std_50_INJ001	Cal Std	10
	cal_std_50	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

   When you submit all samples in this batch, the application acquires all samples (including previously acquired samples).
3. To save this batch with the new samples for reinjection, choose **File > Save > Batch** from the main menu.

   The batch is saved as a prepared batch that is ready to submit. You can open this batch from the Reinject Samples page in the Acquisition mode and submit the batch. The application acquires only the samples that have not been previously acquired.

Submitting a quantitation 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.

For a description of commands in the shortcut menu, see Batch View shortcut menu commands.

Follow these procedures:

- To submit selected peaks for processing
- To submit samples in the batch
- To view the output files

v **To submit selected peaks for processing**

1. In the Peak List, select the **Selected** check box for the peaks that you want to process.
2. Click the **Submit … for Processing** icon, .

   The application processes the selected peaks and updates the data in the Data Review panes.

v 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.

   Note You can also submit only selected peaks for processing. See To submit selected peaks for processing.

2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.
   - When all submitted samples have been previously acquired, this option is (by default) not selected.
   - When one or more samples in the batch have not been acquired, this option is (by default) selected.

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

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

   The application displays processing options for the method.

   If the quantitation method includes unknown screening features, the application also displays unknown screening options. For specifying processing data for batches that also use unknown screening features, see To submit samples in the batch of Chapter 6, "Using the Analysis mode for unknown screening batches."

4. Select the check box for the quantitation options that you want to use.

   Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

   Quantitate: Performs quantitation.

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

6. (Optional with the Multi-Channel LC feature activated) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.

7. (Optional without the Multi-Channel LC feature activated) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   - **Next Available Batch** places the batch immediately after the currently acquiring batch.
   - **Next Available Sample** places the batch immediately after the currently acquiring sample.

   Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.

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

   b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

      This is usually the autosampler.

   c. Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

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

   d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.

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

   The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Analysis mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT When your batch also uses unknown screening features, after the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages for the unknown screening features (refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*) and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Submit Options dialog box for quantitation batches

Use the Submit Options dialog box to submit a batch for acquisition, processing, or reporting.

Figure 30. Submit Options dialog box

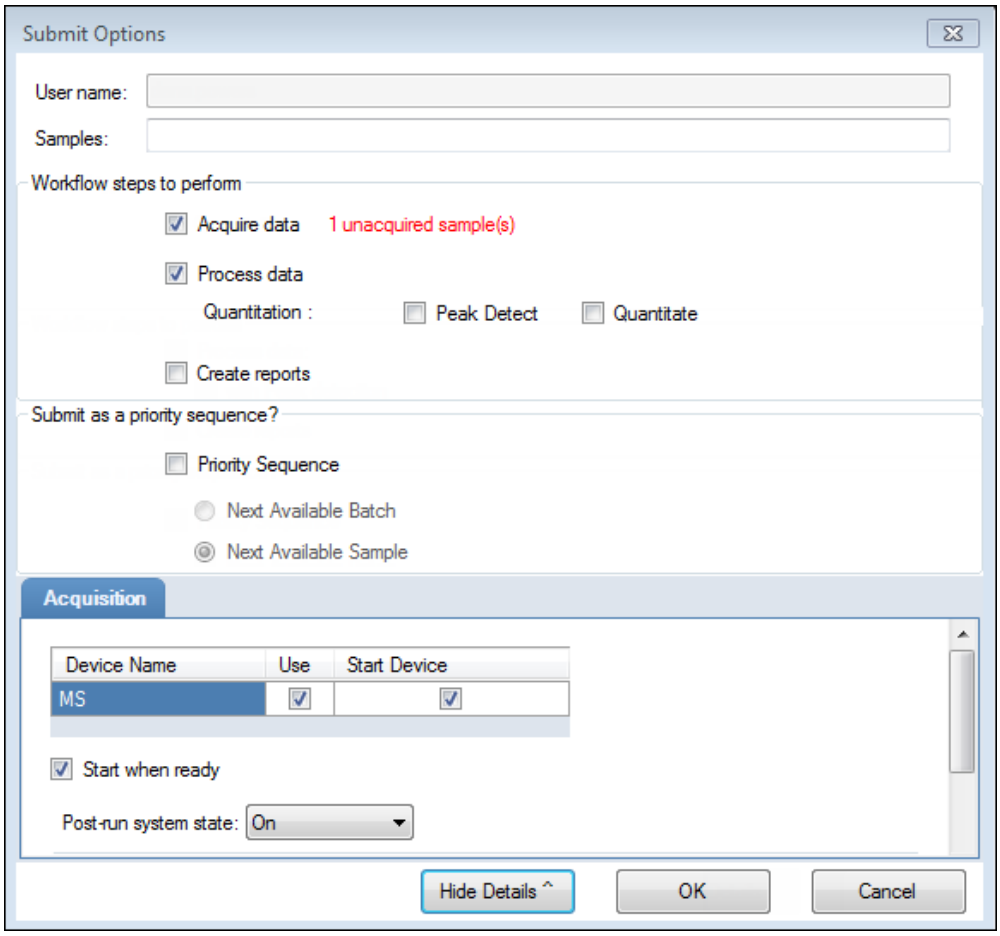


Table 22. Submit Options dialog box parameters (Sheet 1 of 3)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Workflow Steps to Perform	
Acquire Data	Submits the current batch to acquisition. • When all submitted samples have been previously acquired, this option is (by default) not selected. • When one or more samples in the batch have not been acquired, this option is (by default) selected.

Table 22. Submit Options dialog box parameters (Sheet 2 of 3)

Parameter	Description
Process Data	Processes the data for the current batch using any of the following options: Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples. Quantitate: Performs quantitation. **Note** Quantitation methods can include unknown screening features. For specifying processing data for batches that also use unknown screening features, see To submit samples in the batch.
Create Reports	Creates reports for the current batch.
Submit as a Priority Sequence?	
Priority Sequence	With the Multi-Channel LC feature activated, places the batch immediately after the currently acquiring batch. Without the Multi-Channel LC feature 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 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.

Table 22. Submit Options dialog box parameters (Sheet 3 of 3)

Parameter	Description
Start When Ready	Starts the specified device when all the instruments are ready to acquire data. When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
Post-run System State	Specifies the system state after it acquires the last batch: On (default), Standby, or Off.
Buttons	
Hide/Show Details	Collapses or expands the acquisition details of the Submit Options dialog box.
OK	Begins the selected processes.
Cancel	Closes the Submit Options dialog box without submitting any tasks.

v **To view the output files**

- Locate the files to view from the following directories:

  The application writes saved batches to the project folder:

  …\TraceFinderData\Projects\…

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

  …\TraceFinderData\Projects\…\Data

  The application saves method information to the batch Methods folder:

  …\TraceFinderData\Projects\…\Methods

  The application writes the reports to the batch ReportOutput folder:

  …\TraceFinderData\Projects\…*batch*\ReportOutput

Saving a batch to a new location

You can move the current batch to a different project folder, or you can make a copy of the current batch and save the copy to a different project folder.

Follow these procedures:

- To save a batch to another project folder
- To move a batch to another folder
- To create a new project folder
- To delete project folders
- To rename project folders

v To save a batch to another project folder

1. Choose **File > Save > Save Batch As** from the Batch View main menu in the Analysis mode.

   The Save Batch As dialog box opens.

2. (Optional) Select a different repository.

   The default data repository is specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

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.

v To move a batch to another folder

1. Choose **File > Save > Move Batch** from the Batch View main menu in the Analysis mode.

   The Move Batch dialog box opens.

2. (Optional) Select a different repository.

   The default data repository is specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

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.

v To create a new project folder

1. In the Save Batch As dialog box, select the folder for which you will create a new lower-level folder.

   - You can select the main TraceFinderData\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.

v 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.

v 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 and Move Batch dialog box for quantitation batches

Use the features in the Save Batch As dialog box to save a batch to a new name, or use the features in the Move Batch dialog box to move a batch to a different project folder. The features in the two dialog boxes are virtually identical.

Figure 31. Save Batch As dialog box

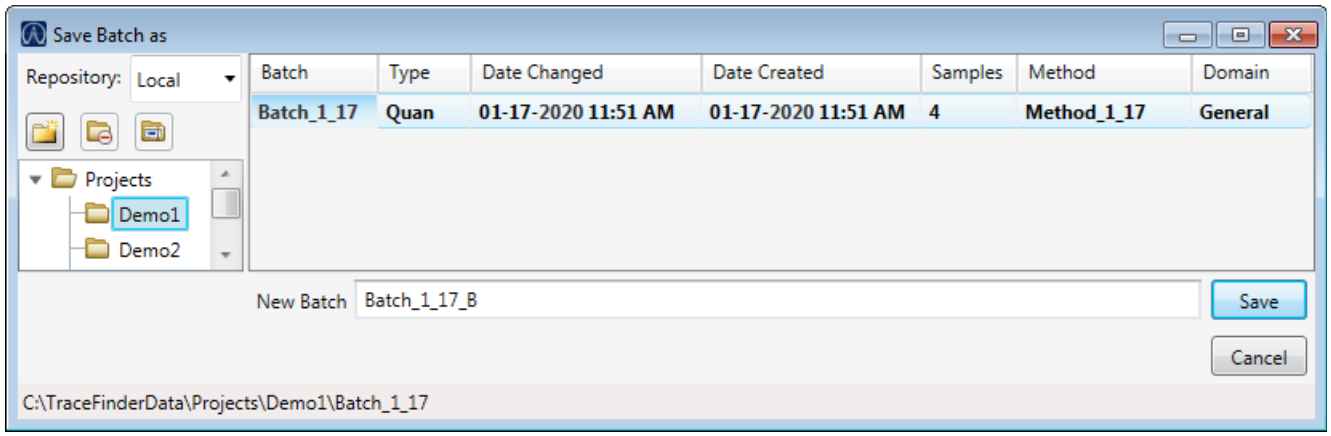


Figure 32. Move Batch dialog box

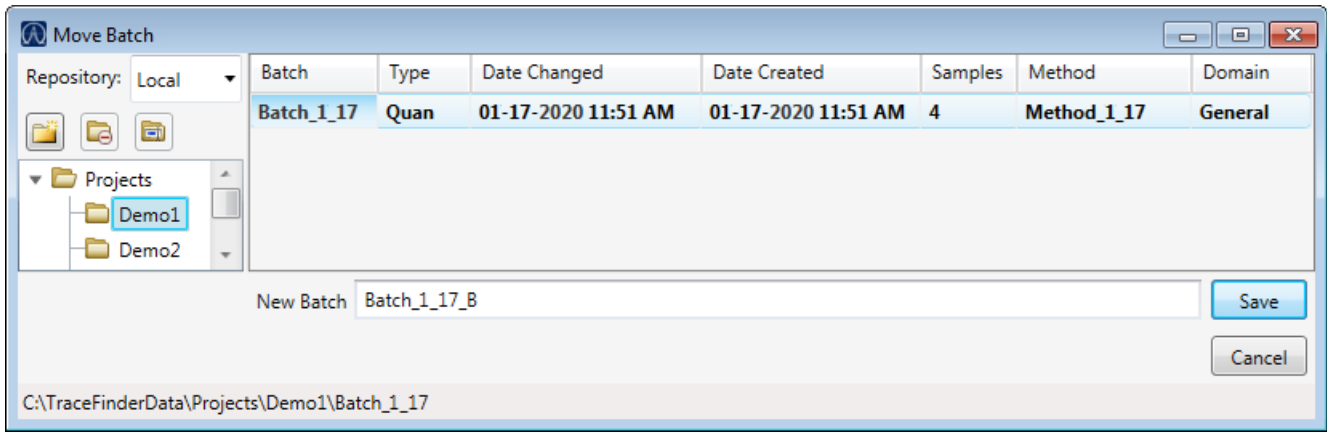


Table 23. Save Batch As dialog box and Move Batch dialog box parameters (Sheet 1 of 3)

Parameter	Description
Repository	The data repository where you want to store the batch.
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, you can right-click and choose Create Folder.

Table 23. Save Batch As dialog box and Move Batch dialog box parameters (Sheet 2 of 3)

Parameter	Description
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, you can right-click and choose Delete.
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, you can right-click and choose Rename.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
New batch parameters	
New Batch	Name of the new batch to create. **Note** If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Path	Path to the project in the TraceFinderData\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.

Table 23. Save Batch As dialog box and Move Batch dialog box parameters (Sheet 3 of 3)

Parameter	Description
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 for quantitation batches

The Auto Samples page identifies the Solvent or Matrix Blank samples to use for any Auto Sample or Auto Sample and Reinject failure actions as specified on the Intelligent Sequencing page of the method. Refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

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.

1. Click **Auto Samples** in the Batch View navigation pane.

   The Auto Samples page opens.

2. Right-click and choose **Add Auto Sample**, or in the toolbar 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 for quantitation batches.

3. To change the sample type to a Matrix Blank, click the Sample Type column and select Matrix Blank from the list.

4. In the Injection Volume column for the sample, type a volume.

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

5. In the Number of Injections column, type the number of injections available in the designated Solvent or Matrix Blank vial.

   After auto sample injections have occurred, you can return to this page to view the number of Injections Used in each vial.

6. In the Vial Position column, type the vial position for the Solvent or Matrix Blank sample.

Auto Samples page

Use the Auto Samples page to specify the sample types to use with Intelligent Sequencing.

Figure 33. 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 24. Auto Samples page parameters

Column	Description
Sample Type	The sample type for the auto sample injection as specified on the Intelligent Sequencing page—either Solvent or Matrix Blank. Default: Solvent
Injection Volume	The injection volume used for the sample acquisition as specified on the Samples page. Valid range: 0.1 through 5000 µL
Injections Used	The number of times a vial has been used. The count is cumulative across all batches.
Number of Injections	The number of injections available in the designated Solvent or Matrix Blank vial.
Vial Position	Vial position for this sample type as specified on the Samples page.

Reference Sample page for quantitation batches

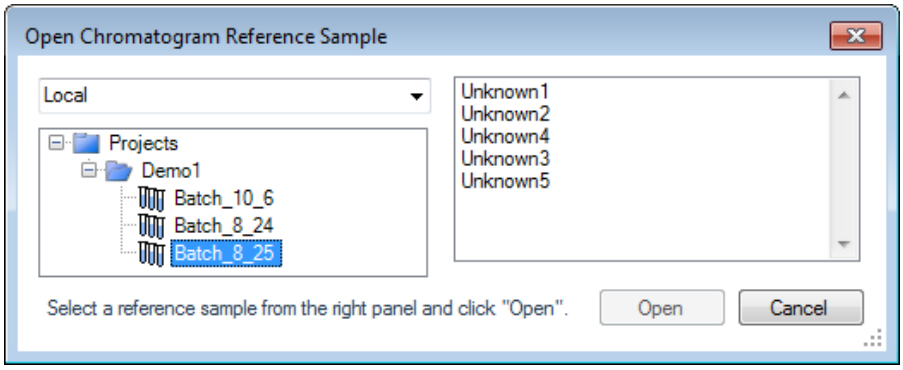
The Reference Sample page displays the reference samples that you selected for this batch.

1. In the Batch View, click **Reference Sample**.

   An empty reference sample table opens.

2. Click the **Add Reference Sample** icon, , in the toolbar, or right-click and choose **Add Reference Sample**.

   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.

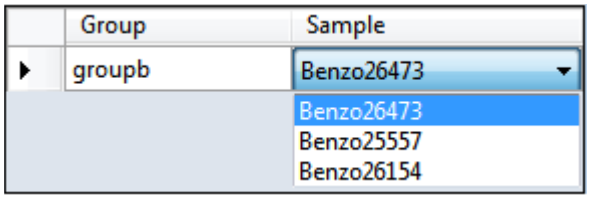
   The application displays all the processed samples in the selected batch. Before using a sample as a reference sample, you must have processed the sample with the current master method.

7. Click **Open**.

Threshold Samples page for quantitation batches

For each group in a batch, you can specify a sample in the group as the threshold sample to use in the Comparative View.

1. In the navigation pane, 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 in the sample peak plots.

To specify the method for creating a threshold guide, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

For information about creating groups, see Groups.

For information about using the threshold guide in the Comparative View, see Comparative View for quantitation batches.

Archiving and importing batches

From any page in the Batch View, you can archive batches or import batches that have been archived.

Import a batch

1. Choose **File > Import Batch** from the main menu.

   The Import Batch dialog box opens.
2. Select a project for the imported batch.
3. Click **Browse** and select a zipped batch file (.zBatch) that contains the batch to import.
4. Type a name for the new batch in the New Batch box.
5. Click **Import**.

   The application extracts the batch from the zipped file in the specified project folder and opens the batch in the Batch View.

Archive the current batch

1. Choose **File > Archive Batch** from the main menu.

   Note You must have an open batch.

   The Browse for Folder dialog box opens.

2. Locate the folder where you want to store the archived batch, and click **OK**.

   The application zips the current batch and moves it to the specified archive folder.

   IMPORTANT The batch is no longer available from its original location. To access the batch, you must import it to your repository. See Import a batch.

   The zipped file includes the processed results, compound database, local method, results, raw data files, report templates, generated reports, and audit logs for the batch.

Working in Data Review for quantitation batches

In the Data Review view, you can view the data generated by the master method. Use Data Review to verify the data for a compound before you generate reports.

Follow these procedures:

- To open the Data Review view
- To restore the default layout

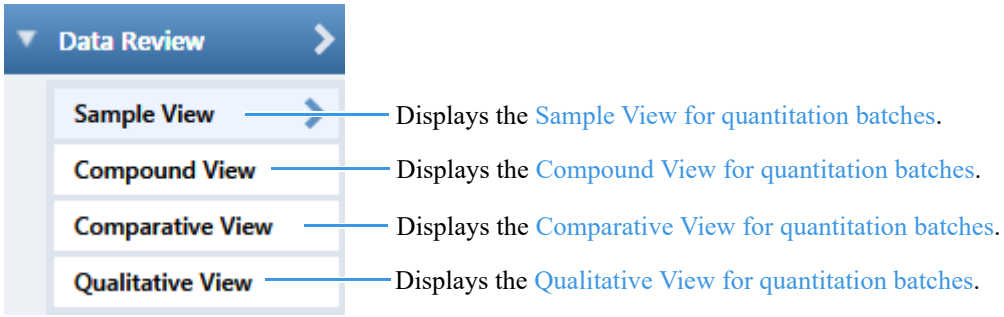
v **To open the Data Review view**

1. Click **Analysis** in the navigation pane.

   The Analysis navigation pane opens.

2. Click **Data Review**.

   The Data Review view opens.



IMPORTANT In the Data Review view, you might be restricted to the Survey Mode display (refer to the *TraceFinder Administrator Console User Guide*).

When you are assigned strict Survey View permission, the Data Review header shows **Survey Mode** and only Cal Std and QC sample types are displayed during processing.

When you are assigned loose Survey View permission, the Data Review header shows **Survey Mode – Loose Restrictions** and only Cal Std and QC sample types are displayed during processing. But after processing is completed, all sample types are available.

Choose from a Sample View, Compound View, Comparative View, or Qualitative View to analyze the data generated by the master method. In any of these views, you might also be restricted to the Survey Mode display (refer to the *TraceFinder Administrator Console User Guide*).

In addition to the information in these views, see the following topics:

- Compound Details for quantitation batches
- Column parameters for Compound Results and Sample Results

v **To restore the default layout**

- Choose **View > Restore Default Layout**.

  The Sample View, Compound View, Comparative View, and Qualitative View have their own defaults for which panes are displayed and in which location.

Survey Mode for quantitation batches

When you are assigned strict Survey View permission, the Sample View, Compound View, and Comparative View headers show **Survey Mode** and only Cal Std and QC sample types are displayed during processing.

When you are assigned loose Survey View permission, the Sample View, Compound View, and Comparative View headers show **Survey Mode – Loose Restrictions** and only Cal Std and QC sample types are displayed during processing. But after processing is completed, all sample types are available.

Sample View for quantitation batches

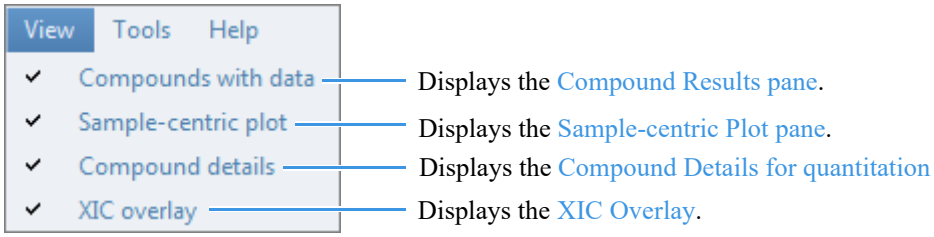
The Sample View displays a list of all samples in the current batch and the compound results for all compounds in the method.

- From the View menu, choose to display or hide any of the following panes.

Note The Samples pane is required for the Sample View display. You cannot hide the Samples pane.

A check mark indicates a displayed pane.

The Sample View display includes the following features:



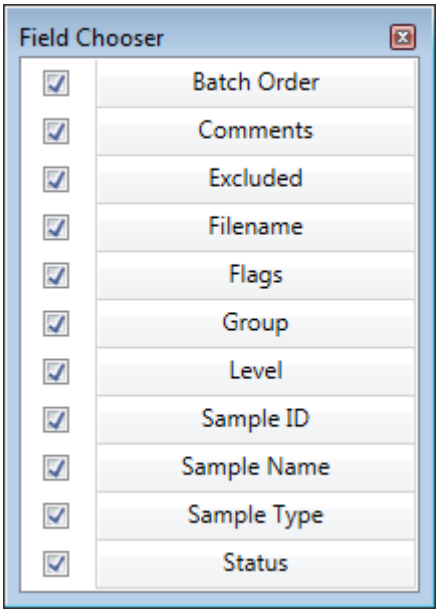
- Samples pane
- Compound Results pane
- Sample-centric Plot pane
- XIC Overlay

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.

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. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

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, close the Field Chooser.

Figure 34. Samples pane

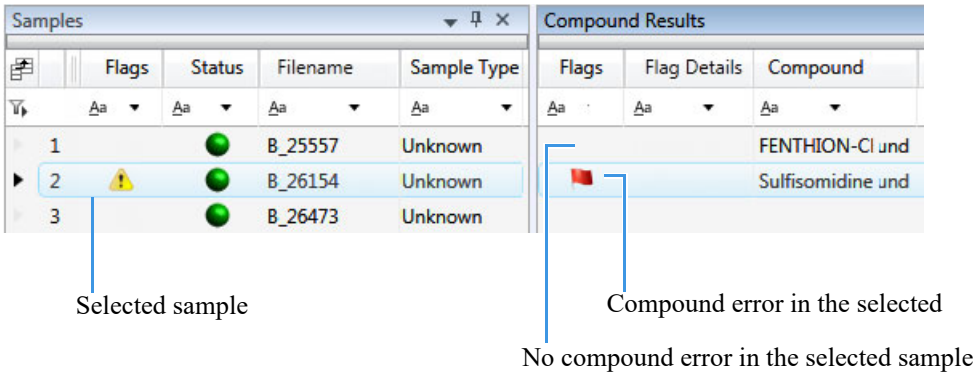


Table 25. Samples pane columns (Sheet 1 of 2)

Column	Description
Batch Order	Sequentially numbers the samples.
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.
Flags	Caution flag displayed when a compound in the sample has an error. See Caution flags.
Group	Threshold group to which a sample belongs. Samples can be viewed by group in the Comparative View of Data Review.
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.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC, or Unknown.

Table 25. Samples pane columns (Sheet 2 of 2)

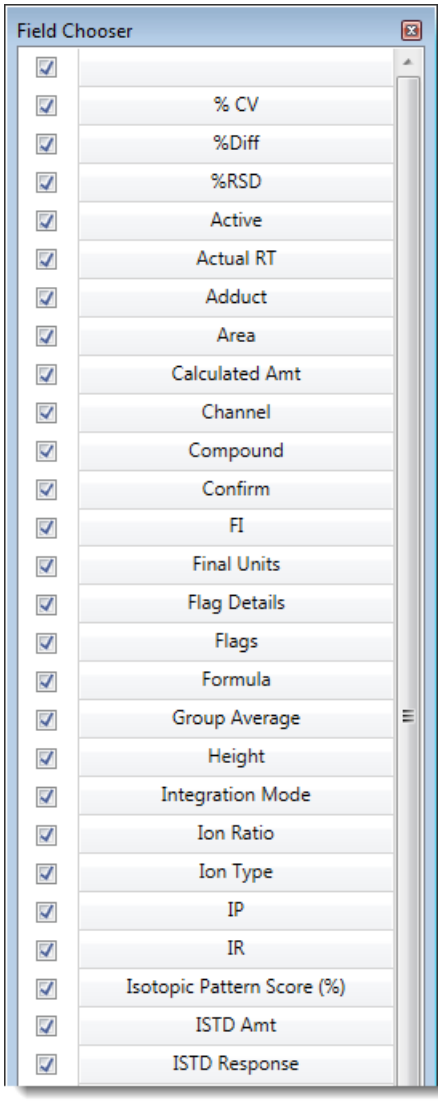
Column	Description
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.
	Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed (), and the Unknown Screening View shows the Status for the samples as acquired but not processed ().
	Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed ().

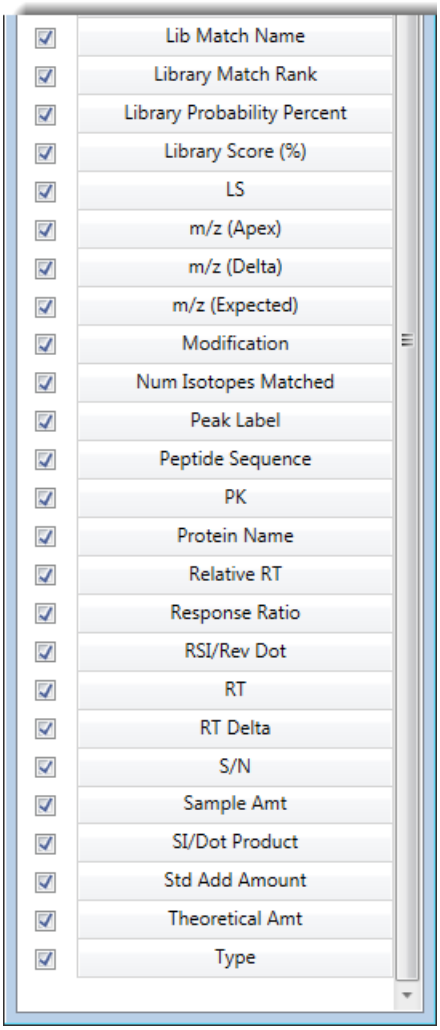
Compound Results pane

Use the Compound Results pane in the Sample View to select a specific compound in the selected sample. The associated Sample-centric Plot pane highlights the selected compound.

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

   The Field Chooser displays all available columns of data for the Compound Results pane.



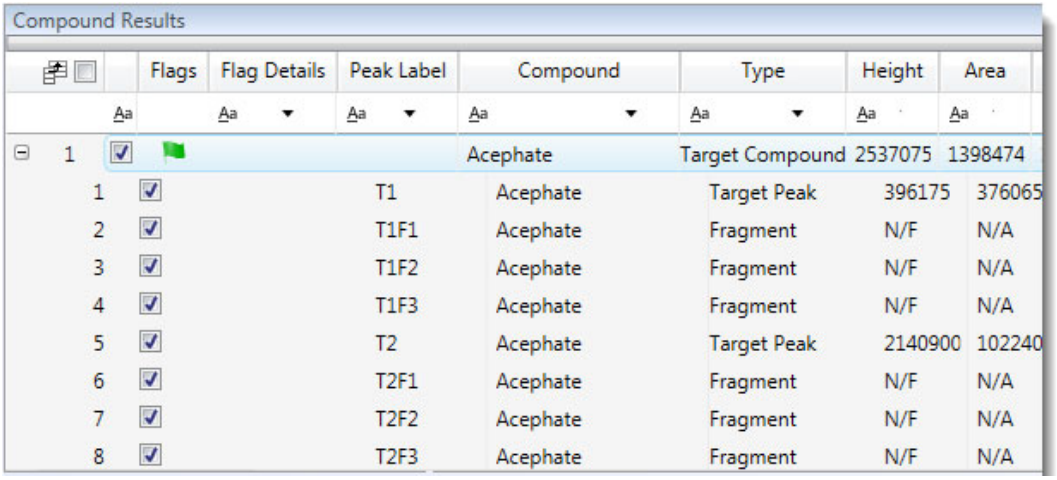


2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   The application displays or hides the column in the Compound Results pane.

3. When you are finished modifying the column display, close the Field Chooser.

Figure 35. Compound Results pane



For descriptions of the column parameters in the Compound Results pane, see Common column parameters.

Sample-centric Plot pane

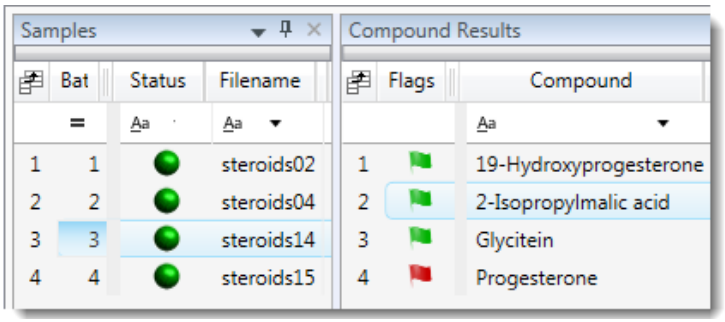
The Sample-centric Plot pane in the Sample View displays the chromatogram, retention time, area, height, and signal-to-noise ratio for each compound in the Compound Results pane. The application highlights the chromatogram for the compound that is currently selected in the Compound Results pane.

Follow these procedures:

- To select a sample to view
- To display details
- To change the number of rows and columns in the display
- To change the displayed y-axis style
- To change the displayed target and confirming peaks
- To zoom in on a peak
- To copy a plot to another format

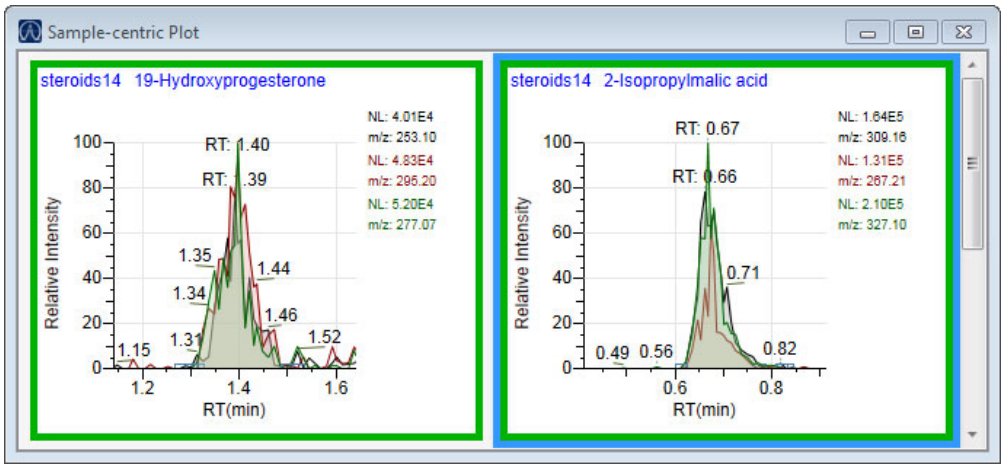
v To select a sample to view

- In the Samples pane, select the sample that you want to view.



The Sample-centric Plot pane displays the compound chromatograms for all compounds in the selected sample. A blue border indicates the compound in the sample that is currently selected in the Compound Results pane.

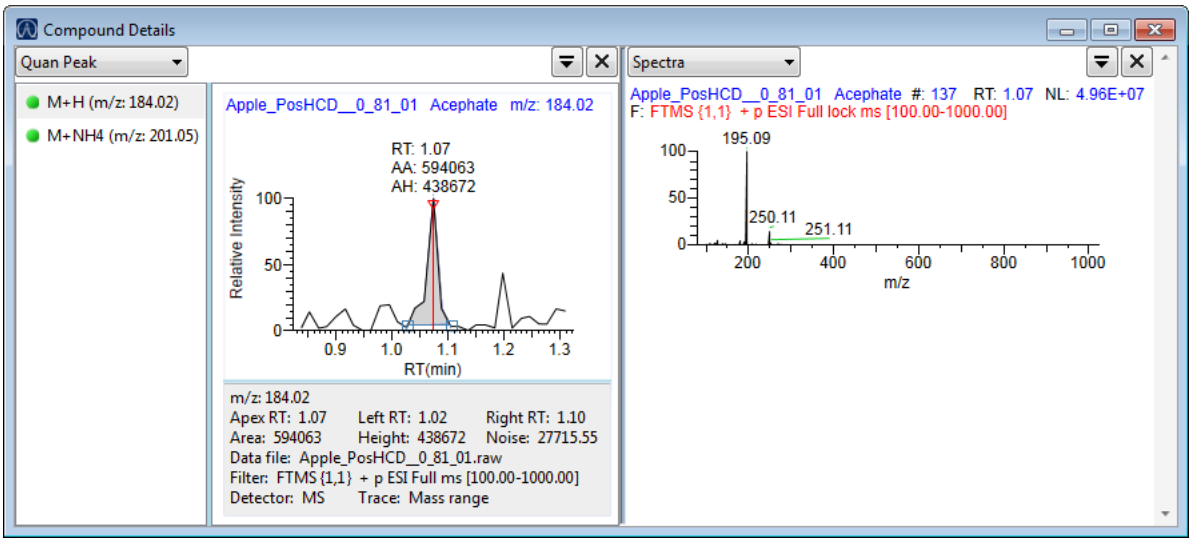
Figure 36. Sample-centric Plot pane



v **To display details**

- Double-click the chromatogram in the Sample-centric Plot pane.

The Compound Details pane opens.



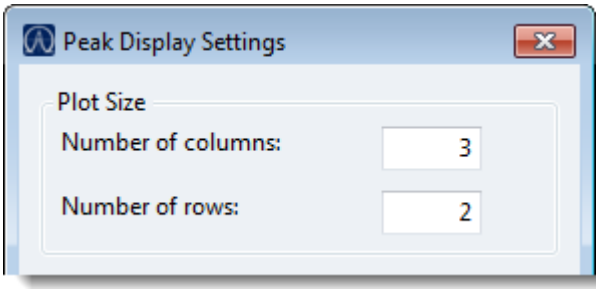
The Compound Details pane displays information about the quantitative peak, calibration curve, confirming ion, internal standard, reference peak, ion overlay, and spectra for the compound.

For a detailed description of the available information in the Compound Details pane, see Compound Details for quantitation batches.

v To change the number of rows and columns in the display

1. Right-click the Sample-centric Plot pane, and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.



2. To change the number of rows or columns to fit in the pane, type new values in the Number of Columns or Number of Rows boxes.

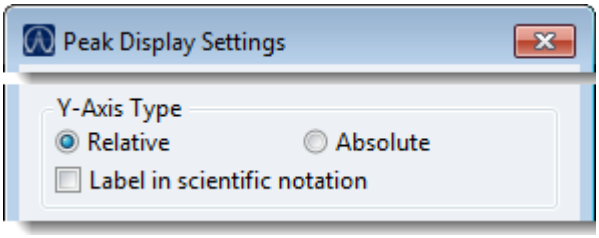
   These values determine how many rows and columns you want to view at one time in the display. The default is two rows and three columns. Use the scroll bar to view all compound chromatograms.

3. Click **OK**.

v To change the displayed *y*-axis style

1. Right-click the Sample-centric Plot pane, and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.



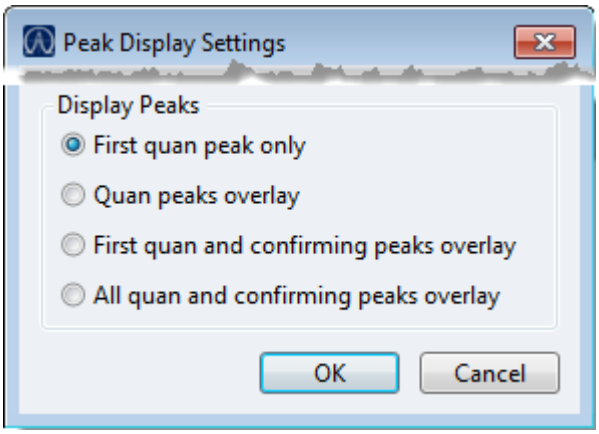
2. Select any of the following:

   - **Relative**: Displays the *y*-axis scale from 0 through 100.
   - **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.

v To change the displayed target and confirming peaks

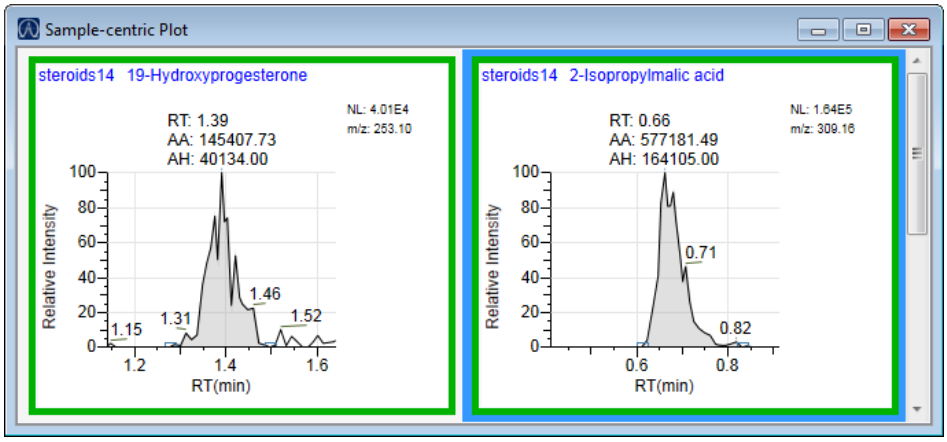
1. Right-click and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.

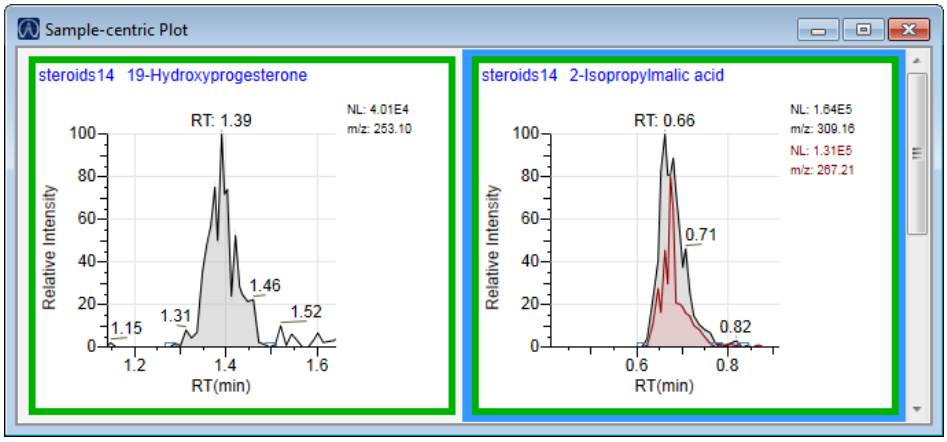


2. Select any of the following display options:

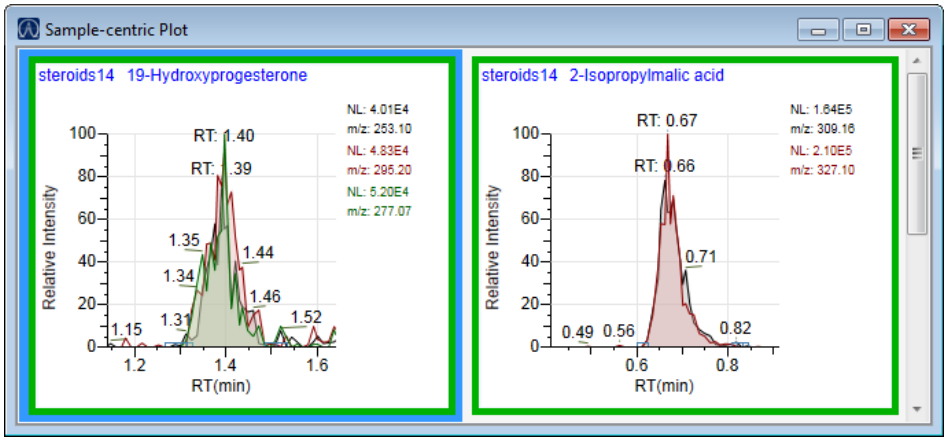
- First Quan Peak Only



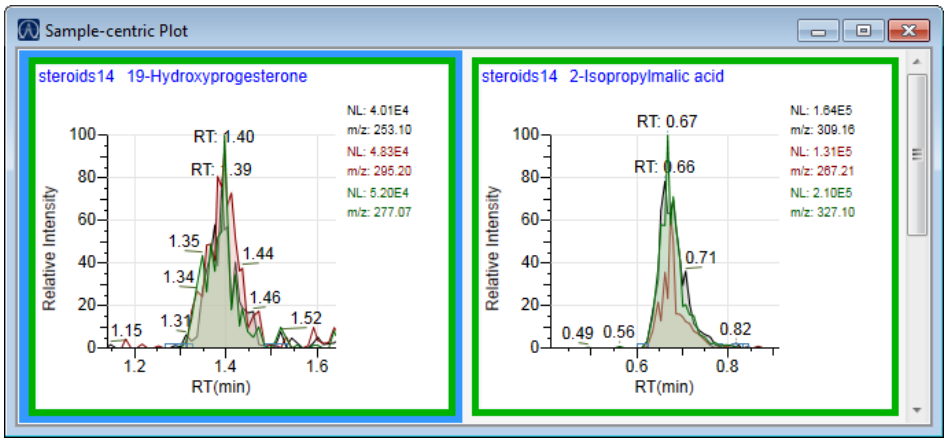
- Quan Peaks Overlay



- First Quan and Confirming Peaks Overlay



- All Quan and Confirming Peaks Overlay



3. Click **OK**.

v **To zoom in on a peak**

1. In any of the chromatogram cells, drag your cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the chromatogram area.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling.**

v **To copy a plot to another format**

1. Right-click the plot that you want to copy and choose **Copy to Clipboard.**

   The application copies the plot graphic to the Clipboard.

2. In the source format (for example, an Excel spreadsheet or email window), right-click and choose **Paste**.

   The application pastes the graphic into the new format.

XIC Overlay

Use the XIC Overlay pane to view the extracted ion current (XIC) of specific groups of peaks. You can choose to view all peaks, selected peaks only, or the top 20 most intense peaks (by area). The XIC Overlay plot is a collection of overlaid, extracted *m/z* ion plots that use a different color for each peak.

Follow these procedures:

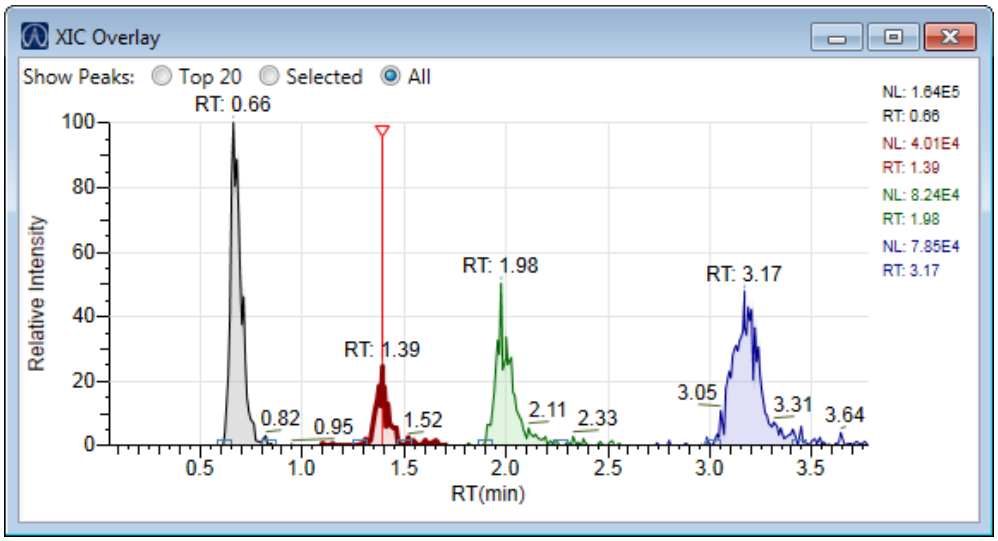
- To display all peaks in a sample
- To display only selected peaks in a sample
- To display the top 20 peaks in a sample
- To focus on a specific peak

v To display all peaks in a sample

1. In the Samples pane, select the sample whose peaks you want to view.
2. In the XIC Overlay pane, select the **All** option.

   The application displays all the peaks in the selected sample.

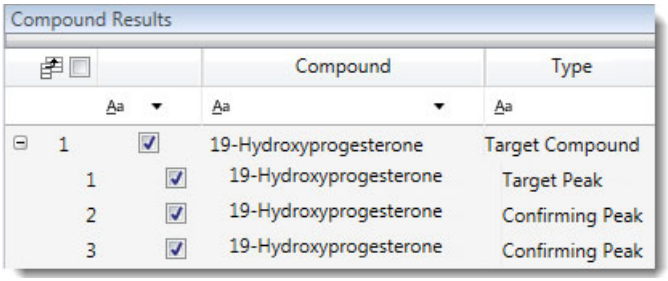
Figure 37. XIC Overlay pane showing all peaks



Note If there are more than 1000 peaks in the sample, performance might be slow.

v To display only selected peaks in a sample

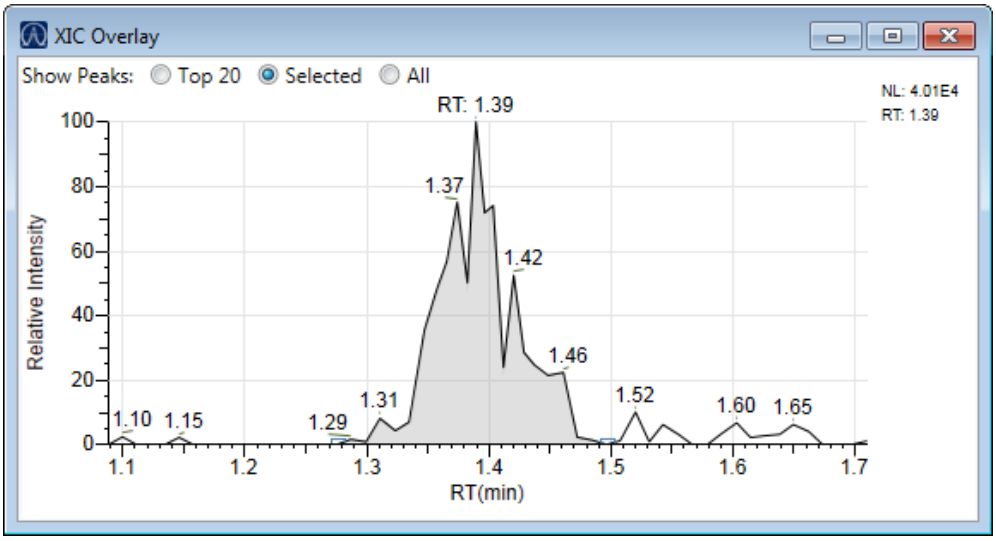
1. In the Samples pane, select the sample whose peaks you want to view.
2. In the Compound Results pane, select the check box for each peak that you want to view.



3. In the XIC Overlay pane, select the **Selected** option.

   The application displays only the selected peaks.

   Figure 38. XIC Overlay pane showing selected peaks

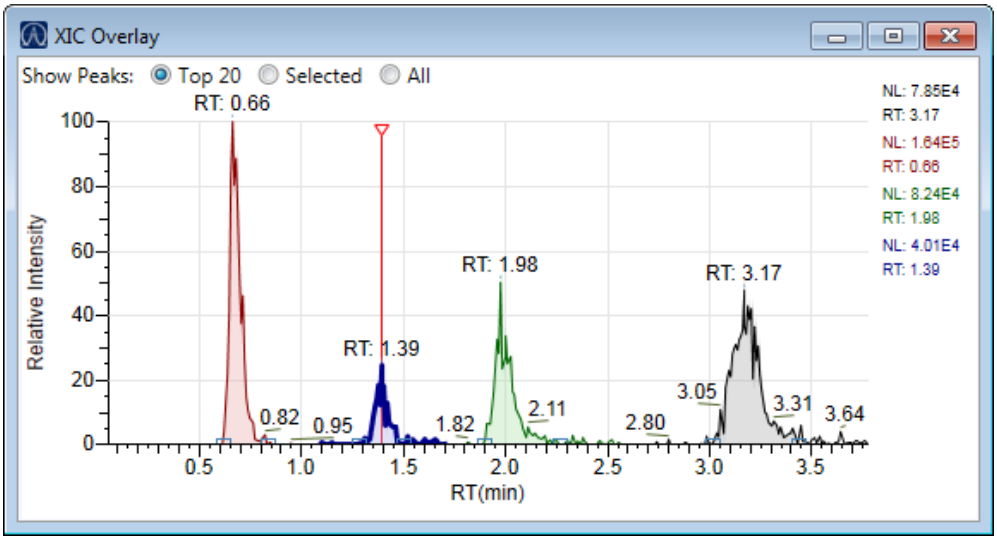


v **To display the top 20 peaks in a sample**

1. In the Samples pane, select the sample whose peaks you want to view.
2. In the XIC Overlay pane, select the **Top 20** option.

   The application displays the top 20 peaks in the selected sample.

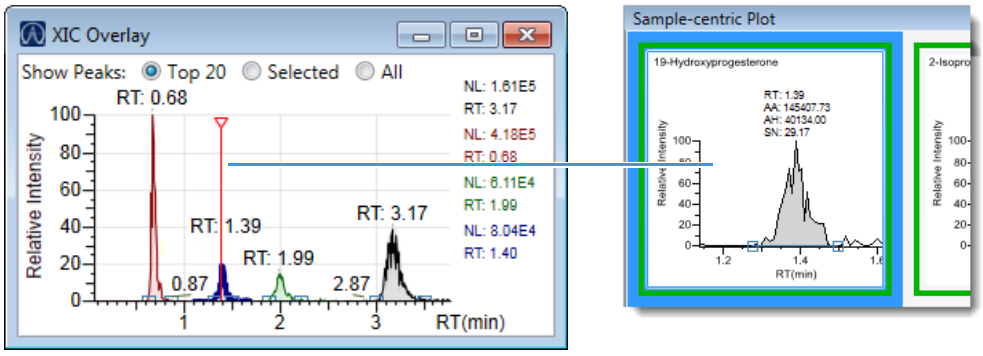
   Figure 39. XIC Overlay pane showing the top 20 peaks



v **To focus on a specific peak**

- In the XIC Overlay pane, click any displayed peak.

The application indicates the selected peak with a red, vertical marker and updates the focus in the other Data Review panes with data for that peak.



Caution flags

In the Sample View, the application displays caution flags in both the Samples pane and the Compound Results pane.

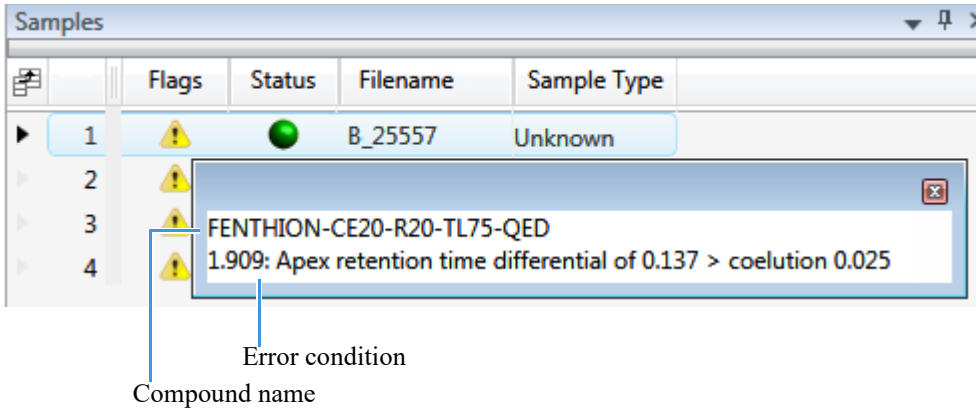
See the following topics:

- Flags in the Samples pane
- Flags in the Compound Results pane
- Error indicators in the Sample-centric Plot pane

Flags in the Samples pane

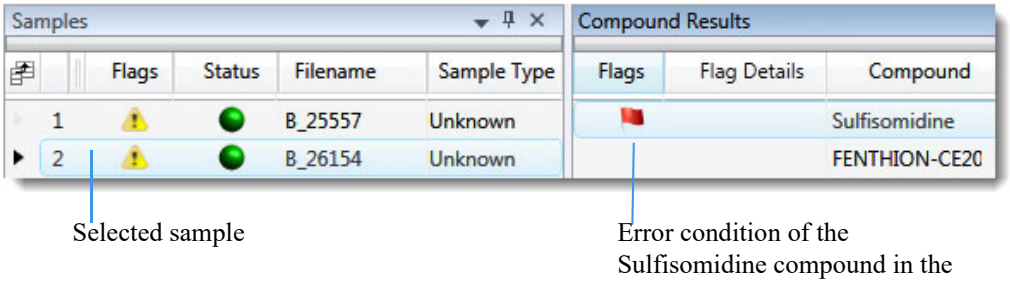
The Flags column in the Samples pane displays a caution flag if any compound in the sample is not in compliance with the method criteria.

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.

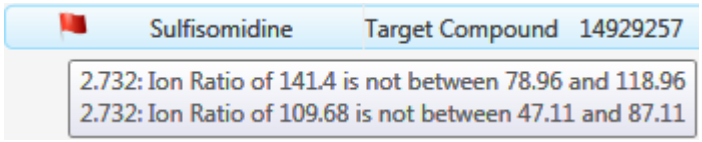


Flags in the Compound Results pane

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.



Point to the flag icon, , to display details for the compound in the selected sample.



Colored flags in the Compound Results pane have the following meaning:

	Red for compounds that have violated (or are activated by) any of the values set in the method. Refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.
	Red for compounds that are outside the specified ion ratio range. See Ion ratio failure flag.
	Orange for compounds that are below the limit of quantitation (LOQ), below the limit of detection (LOD), or between the LOD and LOQ values specified in the method. For descriptions of these limits, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.
	Green for "found" compounds that are over the limit of reporting (LOR) amount specified in the method. For a description of the LOR limit, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.
	Yellow for compounds that are equal to or below the LOR amount specified in the method.
	Yellow for compounds that are not found in Cal Std or QC sample types. The Compound Results pane does not flag compounds that are not found in Unknown sample types.
<no flag>	No flag for compounds where no report options are selected.

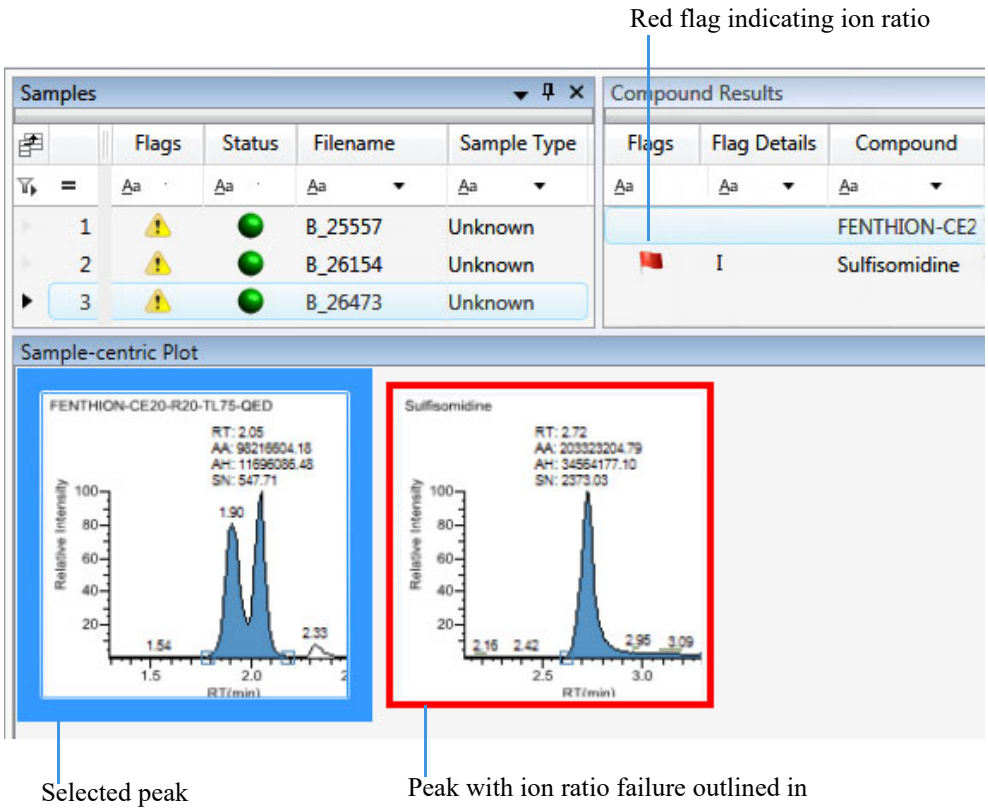
Note These criteria for flag states do not apply to Matrix Blank sample types when the compound is an internal standard.

Error indicators in the Sample-centric Plot pane

In the Sample-centric Plot pane, peak plots are outlined with the color of their associated error flag (red, green. orange, or yellow). In the following figure,

- the FENTHION peak plot indicates no errors and is highlighted in blue to indicate that FENTHION is the selected compound;
- 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 40. Ion ratio failure flag



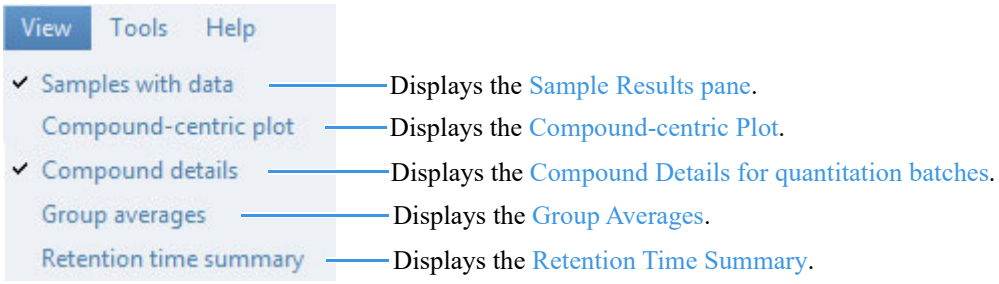
Compound View for quantitation batches

The Compound View displays a list of all compounds available in the method, all samples in the current batch, and the peak plots for all found compounds.

- From the View menu, choose to display or hide any of the following panes.

  Note The Compounds pane is required for the Compound View display. You cannot hide the Compounds pane.

  A check mark indicates a displayed pane.



The Compound View includes the following features:

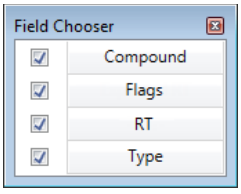
- Compounds pane
- Sample Results pane
- Compound-centric Plot
- Group Averages
- Retention Time Summary
- Caution flags

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.

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, close the Field Chooser.

Figure 41. Compounds pane

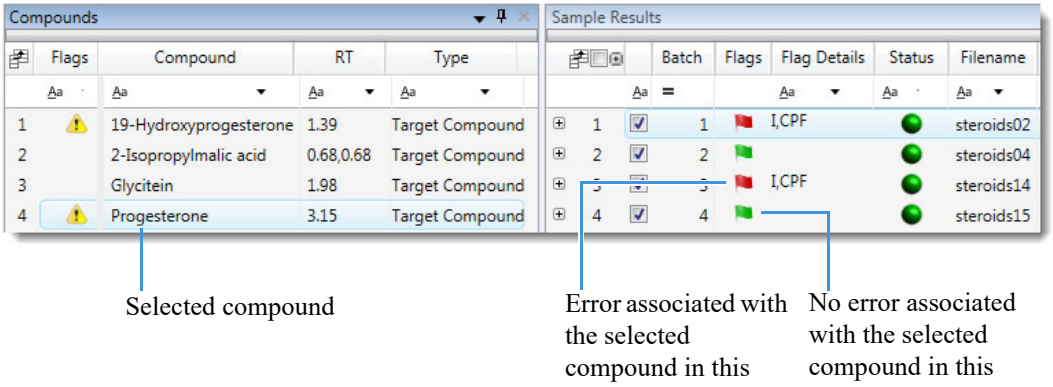


Table 26. Compounds pane columns

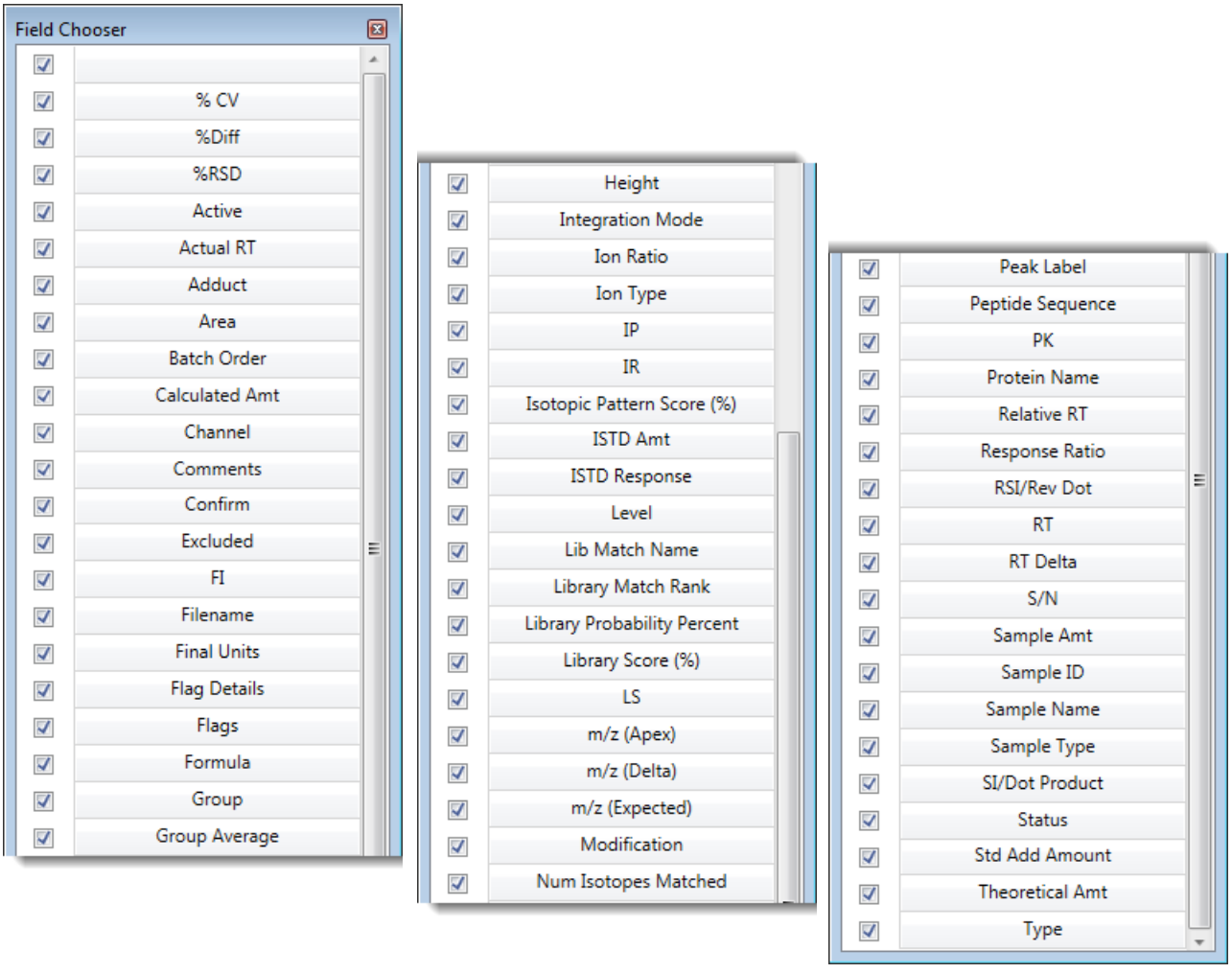
Column	Description
Flags	Caution flag displayed when a compound has an error in any of the samples.
Compound	Compound names as identified in the library. If there is no library selected in the method template, the compound name is identified as *peak@RT.*
RT	Expected retention time for the compound.
Type	Specified compound type: Target Compound or Internal Standard.

Sample Results pane

Use the Sample Results pane in the Compound View to select a specific compound in a specific sample. The Compound-centric Plot pane highlights the selected sample/compound and displays the following information about the compound: chromatogram, retention time, area, height, and signal-to-noise ratio.

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

   The Field Chooser displays all default columns of data for the Sample 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 Sample Results pane.

3. When you are finished modifying the column display, close the Field Chooser.

Figure 42. Sample Results pane

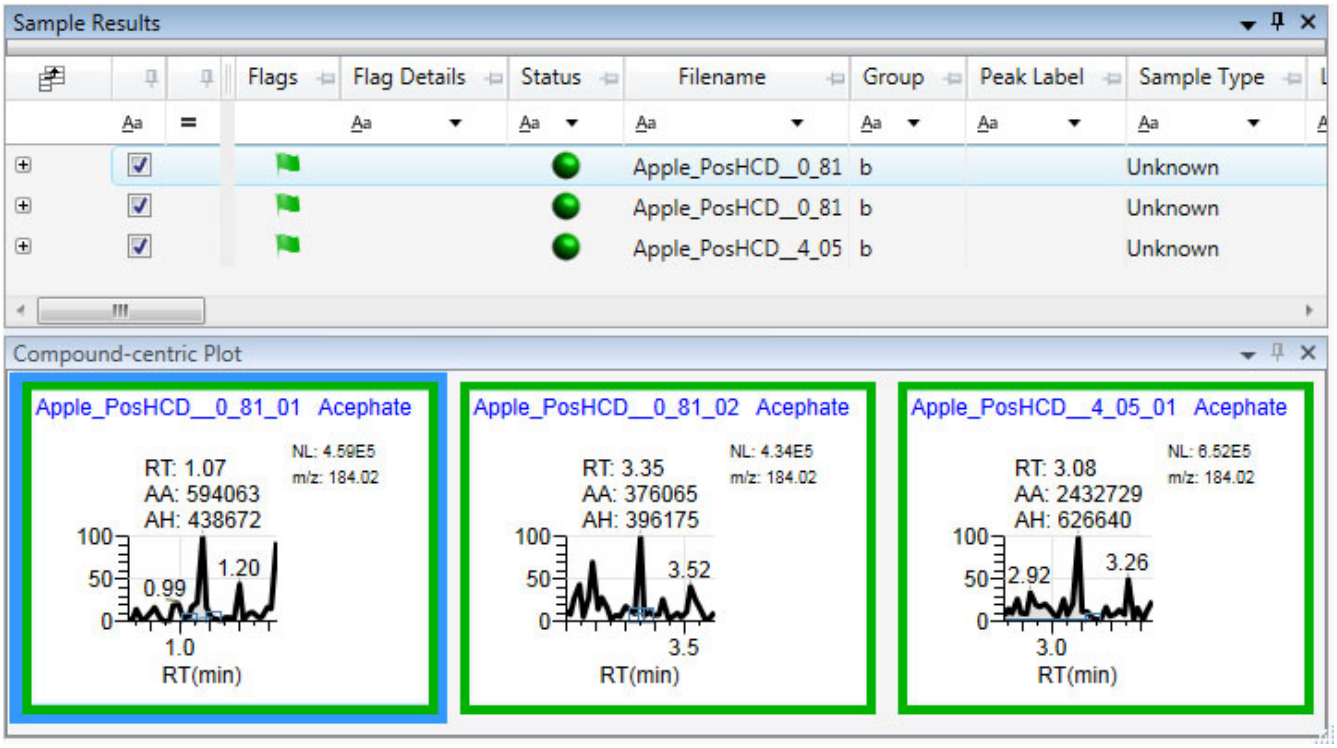


Table 27. Sample Results pane columns (Sheet 1 of 2)

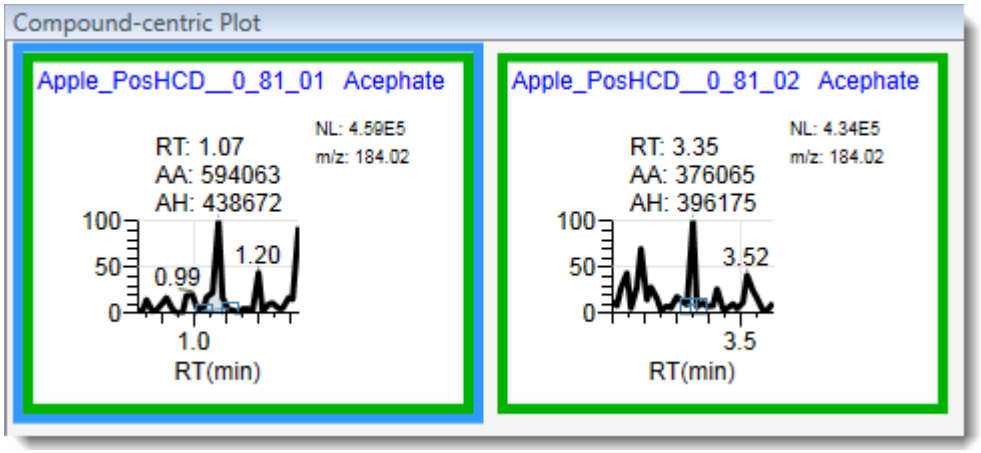
Column	Description
☑	Displays the selected samples in the other Data Review panes.
Flags	Displays a caution flag when a compound within the sample has an error.
Flag Details	Indicates the type of error: • I: Confirming ion coelution failure or Ion ratio failure • A: Amount error • B: Matrix blank error • H: Peak not found

Table 27. 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.
	Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed ( ), and the Unknown Screening View shows the Status for the samples as acquired but not processed ( ).
	Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed ( ).
Filename	Specifies a user-defined name that identifies a sample.
Group	Specifies the threshold group to which a sample belongs. Samples can be viewed by group in the Comparative View of Data Review.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC, or Unknown.
The remainder of the columns in the Sample Results pane are common to both the Sample View and the Compound View displays. See Common column parameters.	

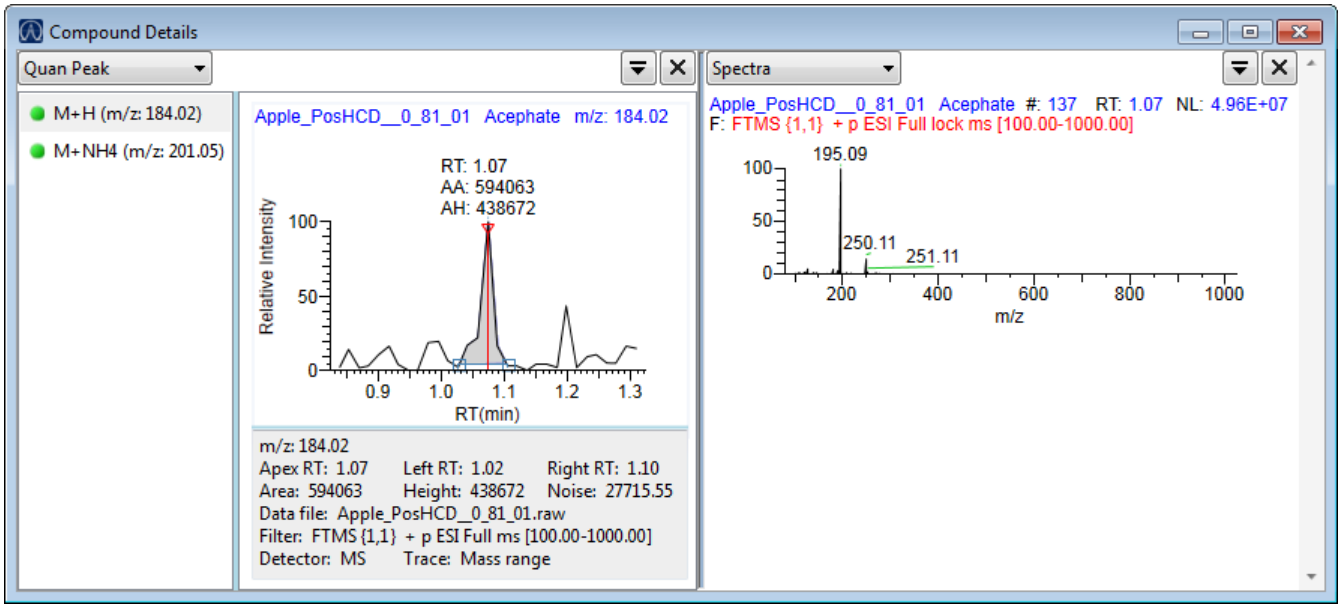
Compound-centric Plot pane

The Compound-centric Plot 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.



- Double-click the chromatogram in the Compound-centric Plot 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 for quantitation batches.

Compound-centric Plot

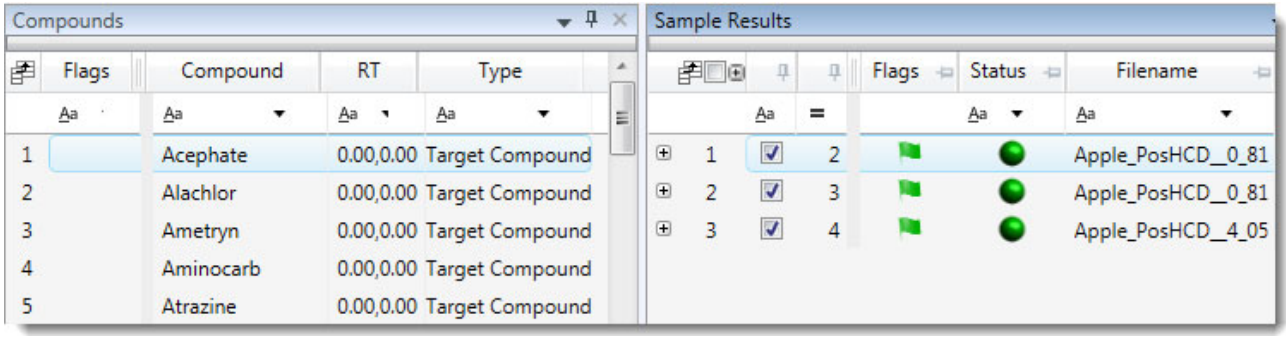
Use the Compound-centric Plot pane to view an overlay of the quantitation and confirming peaks for each sample in the batch.

Follow these procedures:

- To select a sample to view
- To change the displayed number of rows and columns
- To change the displayed y-axis style
- To change the displayed target and confirming peaks
- To zoom in on a peak
- To copy a plot to another format

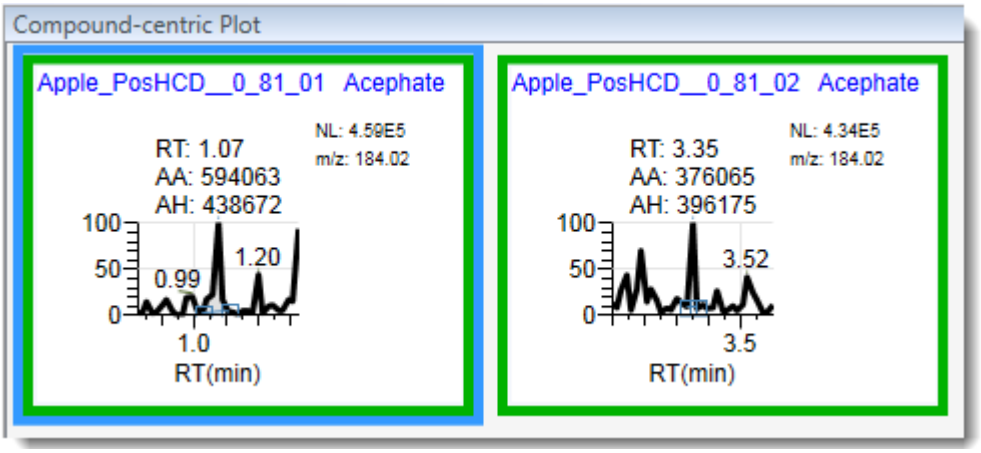
v To select a sample to view

- In the Compounds pane, select the compound that you want to view.



The Compound-centric Plot pane displays the compound chromatograms for the selected compound in each sample in the batch. A blue border indicates the compound in the sample that is currently selected in the Sample Results pane.

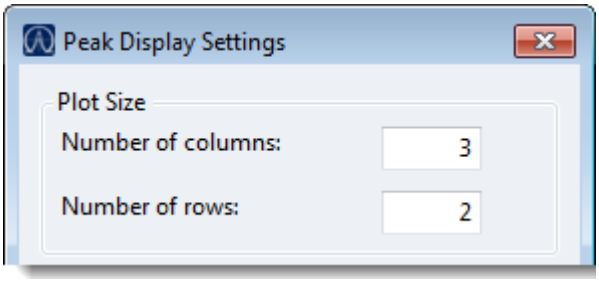
Figure 43. Compound-centric Plot pane



v **To change the displayed number of rows and columns**

1. Right-click the Compound-centric Plot pane and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.



2. To change the number of rows or columns to fit in the pane, type new values in the Number of Columns or Number of Rows boxes.

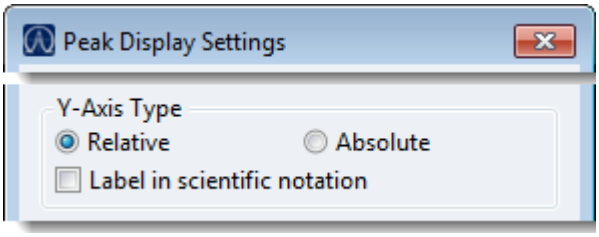
These values do not change the number of rows (compounds) and columns (samples) that are available in the Compound-centric Plot pane. They determine how many rows and columns you want to view at one time in the display. The default is two rows and three columns.

3. Click **OK**.

v **To change the displayed *y*-axis style**

1. Right-click the Compound-centric Plot pane and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.



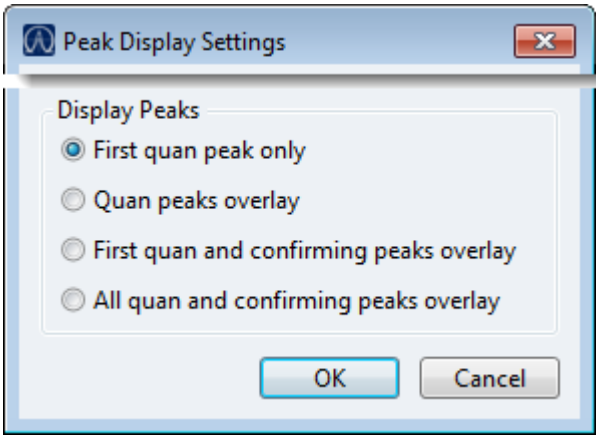
2. Select any of the following:

   - **Relative**: Displays the *y*-axis scale from 0 through 100.
   - **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.

v **To change the displayed target and confirming peaks**

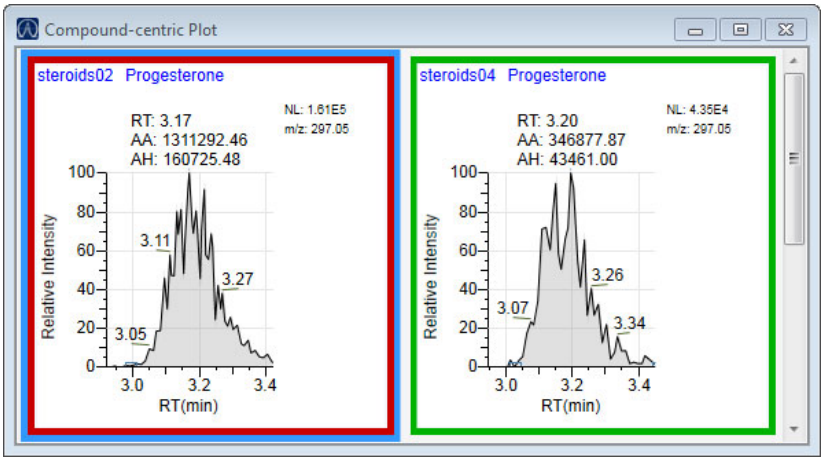
1. Right-click the Compound-centric Plot pane and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.

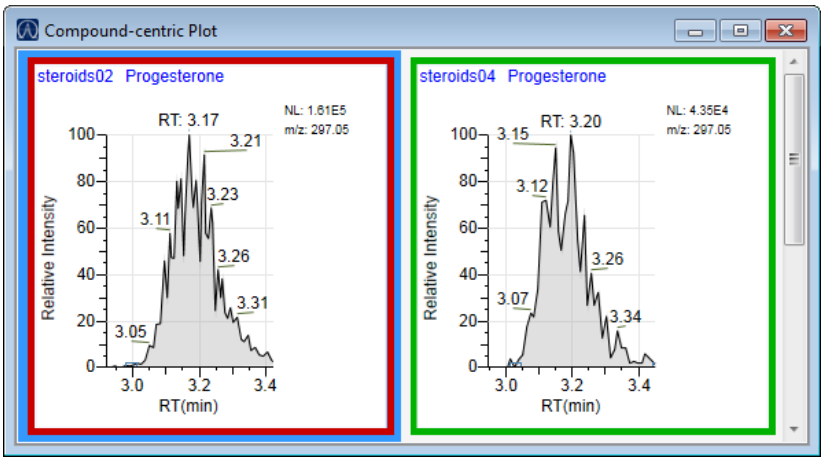


2. Select any of the following display options:

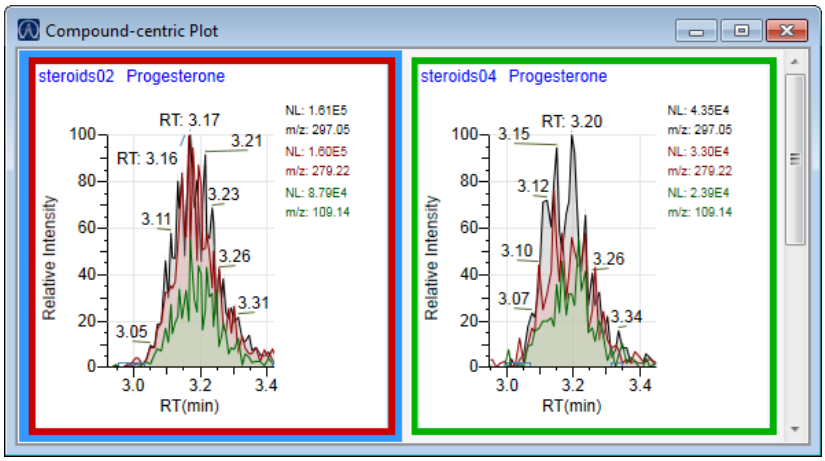
- First Quan Peak Only



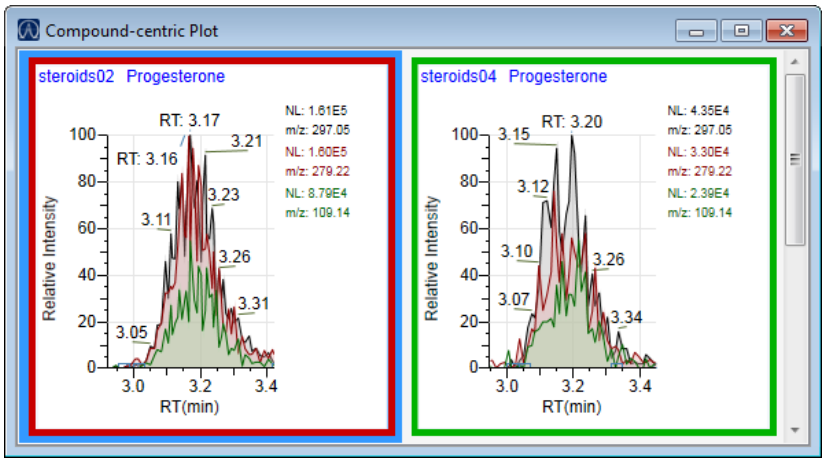
- Quan Peaks Overlay



- First Quan and Confirming Peaks Overlay



- All Quan and Confirming Peaks Overlay



3. Click **OK**.

v **To zoom in on a peak**

1. In any of the chromatogram cells, drag your cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the chromatogram area.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling.**

v **To copy a plot to another format**

1. Right-click the plot that you want to copy and choose **Copy to Clipboard.**

   The application copies the plot graphic to the Clipboard.

2. In the source format (for example, an Excel spreadsheet or email window), right-click and choose **Paste**.

   The application pastes the graphic into the new format.

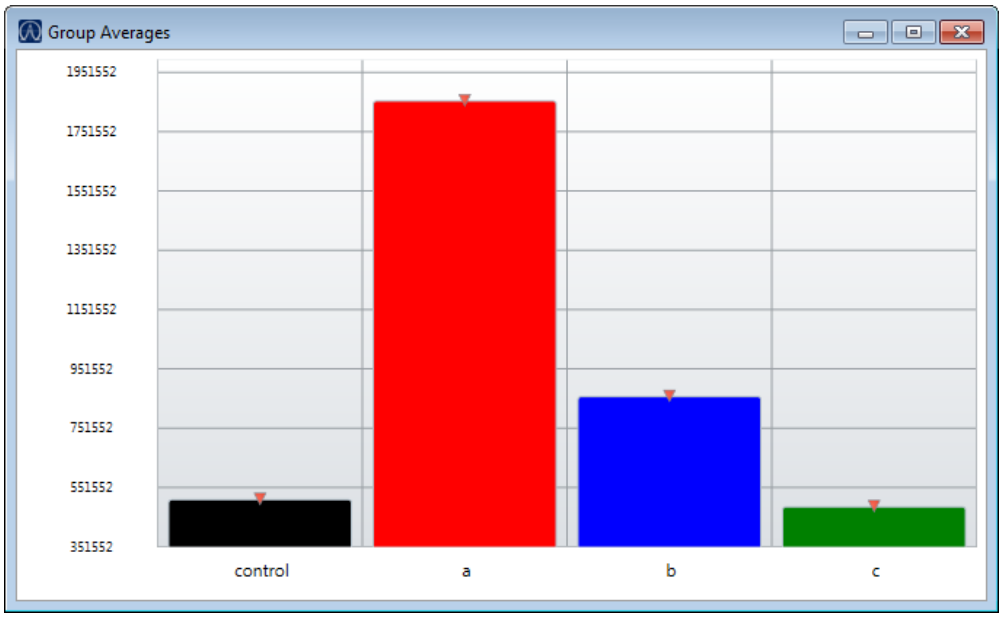
Group Averages

Use the Group Averages pane to compare the peak areas of different samples to a control group of samples. You must have at least two groups defined, and one group must be a control group.

The control group is displayed to the left, and other samples and groups are listed in the order in which they appear in the Batch View. To specify a group as the control group, see Groups.

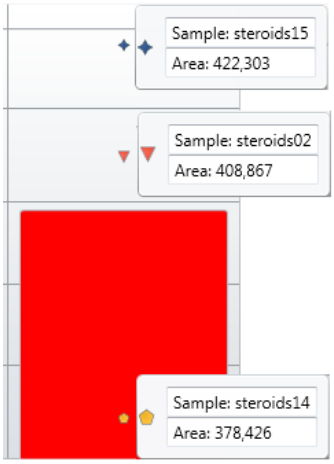
Each group displays a colored bar that indicates the average response of the group.

Figure 44. Group Averages pane



- Point to an indicator icon (,).

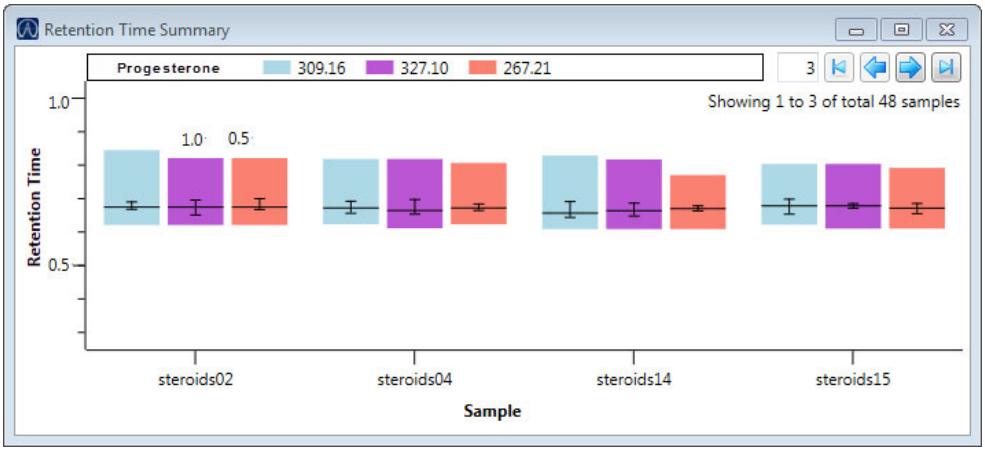
  The application displays the area for the selected compound in each represented sample.

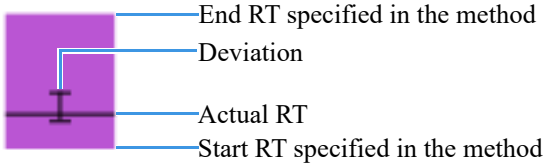


Retention Time Summary

Use the Retention Time Summary pane to view variations of the retention times for a compound across all samples in a batch. The Retention Time Summary pane displays each color-coded compound for each sample in the batch.

Figure 45. Retention Time Summary pane





Caution flags

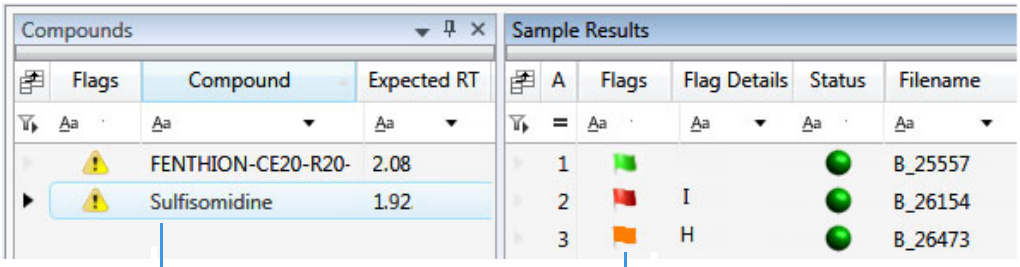
In the Compound View, the application displays caution flags in both the Compounds pane and in the Sample Results pane.

See the following topics:

- Flags in the Compounds pane
- Flags in the Sample Results pane
- Error indicators in the Compound-centric Plot pane

Flags in the Compounds pane

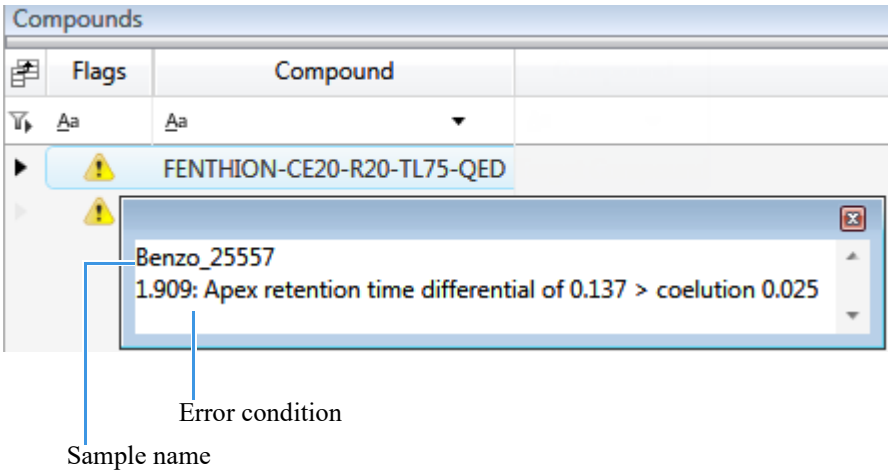
The Flags column in the Compounds pane displays a caution flag if the compound in any of the samples is not in compliance with the method criteria.



Selected Sulfisomidine compound

Flags for the Sulfisomidine compound in each sample

Click the caution flag icon, , to display the details. Information in the pop-up box shows the sample where the compound is in error and describes the exact error condition.



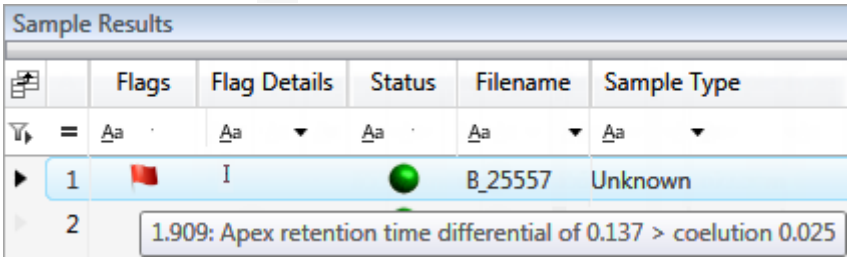
Error condition

Sample name

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.

Point to the flag icon, , to display the details for the selected compound in the sample.



Colored flags in the Sample Results pane have the following meaning.

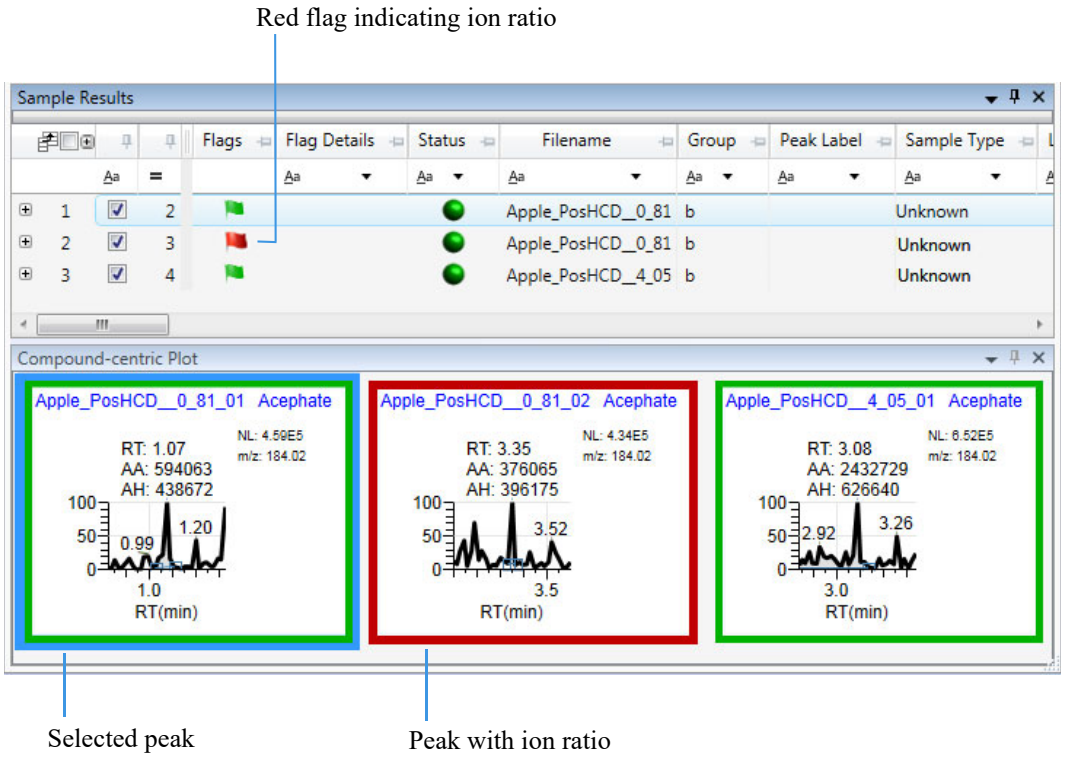
Flag	Description
	Green for compounds that are over the LOR amount specified in the method.
	Red for compounds that have violated (or are activated by) any of the values set in the method. Refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.
	Red for compounds that are outside the specified ion ratio range. See Ion ratio failure flag.
	Orange for compounds that are not found in Cal Std 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 Unknown sample types.
	No flag for compounds where no report options are selected.

Note These criteria for flag states do not apply to Matrix Blank sample types when the compound is an internal standard.

Error indicators in the Compound-centric Plot pane

In the Compound-centric Plot 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 46. Ion ratio failure flag



Compound Details for quantitation batches

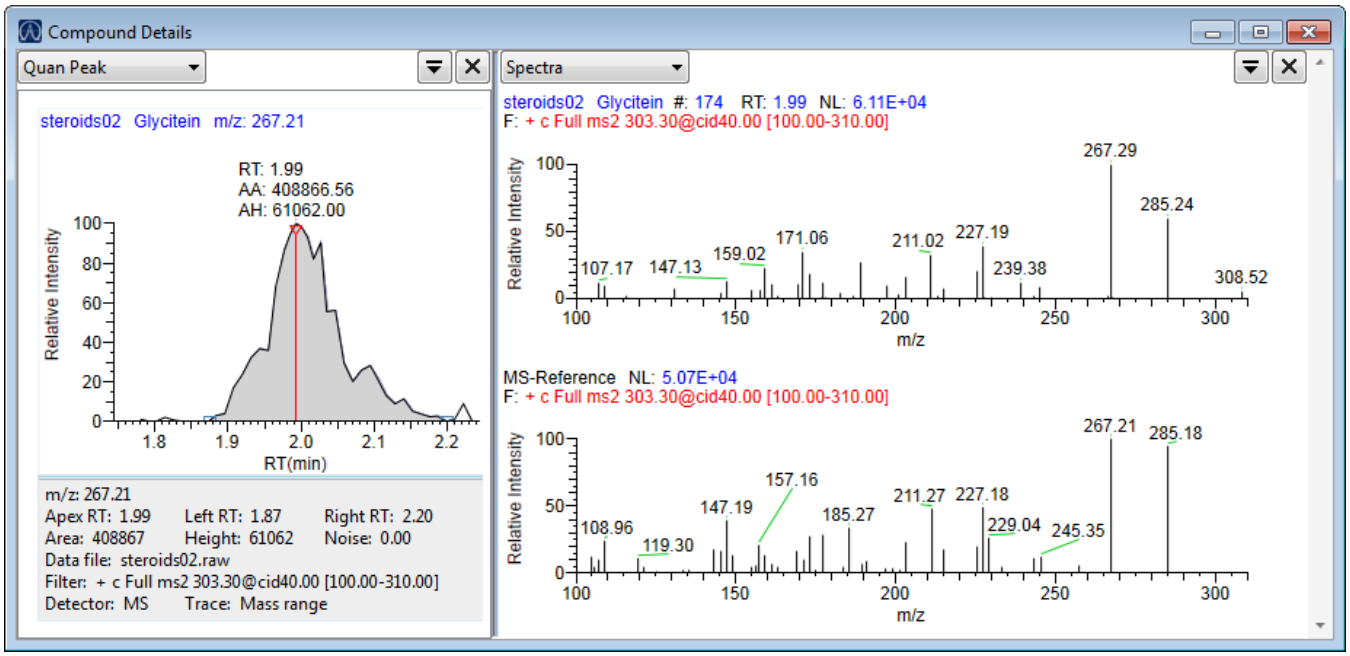
The Compound Details pane is identical for Sample View and Compound View. Use the Compounds Details pane to display any of the following types of data:

- Quan Peak
- Confirming Ions
- Calibration Curve
- Ion Overlay
- ISTD
- Reference Peak
- Spectra
- Library Match
- Isotope
- Fragments
- Quan Peaks Overlay
- Caution flags

v To open the Compound Details pane

1. Double-click the chromatogram in the Sample-centric plot or the Compound-centric plot.

   The Compound Details pane opens.



   By default, the first display pane shows the quantitative peak for the selected compound.

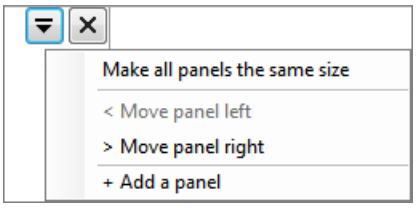
2. In the second pane, select the additional type of data that you want to display.

Follow these procedures to change the display of the peak data in either of the panes:

- To change the peaks pane
- To zoom in on a peak

v To change the peaks pane

- 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 pane one space to the left. This command is not available when the current pane is the leftmost pane.
Move Panel Right	Moves the current pane 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.

v To zoom in on a peak

1. In any of the views, drag your cursor to delineate a rectangle around the peak or spectrum.

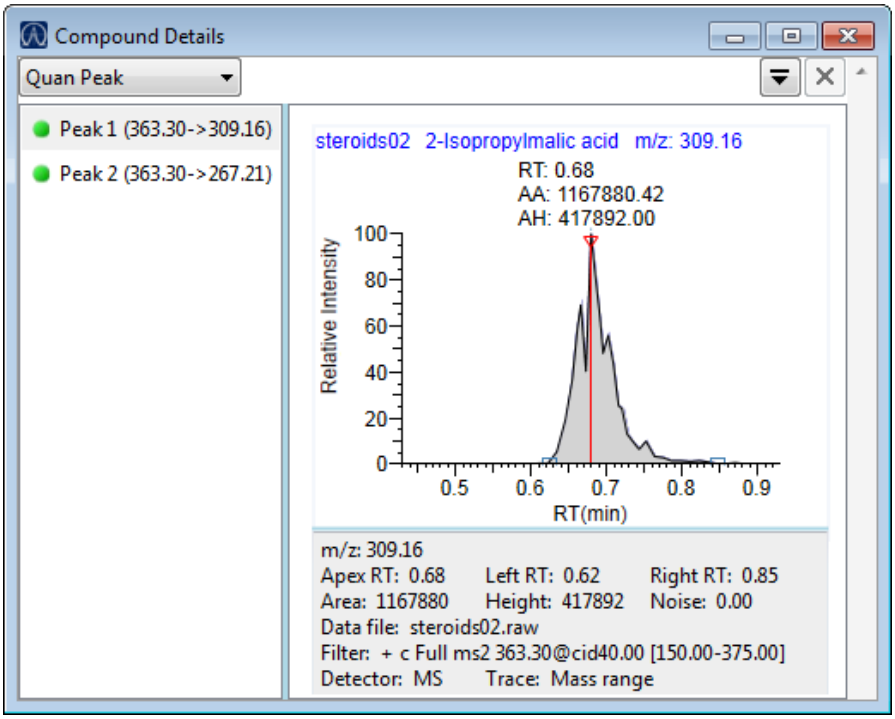
   The delineated area expands to fill the view.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling.**

Quan Peak

A compound can have multiple quantitative peaks. You can switch between quantitative peaks, but you cannot view multiple quantitative peaks at the same time. The Quan Peak pane uses a unique shortcut menu. See Quan Peak pane shortcut menu commands.

Figure 47. Quantitative peak pane with multiple quantitative peaks



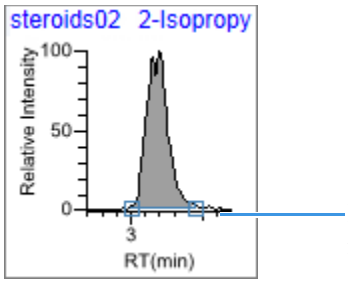
Follow these procedures to modify the quantitative or confirming ion peak data:

- To manually integrate a peak by swiping the peak
- To manually integrate a peak by moving the peak delimiters
- To remove a manually created peak
- To switch between method, manual, and user integration modes
- To customize the labels in the display
- To modify the peak detection settings

v To manually integrate a peak by swiping the peak

1. Right-click anywhere in the quantitative peak pane and then choose **Swipe Manual Integration,** or click the icon in the upper right corner, .
2. Click the left base of the peak that you want to identify.
3. Drag to the right base and release the mouse.

The application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



v **To manually integrate a peak by moving the peak delimiters**

1. Point to 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 edited.

v **To remove a manually created peak**

- Right-click the pane and then choose **Delete Peak**, or click the icon in the upper right corner, .

  The application removes the manual integration from the selected peak.

v **To switch between method, manual, and user integration modes**

- Right-click the chromatogram pane and choose **Toggle Integration Mode > Method/Manual/User**.

  Initially, the method integration and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the chromatogram plots update and the result set updates as you switch between modes.

  Each pane in Data Review reflects the changes when you switch between modes. The generated reports for these data identify any manual modifications.

v To customize the labels in the display

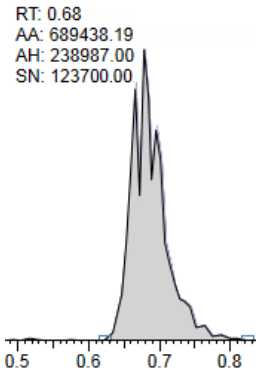
1. Right-click and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.

2. To display labels for the peak retention time (RT), area (AA), height (AH), or signal-to-noise (SN), select the appropriate check box.

3. Click **OK** in the Peak Display Settings dialog box.

   Figure 48. Example of displayed labels



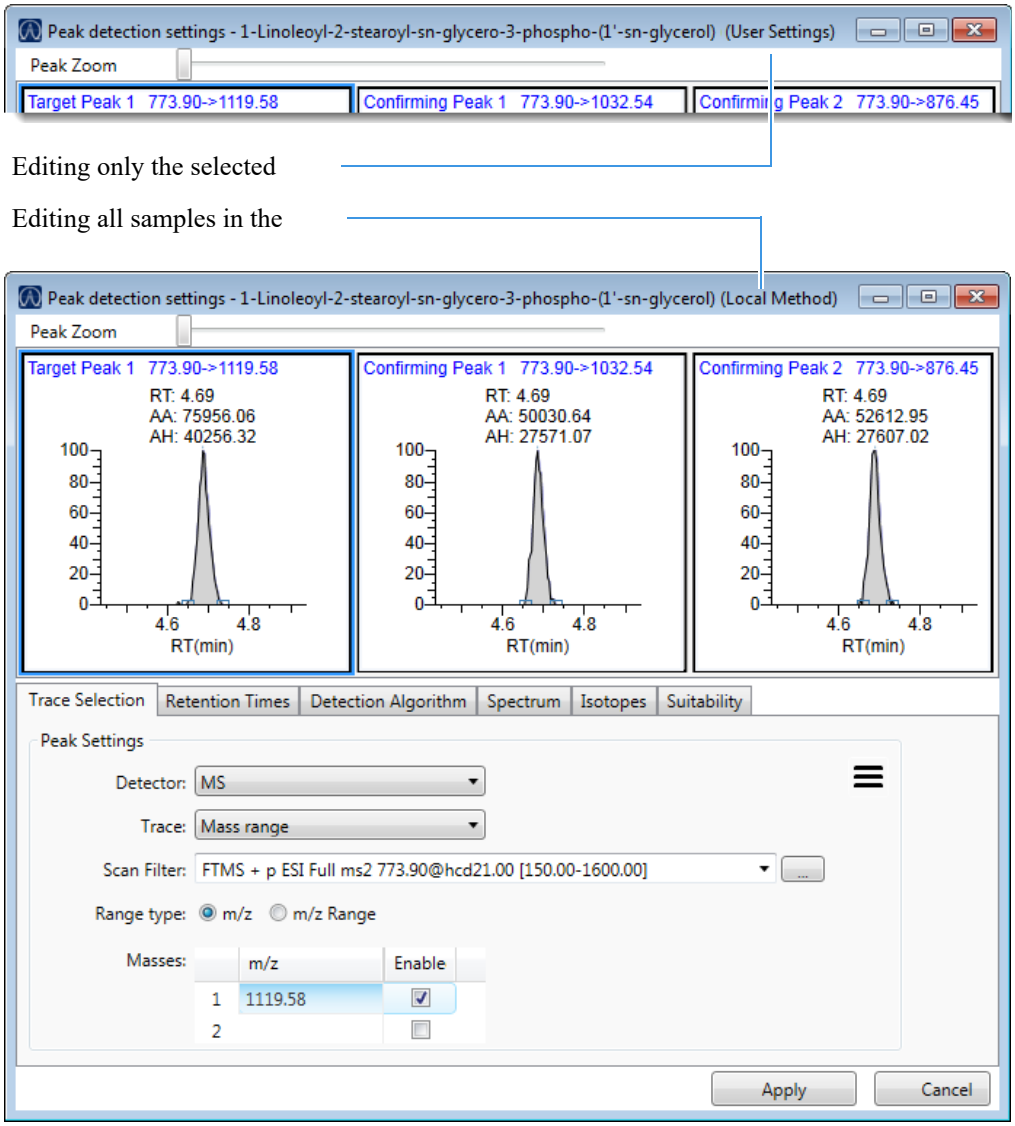
v To modify the peak detection settings

1. Right-click the chromatogram view and choose one of the following:

   - **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 Peak Detection Settings**: Makes changes to the selected compound for only the selected sample. The application saves these changes with the batch and stops applying the local method detection settings to the compound for this sample only.

   The Peak Detection Settings dialog box opens where you can adjust detection settings that were specified in the method. The title bar of the dialog box lists the selected compound and indicates whether you are making changes to only the selected sample or to the local method.

Figure 49. Peak Detection Settings dialog box



2. Edit any of the detection settings.

   For detailed descriptions of all detection settings, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

   Note You can enable the pharmacopeia S/N calculation in the peak detection settings.

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.

Table 28. Quan Peak 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.
Send RT to Method	Sets the current retention time as the expected retention time for the compound in the local method.
Swipe Manual Integration	Switches to manual integration mode, where you can manually define the peak. Also available from the icon in the upper right corner, .
Toggle Integration Mode (Method, Manual, or User)	Switches the display between local method integration, manual integration, and user-defined peak detection settings. You can edit the *method* or *user* peak detection settings from the Peak Detection Settings menu. See To modify the peak detection settings. You can manually edit a peak with the Swipe Manual Integration command. See To manually integrate a peak by swiping the peak.
Delete Peak	Removes the peak and all data for this peak from all Compound View panes. Also available from the icon in the upper right corner, .
Peak Display Settings	Select the confirming ions to be viewed. Not available for analog compounds. See Peak Display Settings dialog box.
Peak Detection Settings	Edit User 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. The changes that you make on the Signal page in the Peak Detection Settings dialog box can affect all quantification and ion ratio calculations and are not auto-reversible. These changes can also create a mismatch with calibration files that are not fully defined in the batch. Enable the pharmacopeia S/N calculation in the peak detection settings. Calculate the time range for the noise determination in relation with the peak width at 50% of the peak height at half height (time span) and a multiply factor. **Note** The Peak Detection Settings commands are also available in the Confirming Ions pane.

Confirming Ions

The Confirming Ions pane displays a list of peaks, a graphical view of all qualifying/confirming ions for the selected compound, and calculated ion ratios and ion ratio acceptance windows. A red border indicates that an ion ratio is outside of its window. See Quantitative peak with multiple confirming ions. The Confirming Ions pane uses a unique shortcut menu. See Confirming Ions pane shortcut menu commands.

In the peaks list, the application displays the mass of each confirming ion peak. When a peak is within the tolerance set, the peak status is green. When a peak is not within the tolerance set, the peak status is red.

Note For compounds with an analog detection type, the application displays "No Confirming Ions are Enabled" in the Confirming Ions pane.

Follow these procedures:

- To zoom in on a peak
- To remove a peak
- To customize the labels in the display
- To display surrounding apex times
- To manually integrate a peak
- To modify the peak detection settings
- To switch between method, manual, and user integration modes

v 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**.

v To remove a peak

- Right-click the Confirming Ions pane and choose **Delete Peak**.

  The application removes the peak displayed in the Confirming Ions pane. All data for this peak are removed from the Compound View panes.

v To customize the labels in the display

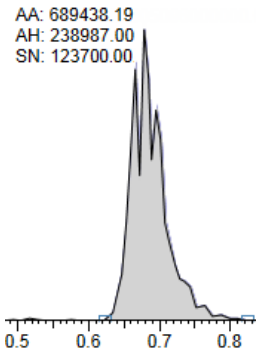
1. Right-click the Confirming Ions pane and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.

2. To display labels for the peak retention time (RT), mass area (MA), mass height (MH), or signal-to-noise (SN), select the appropriate check box. See Example of displayed labels.

3. Click **OK** in the Peak Display Settings dialog box.

Figure 50. Example of displayed labels



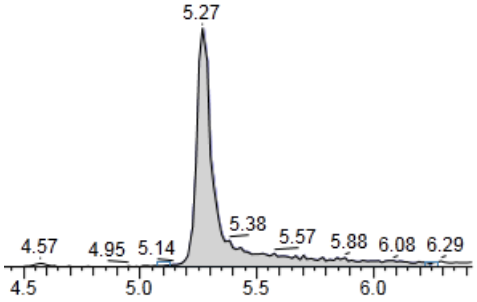
v **To display surrounding apex times**

1. Right-click the Confirming Ions pane and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.

2. Select the **Show All Apex Times** check box.
3. Click **OK** in the Peak Settings dialog box.

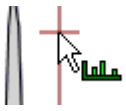
Figure 51. Example of displayed apex times



v **To manually integrate a peak**

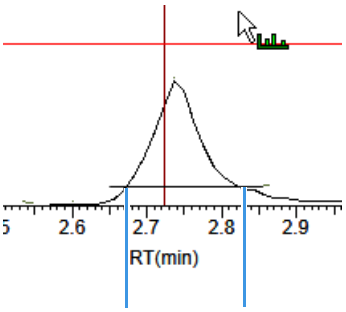
1. Right-click the Confirming Ions pane and then choose **Swipe Manual Integration**, or click the **Swipe Manual Integration** icon, .

   The cursor changes to indicate the manual integration mode.

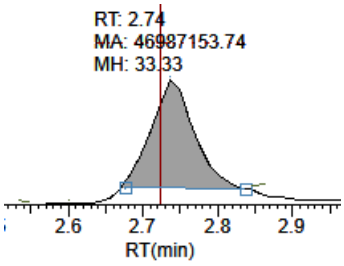


2. Drag the cursor to define the beginning and ending base points for the new peak.

Note You must drag the cursor inside the *x* axis and *y* axis.



Drag the cursor across the peak at the base points for the



The application identifies the peak and indicates the manual integration in the labels.

The application updates the area of the peak to the baseline that you have just added. When you regenerate the reports, they display the manually modified data.

You can store two peak value sets (method and manual integration settings) with each compound in each file. These settings can result in a different set of stored values. The application originally calculates the method values based on the processing method parameters. The manual values are a result of what you edited.

Note Because a Blank Report displays only the quantitation mass, when you manually integrate a confirming ion, the manual integration flag in the report is displayed on the quantitation mass.

v To modify the peak detection settings

1. Right-click the chromatogram view and choose one of the following:

   - **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 Peak Detection Settings**: Makes changes to the selected compound for only the selected sample. The application saves these changes with the batch and stops applying the local method detection settings to the compound for this sample only.

   The Peak Detection Settings dialog box opens where you can adjust detection settings that were specified in the method. The title bar of the dialog box lists the selected compound and indicates whether you are making changes to only the selected sample or to the local method.

v To switch between method, manual, and user integration modes

- Right-click the Confirming Ions pane and choose **Toggle Integration Mode > Method/Manual/User**.

Initially, the method integration and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the plots for the Confirming Ions update and the result set updates as you switch between modes.

Each pane in Data Review reflects the changes when you switch between modes. The generated reports for these data identify any manual modifications.

Figure 52. Quantitative peak with multiple confirming ions

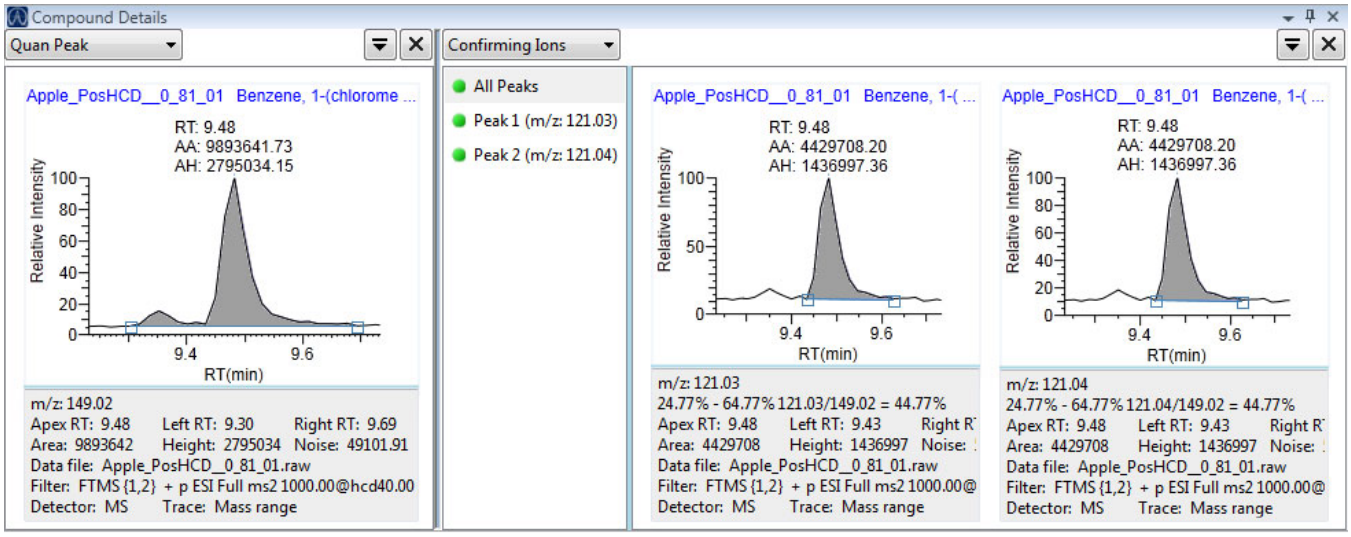


Figure 53. Confirming ion with coelution failure

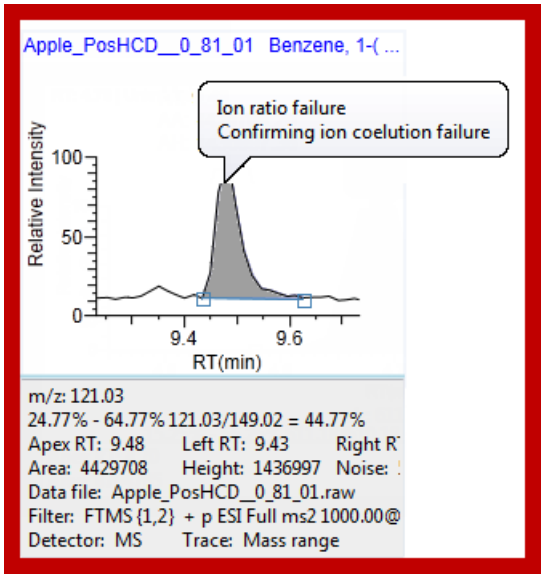


Table 29. Confirming Ions pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Swipe Manual Integration	Switches to manual integration mode, where you can manually define the peak. Also available from the icon in the upper right corner, .
Toggle Integration Mode (Method, Manual, or User)	Switches the display between local method integration, manual integration, and user-defined peak detection settings. You can edit the *method* or *user* peak detection settings from the Peak Detection Settings menu. See To modify the peak detection settings. You can manually edit a peak with the Swipe Manual Integration command. See To manually integrate a peak.
Delete Peak	Removes the peak and all data for this peak from all Compound View panes. Also available from the icon in the upper right corner, .
Peak Display Settings	Opens the Peak Display Settings dialog box.
Peak Detection Settings	Edit User 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. **IMPORTANT** The changes that you make on the Signal page in the Peak Detection Settings dialog box can affect all quantification and ion ratio calculations and are not auto-reversible. These changes can also create a mismatch with calibration files that are not fully defined in the batch.

Peak Display Settings dialog box

Use the features in the Peak Display Setting dialog box to change the labels in the Confirming Ions pane display.

Figure 54. Peak Display Settings dialog box

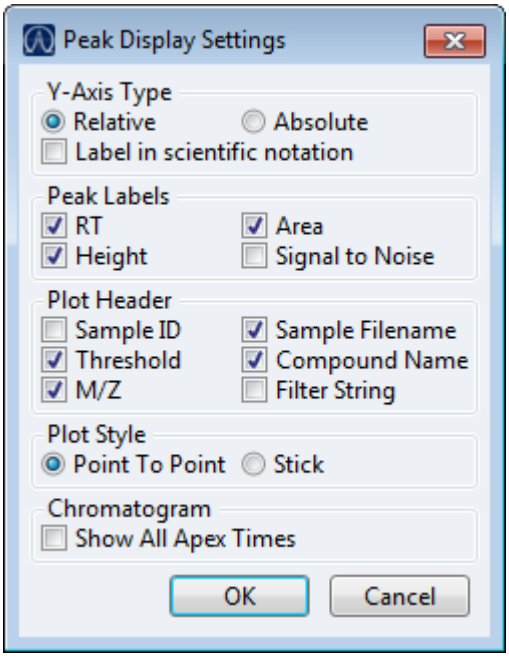
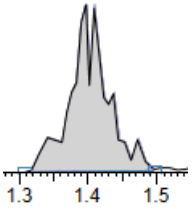
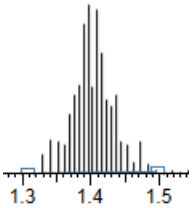


Table 30. Peak Display Settings dialog box parameters (Sheet 1 of 2)

Command	Description
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.
Peak Labels	
RT	Displays the retention time (RT) label in the peak chromatogram pane.
Height	Displays the peak height (AH) label in the peak chromatogram pane.
Area	Displays the peak area (AA) label in the peak chromatogram pane.
Signal to Noise	Displays the signal-to-noise (SN) label in the peak chromatogram pane.
Plot Header	
Sample ID	Displays a user-defined, alphanumeric string that identifies a sample.
Threshold	Displays the peak threshold.

Table 30. Peak Display Settings dialog box parameters (Sheet 2 of 2)

Command	Description
m/z	Displays the mass-to-charge ratio found in the spectrum for the peak. Assumes the charge is 1.
Sample Filename	Displays the name of the current, selected sample where the peak was found.
Compound Name	Displays the matched compound name found in the library or compound database.
Filter String	Displays the filter used to identify the peak. Specified in the raw data file or the master method.
Plot Style	
Point To Point	Displays chromatograms in the following format: 
Stick	Displays chromatograms in the following format: 
Chromatogram	
Show All Apex Times	Displays all surrounding apex times in the plot.

Calibration Curve

The Calibration Curve pane displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration. The Calibration Curve pane uses a unique shortcut menu. See Calibration Curve pane shortcut menu commands.

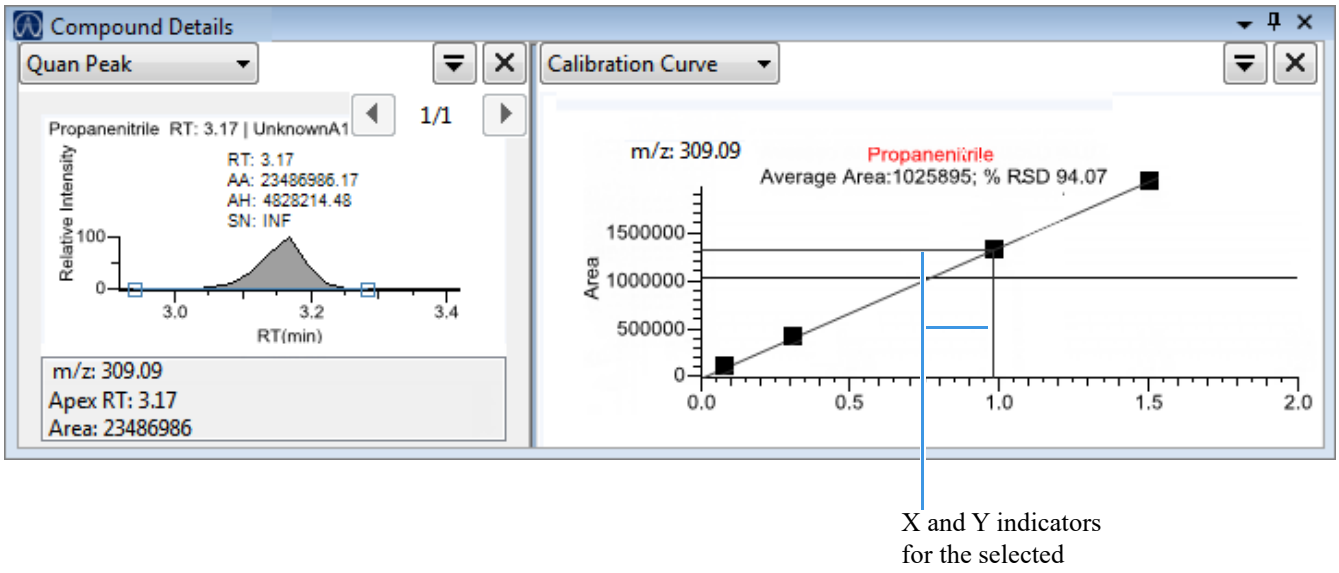
Note The field calculations related to calibration group are based on the selected group instead of the whole batch. The calibration is performed on each calibration group.

The calibration plot shows up for the selected sample based on the corresponding calibration group you have setup in the sample list. It will display the calibration group name in the plot as part of the heading.

The calibration curve plot shows X and Y indicators for the selected sample. The *x* axis represents the calculated amount, and the *y* axis represents the Response Via (area or height).

- The calibration curve plot displays the X and Y indicators when the Standard Type is Internal, External, or Estimated or when the Calibration Curve Type is Linear or Quadratic.
- The calibration curve plot does not display the X and Y indicators when the Standard Type is Std Addition or when the Calibration Curve Type is Average RF.
- Calibration plots in reports do not display the X and Y indicators.

Figure 55. Quantitative peak with a calibration curve plot



Manually exclude a calibration point

- In the Sample Results pane, select the **Excluded** check box for the sample.

  You might need to use the horizontal scroll bar at the bottom of the table to scroll to the Excluded column. See Inactive and Excluded compounds.

  When the application no longer uses a calibration point, its value appears as an empty box in the graphical view of the calibration curve.

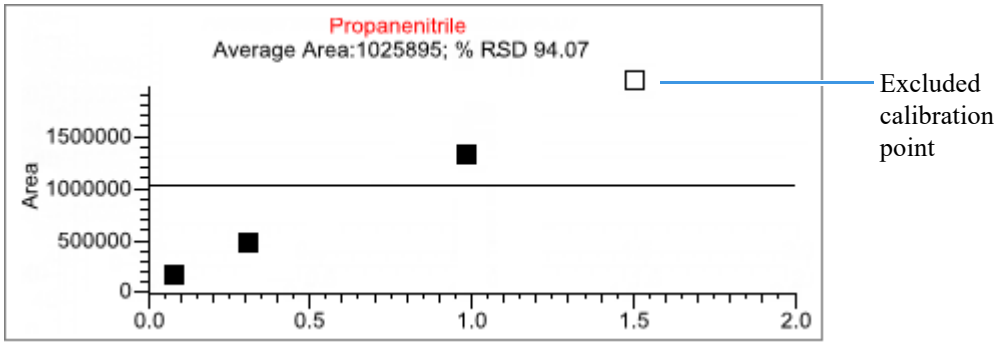


Table 31. Calibration Curve pane shortcut menu commands

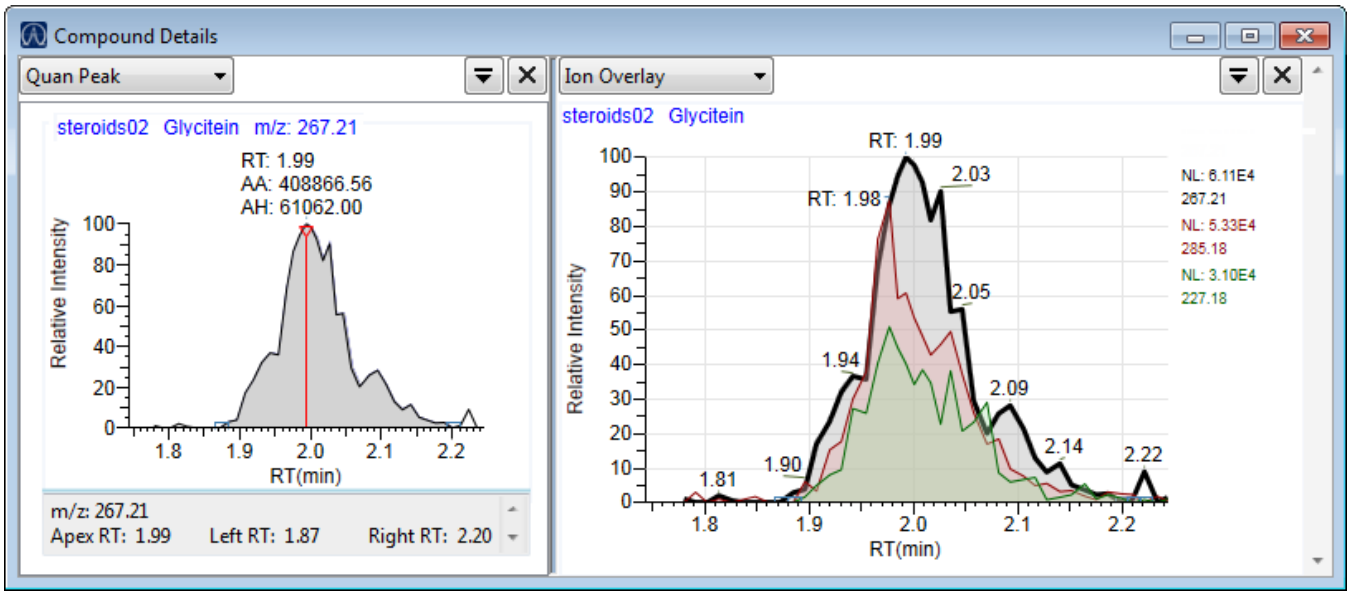
Command	Description
Standard Type	Sets the standard type to External or Internal.
Calibration Curve Type	Sets the calibration curve type to one of the following: • Linear: Uses all settings with this exception: When Origin is set to Include, all Weighting values are grayed out and Weighting is set to Equal. • Quadratic: Uses 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: Uses 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—target and 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.

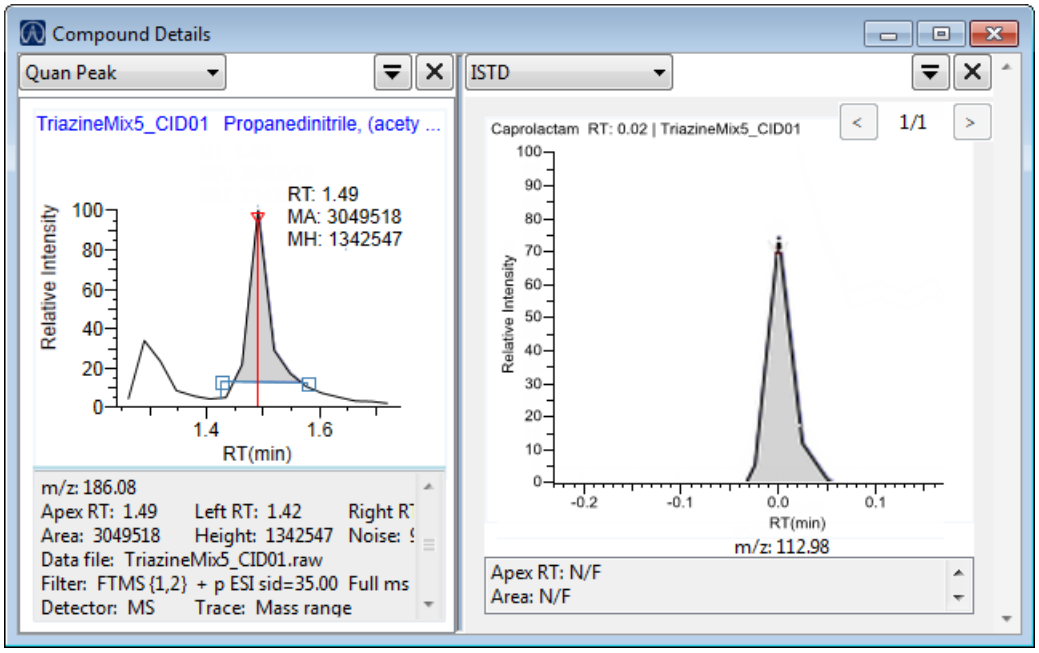
Figure 56. Target peak with a confirming ion overlay



ISTD

The ISTD pane displays the internal standard specified for the compound in the method. Refer to the instructions "To specify an internal standard type for a compound" in Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

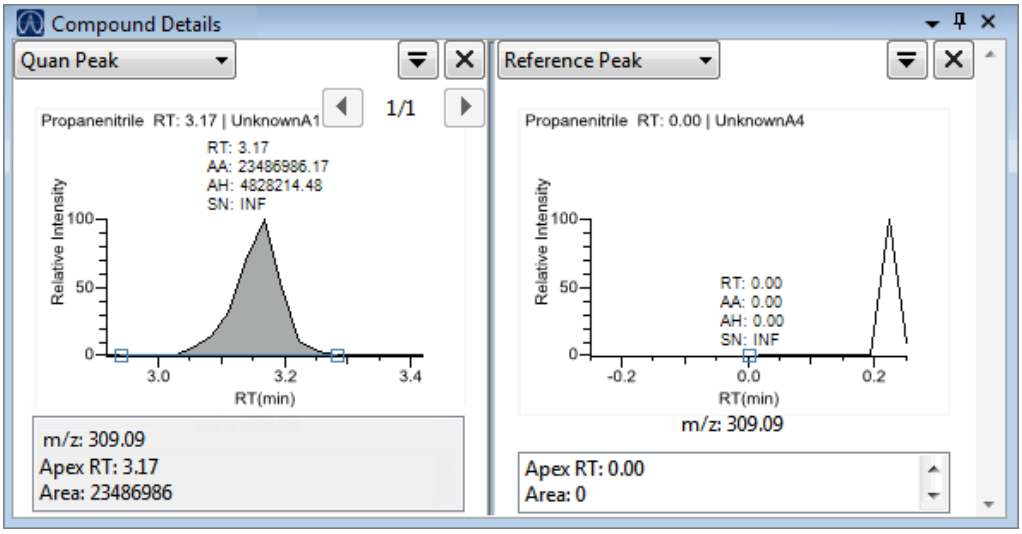
Figure 57. Quantitative peak with an internal standard



Reference Peak

The Reference Peak pane displays the reference peak as specified in the method.

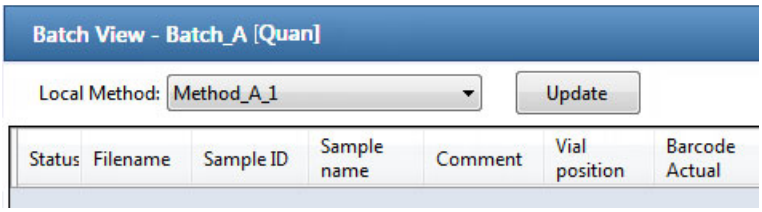
Figure 58. Quantitative peak with a reference peak



Specify a chromatogram reference peak

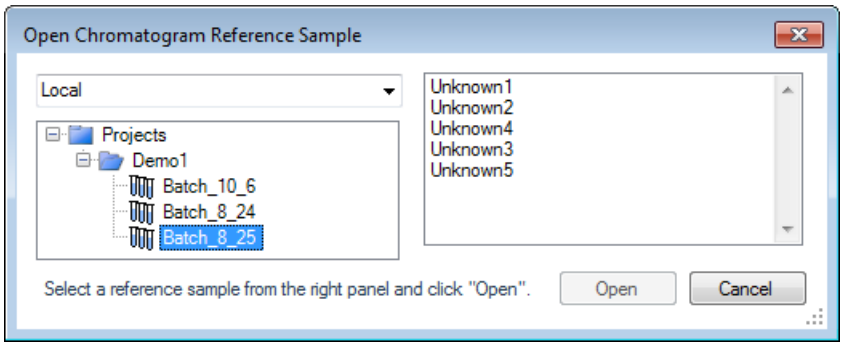
1. In the Batch View navigation pane, click **Reference Sample**.

   An empty reference sample table opens.



2. Right-click the sample table and choose **Add Reference Sample**.

   The Open Chromatogram Reference Sample dialog box opens.



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

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

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

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

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

8. 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, right-click and choose **Delete Selected**.

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.

Follow these procedures:

- To zoom in on a peak
- To copy a plot to another format
- To display the MS reference
- To customize the labels in a small molecule or peptide spectrum

v To zoom in on a peak

1. In the Spectra 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 Spectra pane and choose **Reset Scaling.**

v To copy a plot to another format

1. In the data spectrum or the reference spectrum, right-click and choose **Copy to Clipboard.**

   The application copies the specified plot graphic to the Clipboard.

   Note The application copies only the indicated data spectrum or the reference spectrum. It does not copy the entire Spectra pane.

2. In the source format (for example, an Excel spreadsheet or email window), right-click and choose **Paste**.

   The application pastes the graphic into the new format.

v To display the MS reference

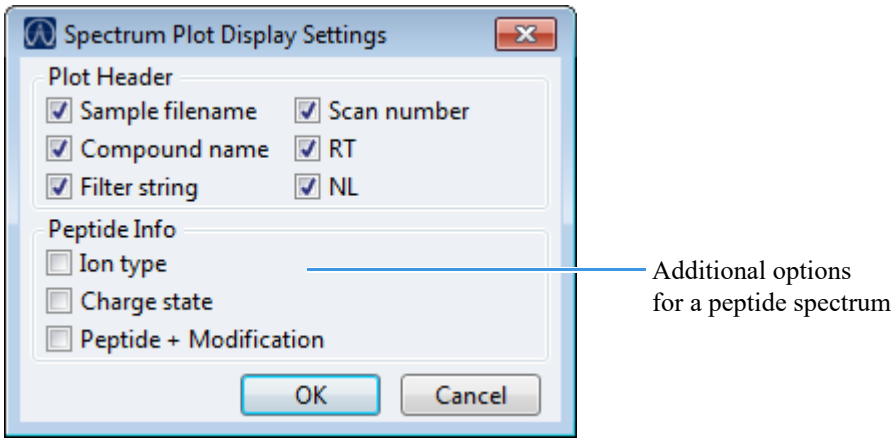
- Right-click the Spectra pane and choose **Show MS-Reference.**

  The application displays or hides the reference spectrum in the Spectra pane.

v To customize the labels in a small molecule or peptide spectrum

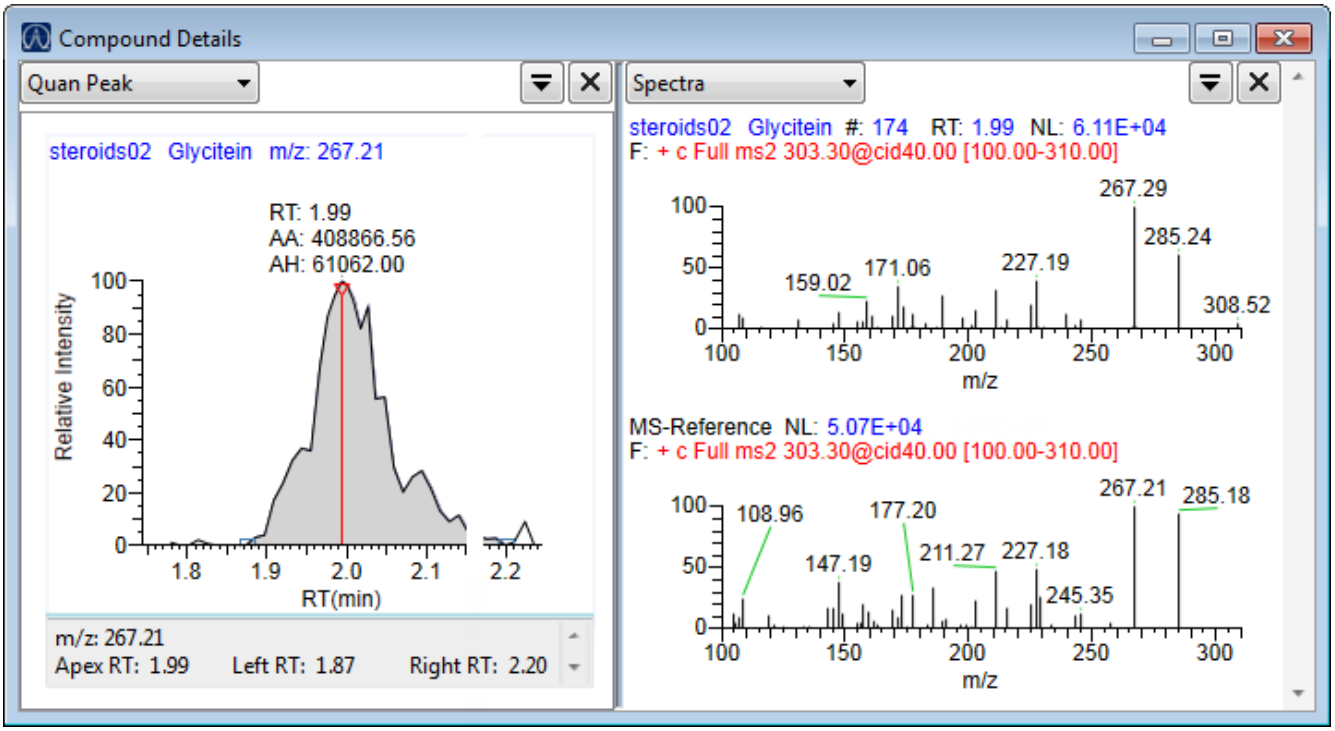
1. Right-click the Spectra pane and choose **Display Settings**.

   The Spectrum Plot Display Settings dialog box opens.



2. Select the check box for each label that you want to display and click **OK**.

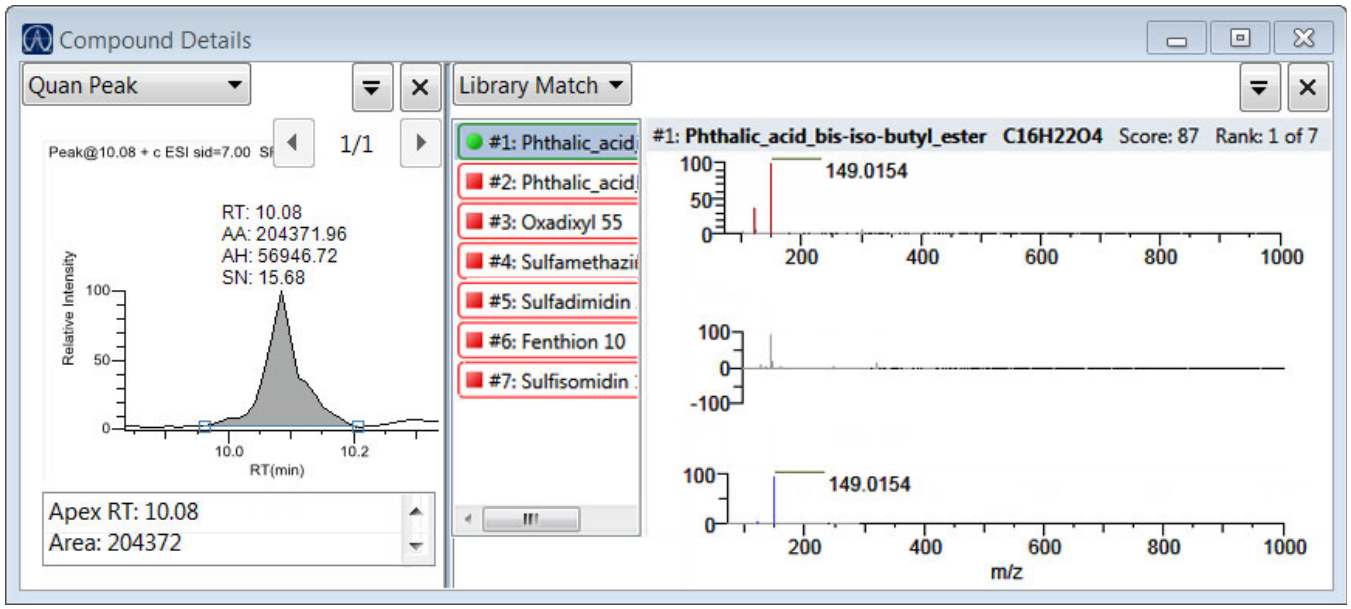
Figure 59. Quantitative peak with data and reference spectra



Library Match

The Library Match pane displays all library matches for the selected compound.

Figure 60. Library Match for the selected compound



If you have no matches for any of your compounds, make sure you have completed all of the following:

- Installed a library.
- Selected screening libraries in the Configuration console. Refer to Chapter 1, “Using the Configuration Console,” in the *TraceFinder Lab Director User Guide*.
- Enabled Library Matching in the method. Refer to Chapter 4, “Using the Method Development Mode for Quantitation Methods,” in the *TraceFinder Lab Director User Guide*.

Isotope

The Isotope pane displays all isotopes for the selected compound. The Isotope pane includes a shortcut menu. See Isotope pane shortcut menu commands.

Note When you select different samples, the current compound remains selected (as long as that compound is found in the sample).

The isotopes pane displays isotopic pattern results for all adducts of a compound according to the threshold and deviation parameters defined in the method.

To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

- An isotope peak is not found if its intensity, relative to the monoisotopic ion's intensity, is more than the specified intensity deviation percentage away from the theoretical relative intensity of the isotope ion.
- An isotope peak is found if its measured *m/z* is less than the specified mass deviation amount away from its expected *m/z*.

To specify isotopic criteria in a method, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

Figure 61. Isotope pane

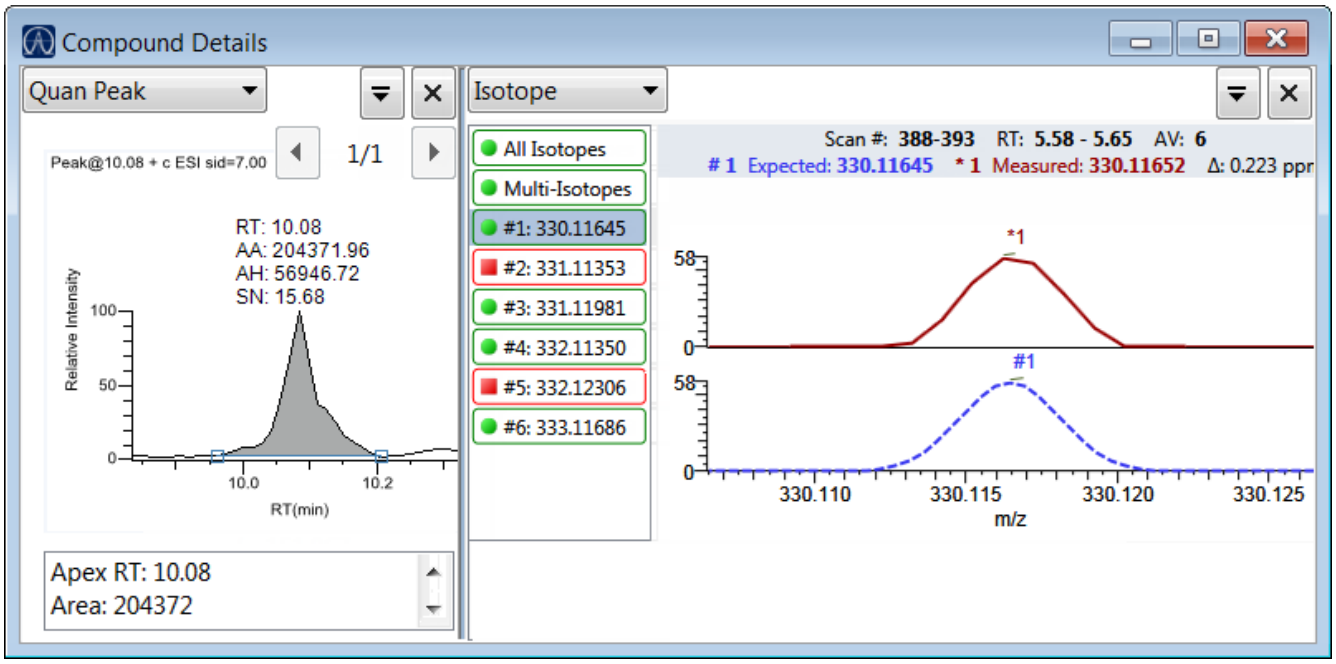


Table 32. Isotope pane shortcut menu commands

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 peak apex spectrum over the simulated 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

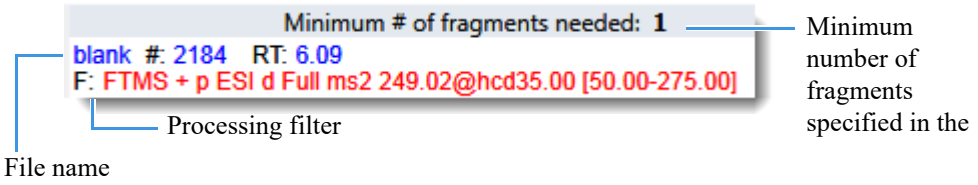
The Fragments pane displays fragments in one of two ways:

- All Fragments
- Individual fragments

All Fragments

The All Fragments view displays a composite of all fragments found in the peak. The application displays the measured peak as a red line; it displays the expected peak as a blue line.

These are the headers for the All Fragments view.



You can display all fragments as either stacked spectra or overlaid spectra.

Figure 62. Fragments pane with stacked spectra for all fragments

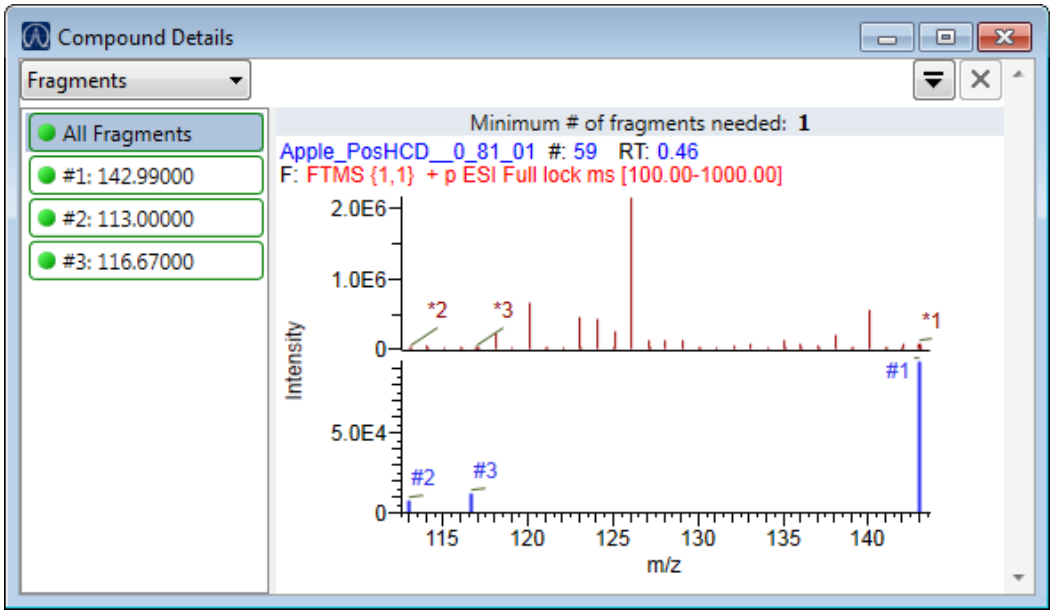
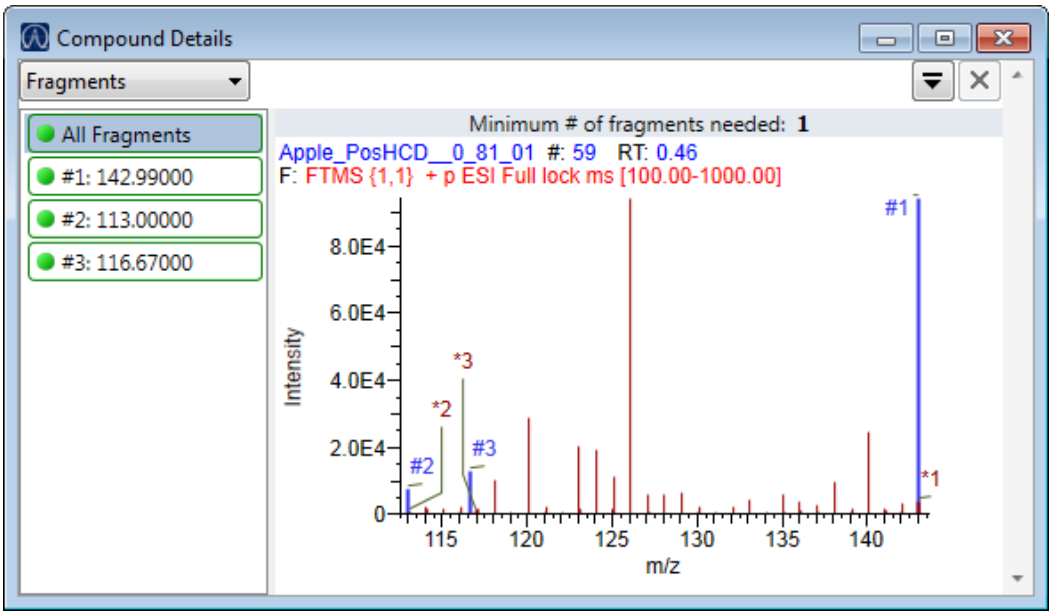


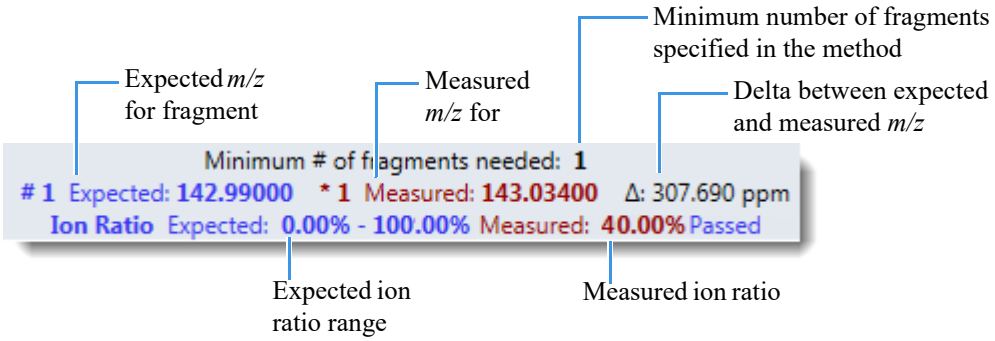
Figure 63. Fragments pane with overlaid spectra for all fragments



Individual fragments

The individual fragments view displays the expected and measured peaks for a single fragment.

These are the headers for the individual fragments view:



You can display the fragment as either stacked spectra or overlaid spectra.

Figure 64. Fragments pane with stacked spectra for a single fragment

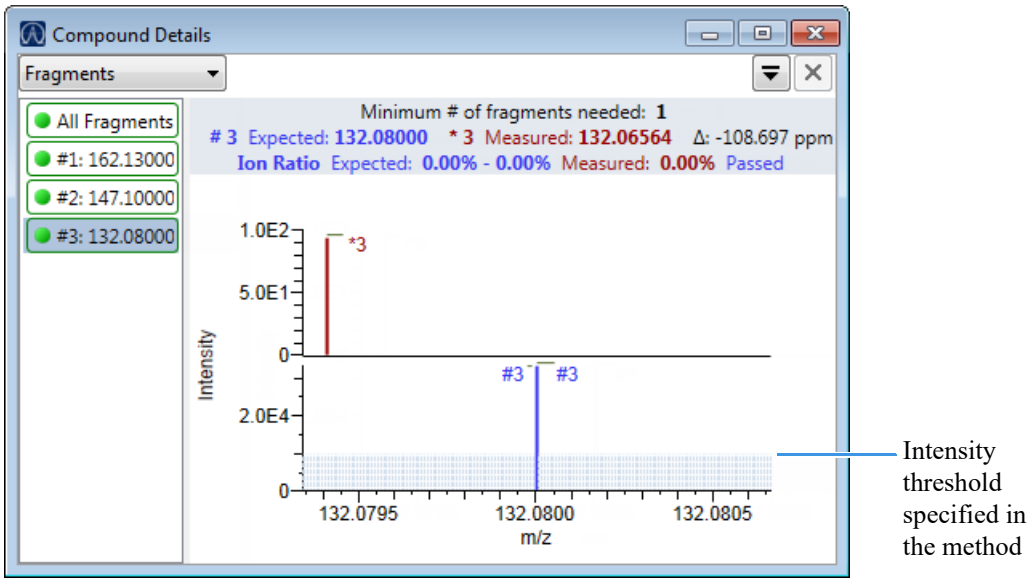
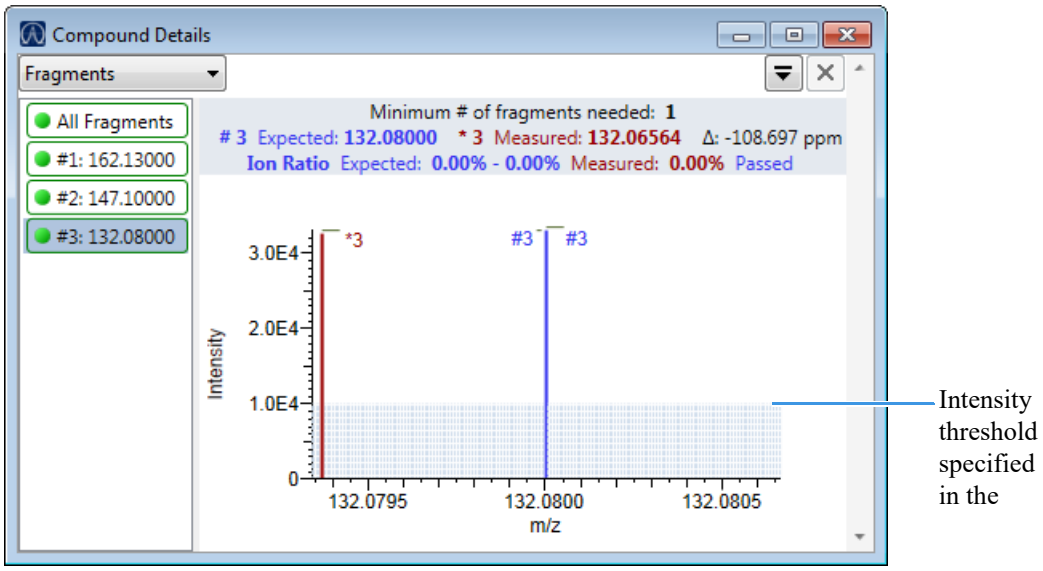


Figure 65. Fragments pane with overlaid spectra for a single fragment

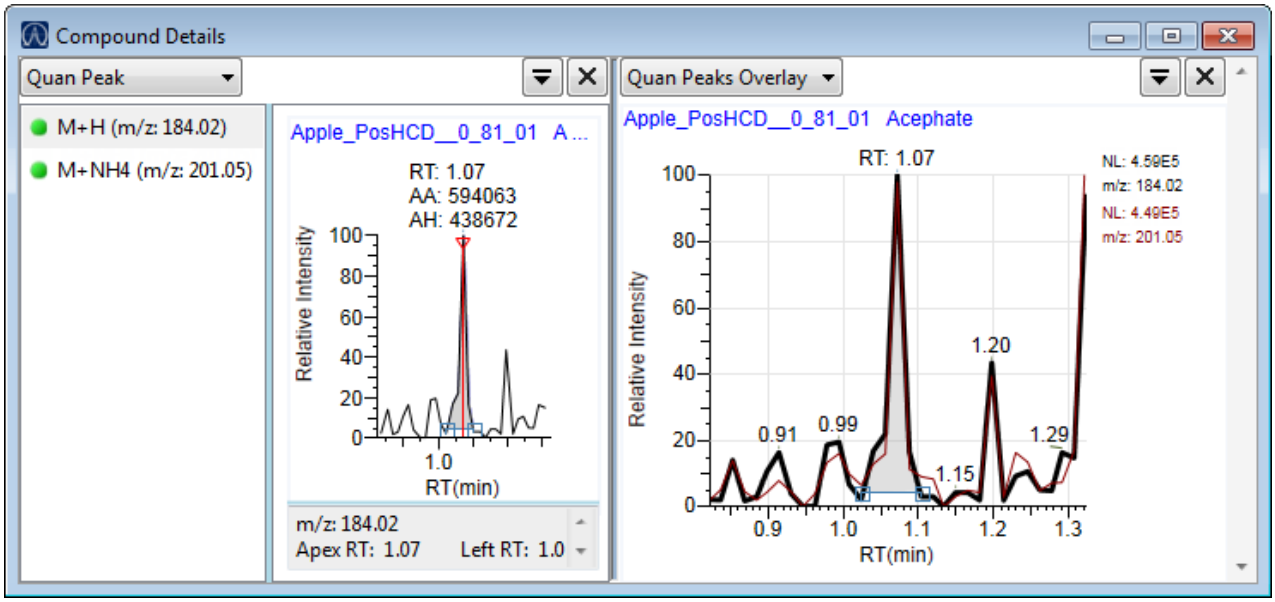


Quan Peaks Overlay

The Quan Peaks Overlay page displays overlaying quantitation peaks for compounds with multiple target peaks.

- The first target peak in the peak list appears in black in the overlay pane.
- The second target peak in the peak list appears in red in the overlay pane.
- The selected peak is bolded in the overlay pane.

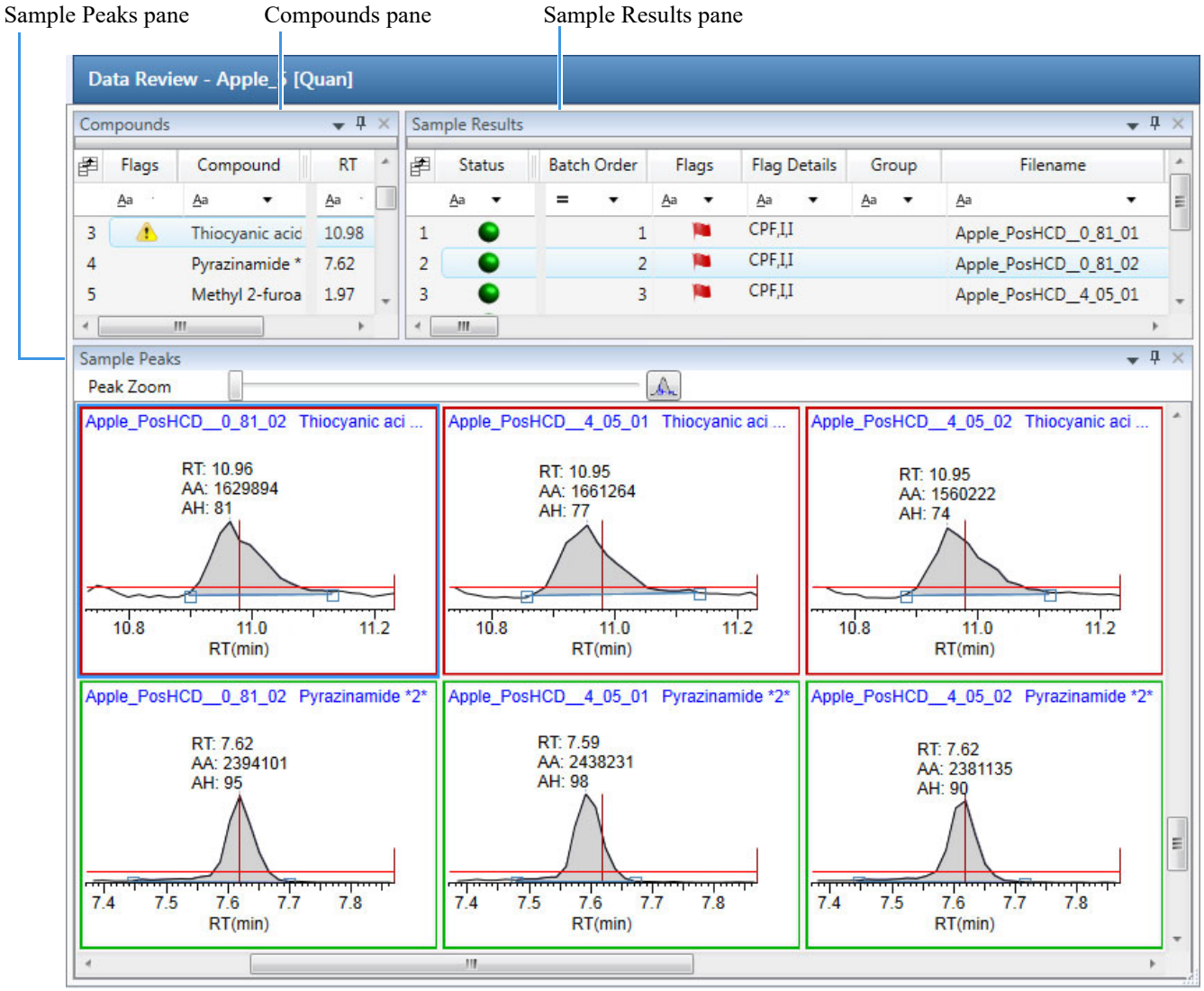
Figure 66. Quan Peaks Overlay page



Comparative View for quantitation batches

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.

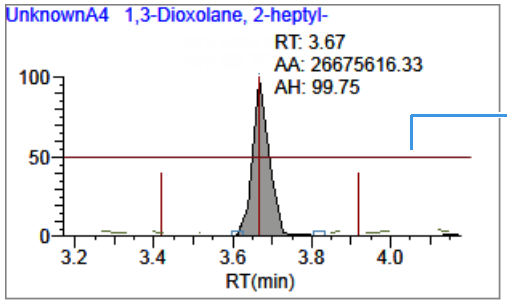
These are the default panes and their locations:



Using the Threshold Guide

The following factors define the threshold guide that the Comparative View displays in the sample peak plots:

- The threshold method and amount that you specified in the method
- The group that you created on the Sample page
- The threshold sample that you selected on the Threshold Samples page



The horizontal guide indicates the threshold value as specified in the method.

For information about creating groups, see Groups.

For information about specifying a threshold sample, see Threshold Samples page for quantitation batches.

For information about specifying the method to use for creating a threshold guide, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

IMPORTANT If the peaks are not displayed in the Comparative view when you are connected through a remote desktop, change the size of the text on the Windows Display settings page from 125% to 100% on the computer running Trace Finder application.

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.

Change the Sample Peaks pane display

1. From the View menu, choose **Chromatogram Pane Settings**.

   The Chromatogram Plot Settings dialog box opens.

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 67. Number of Rows equals 1 and Number of Columns equals 1

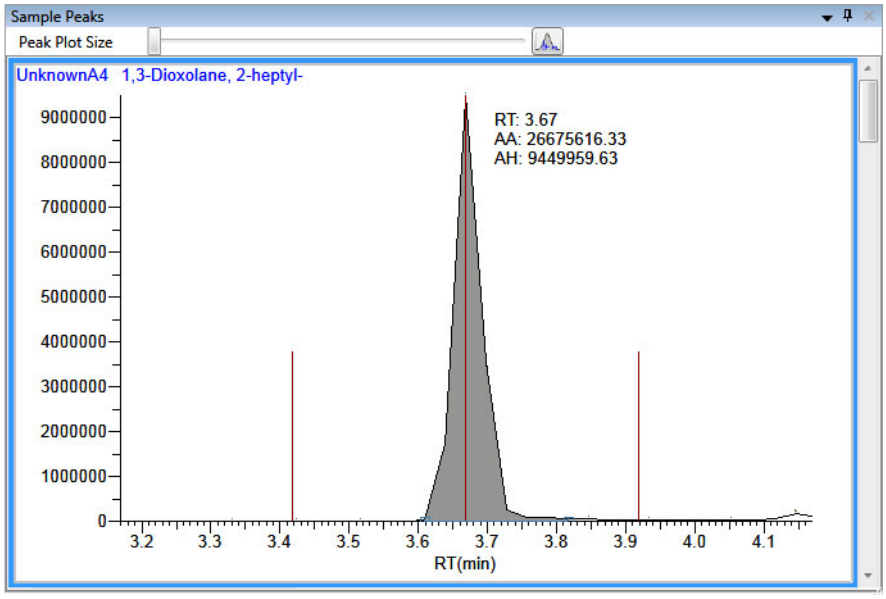
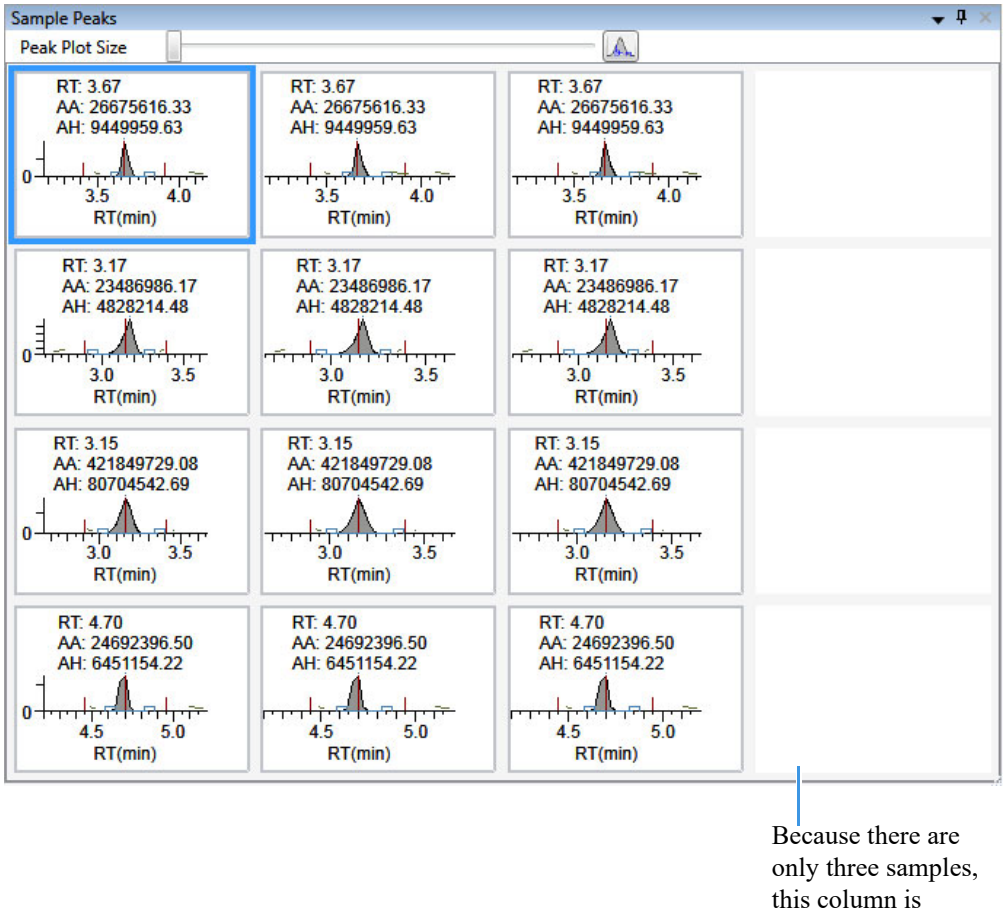
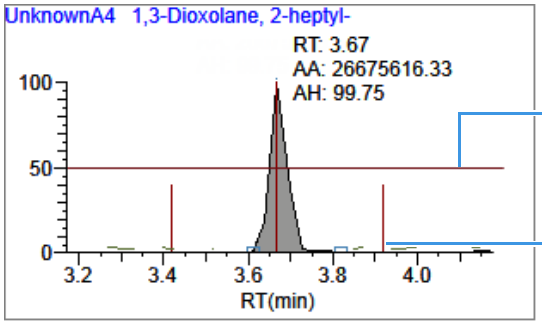


Figure 68. Number of Rows equals 4 and Number of Columns equals 4

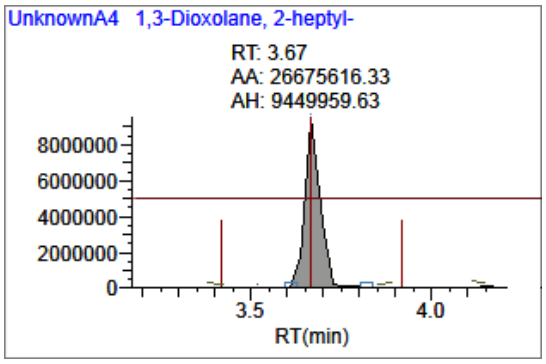


3. To change the display type for the *y*-axis scale, select one of the following:

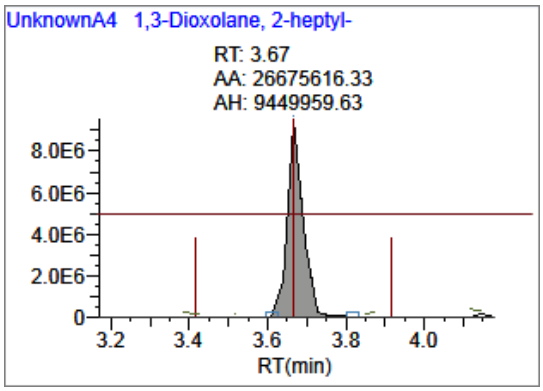
   - **Relative**: Displays the *y*-axis scale from 0 through 100.



- **Absolute**: Displays the *y*-axis scale from 0 to the actual value of the most intense peak in the group.



- **Label in Scientific Notation**: Displays the *y*-axis scale in scientific notation.



Note The Sample Peaks pane displays a *y* axis only in the first chromatogram in each row. The limits of the scale are determined by the most intense peak in the group.

4. Specify which labels you want to display in the sample peak plots.

   For an example of all available peak plot labels, see Peak Plot Labels.

Chromatogram Plot Settings dialog box

Use the Chromatogram Plot Settings dialog box to change the Sample Peaks pane display.

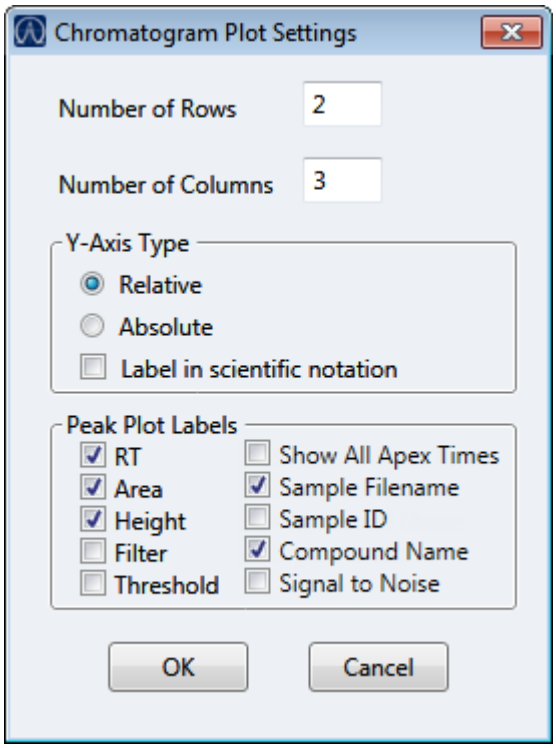
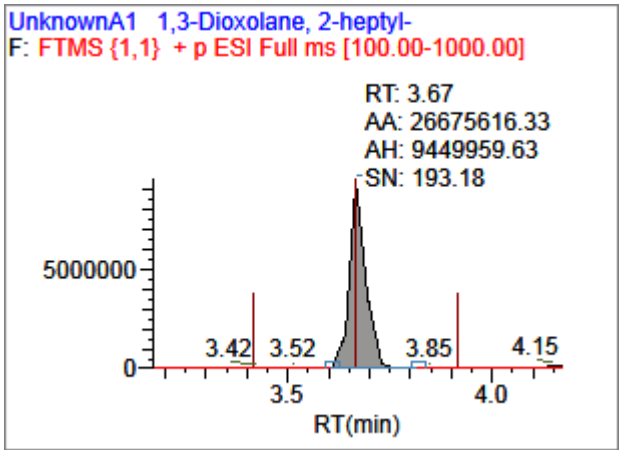


Table 33. Chromatogram Plot Settings dialog box parameters (Sheet 1 of 2)

Parameter	Description
Number of Rows	Specifies the number of rows visible in the Sample Peaks pane. When Number of Rows equals 1, the application scales the height of all chromatograms to fill the Y dimension of the Sample Peaks pane. Default: 3
Number of Columns	Specifies the number of columns visible in the Sample Peaks pane. When Number of Columns equals 1, the application scales the width of all chromatograms to fill the X dimension of the Sample Peaks pane. Default: 3
Y-Axis Type	Displays the *y*-axis scale as Relative (to the most intense peak), Absolute, or in scientific notation.

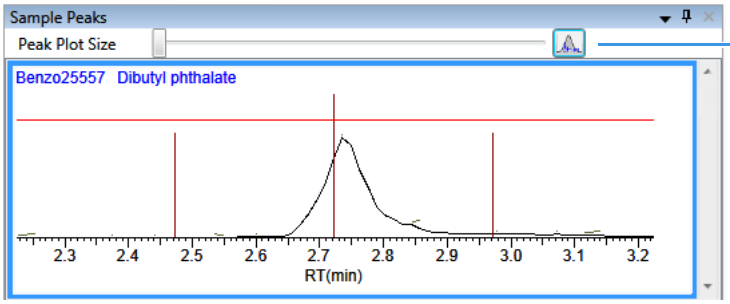
Table 33. Chromatogram Plot Settings dialog box parameters (Sheet 2 of 2)

Parameter	Description
Peak Plot Labels	Displays or hides the following peak labels: • RT • Area • Height • Filter • Threshold • Show All Apex Times • Sample Filename • Sample ID • Compound Name • Signal to Noise Example with all peak labels displayed: 

Manually integrate 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.

1. In the Sample Peaks plot, click the **Manual Integration** icon.

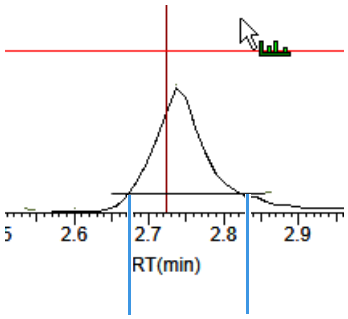


The cursor changes to look like this:

2. Integrate a peak as follows:
   a. Drag the cursor to define the beginning and ending base points for the new peak.

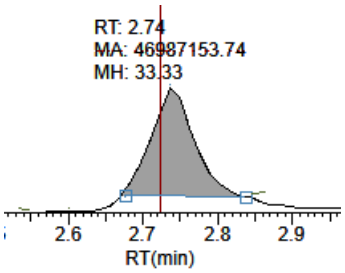
   Note You must drag the cursor inside the *x* axis and *y* axis.

   b. Click outside the plot to refresh the display.



Click the first base point, and then drag to the second base

Click outside the plot to refresh the view.



The application identifies the peak and indicates the manual integration in the labels.

3. To zoom in on an area, do the following:
   a. Drag the cursor below the *x* axis or to the left of the *y* axis.

   The plot zooms to fit the defined X or Y dimension into the entire pane. The application zooms all compounds in the row to the same scale.

   b. To return to the original view, right-click and choose **Reset Scaling**.

Qualitative View for quantitation batches

The Qualitative View uses several different panes to display qualitative information for the selected sample. See Display 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.

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 Chromatogram pane
- Spectrum pane (library and data)
- Library Hits pane

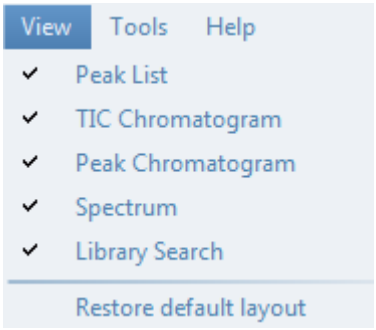
Display Qualitative View panes

The Qualitative View displays data using multiple panes: Samples, Peaks, Sample Chromatogram, Peak Chromatogram, Spectrum, and Library Hits. You can display, hide, or move any of these panes.

- From the View menu, choose to display or hide the following:
  - **Peak List**: Displays the Peaks pane
  - **TIC Chromatogram**: Displays the Sample Chromatogram pane
  - **Peak Chromatogram**: Displays the Peak Chromatogram pane
  - **Spectrum**: Displays the Spectrum pane
  - **Library Search**: Displays the Library Hits pane

Note The Samples pane is required for the Qualitative View display. You cannot hide the Samples pane.

A check mark indicates a displayed pane.



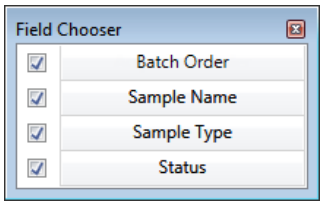
Samples Pane

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.

v **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 69. Samples pane

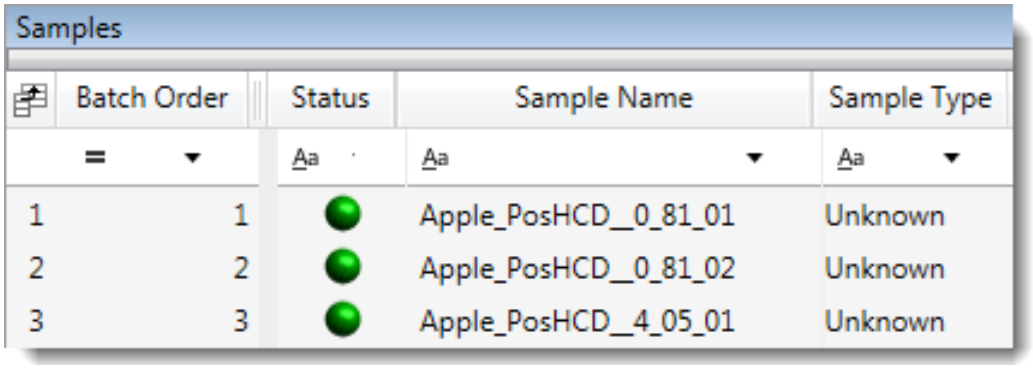


Table 34. Samples pane columns (Sheet 1 of 2)

Column	Description
Batch Order	Sequentially numbers the samples.
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.
	Note When you include unknown screening features in the quantitation method and you choose to process with only the quantitation criteria, the Sample View shows the Status for the samples as acquired and processed (), and the Unknown Screening View shows the Status for the samples as acquired but not processed ().
	Note When you include unknown screening features in the quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed ().

Table 34. Samples pane columns (Sheet 2 of 2)

Column	Description
Sample Name	A user-defined name that identifies a sample.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC, or Unknown.

Peaks pane

The Peaks pane in the Qualitative View works with the Samples pane to display graphical values for a unique sample and peak combination.

Follow these procedures:

- To display peaks for a specific compound
- To hide or display columns in the Peaks pane

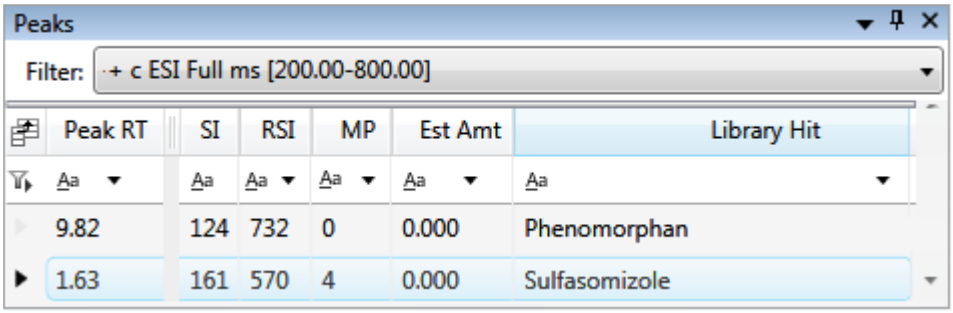
v To display peaks for a specific compound

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. Refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

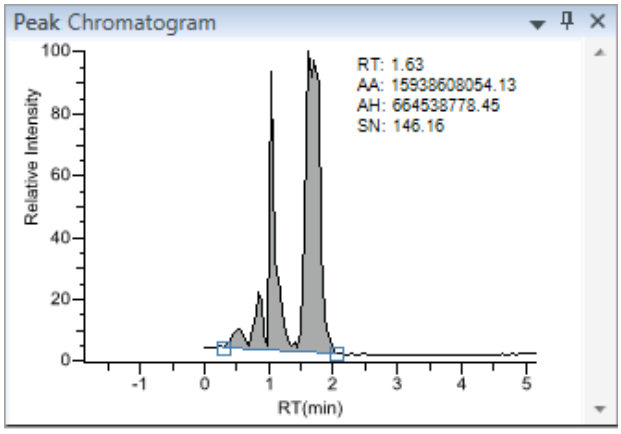
2. In the Peaks pane, select a peak in the sample.



   The application displays the selected peak in the Peak Chromatogram pane, displays the Qual Data and Qual Library sections in the Spectrum pane, and locates the selected peak in the Sample Chromatogram pane.

   - The Qual Data section shows spectrum data for the peak in the raw data file.
   - The Qual Library section shows actual spectrum for the identified library compound.

Figure 70. Peak Chromatogram pane



Note When you select a data-dependent sample, the peak can be from either a full scan or a QED spectrum of an SRM-filtered chromatogram.

Figure 71. Spectrum pane

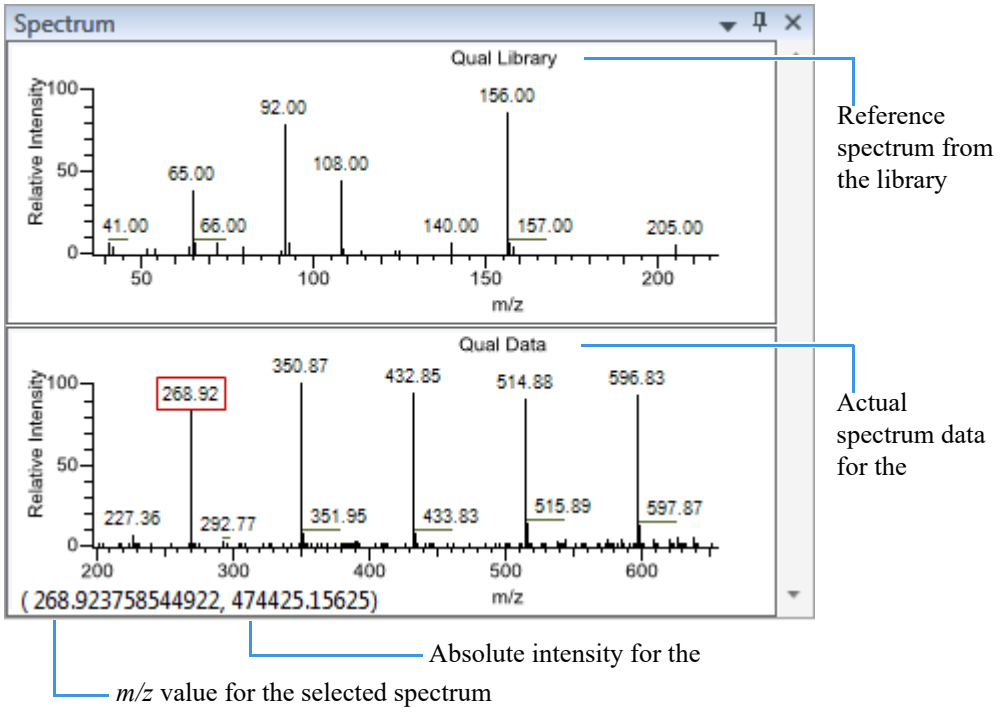
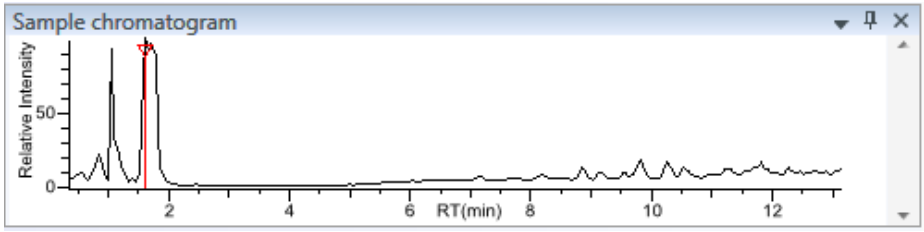


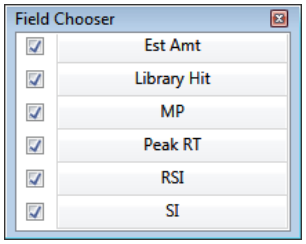
Figure 72. Selected peak in the Sample Chromatogram pane



v 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 73. Peaks pane

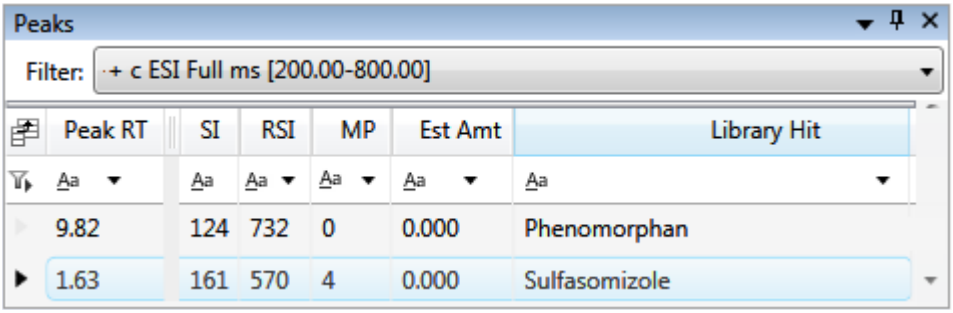


Table 35. Peaks pane parameters (Sheet 1 of 2)

Parameter	Description
Filter	Filter used to identify the peaks. Specified in the raw data file or the master method. When your raw data file is data-dependent, the filter indicates this with a "d".
Peak RT	Peak retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.

Table 35. Peaks pane parameters (Sheet 2 of 2)

Parameter	Description
SI	Search index method used to search the NIST library.
RSI	(Reverse search index) A method used to search the NIST library. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
MP	Match probability.
Est Amt	Estimated amount of the compound.
Library Hit	Library compound that matches the identified peak.

Sample Chromatogram pane

The Sample Chromatogram pane in the Qualitative View displays all peaks in the selected sample. The peak selected in the Peaks pane displays a red marker.

v **To zoom in on a peak**

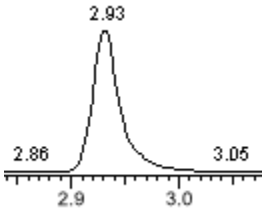
1. In the Sample Chromatogram pane, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the Sample Chromatogram pane and choose **Reset Scaling.**

v **To manually add a peak**

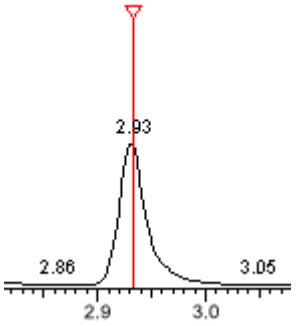
1. Zoom in to better identify which peak to add to the results set.



2. Right-click the Sample Chromatogram pane, and choose **Add Qual Peak**.

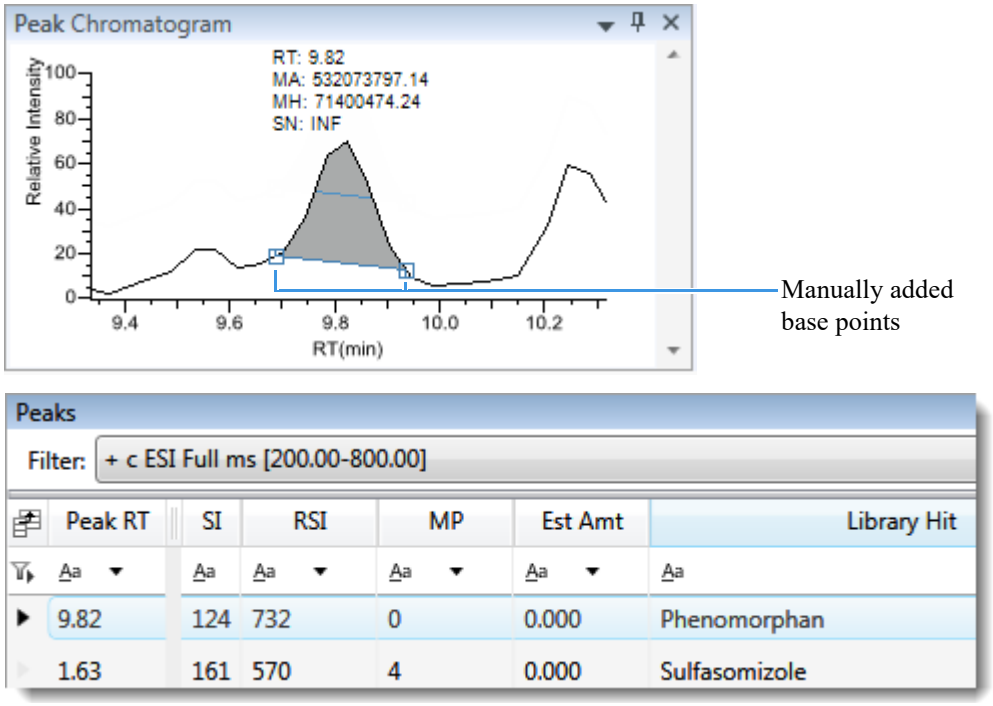
3. Click to indicate the left and right base points for the peak.

   The application marks the peak in the Sample Chromatogram pane.



The application places the peak delimiter tags at the base point locations and automatically updates the peak values in the Peaks pane and Peak Chromatogram pane. See Peak Chromatogram pane with a manually added peak.

Figure 74. Peak Chromatogram pane with a manually added peak



Sample Chromatogram pane

Use the features in the Sample Chromatogram pane to display peaks in the selected sample.

Figure 75. Sample Chromatogram pane

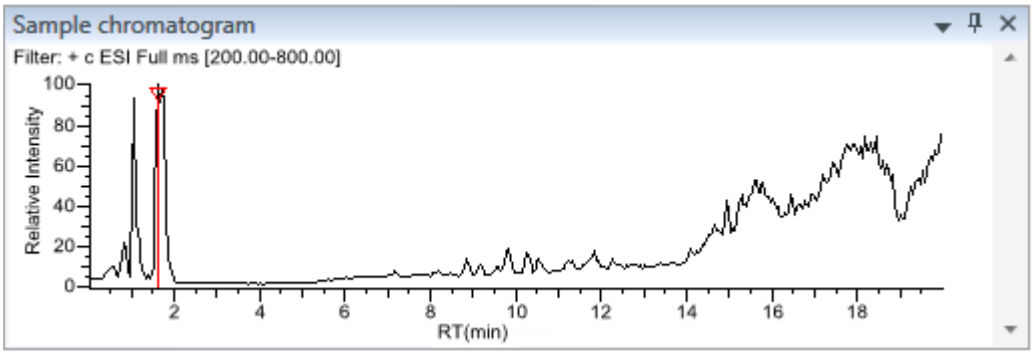


Table 36. Sample chromatogram pane shortcut menu commands

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.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Peak Chromatogram pane

The Peak Chromatogram pane in the Qualitative View displays the selected peak.

Follow these procedures:

- To zoom in on a peak
- To remove a peak
- To switch between method, manual, and user integration modes
- To customize the labels in the display

v **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.**

v **To remove a peak**

- Right-click the Peak Chromatogram pane, and choose **Remove Qual Peak**.

  The application removes the peak displayed in the Peak Chromatogram pane. All data for this peak are removed from the Qualitative View panes.

v To switch between method, manual, and user integration modes

- Right-click the Peak Chromatogram pane and choose **Toggle Integration Mode > Method/Manual/User**.

  Initially, the method integration and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the Peak Chromatogram plots update and the result set updates as you switch between modes.

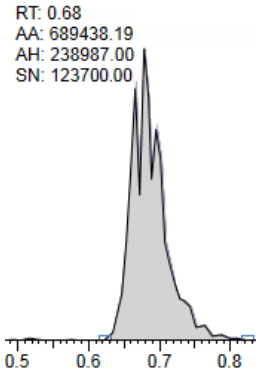
  Each pane in Data Review reflects the changes when you switch between modes. The generated reports for these data identify any manual modifications.

v To customize the labels in the display

1. Right-click the peak plot and point to **Peak Labels**.
2. To display labels for the peak retention time (RT), area (AA), height (AH), or signal-to-noise (SN), select the appropriate check box.

   See Example of displayed labels.

   Figure 76. Example of displayed labels



Peak Chromatogram pane

Use the features in the Peak Chromatogram pane to display the selected peak.

Figure 77. Peak Chromatogram pane

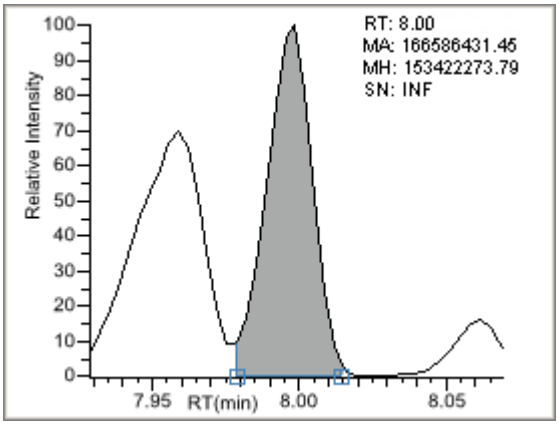


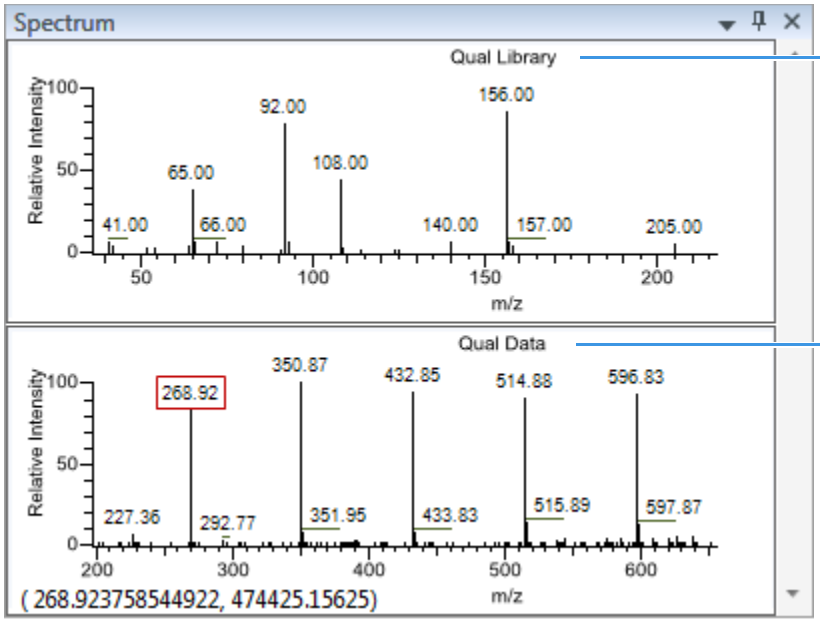
Table 37. Peak Chromatogram pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Method Integration	Displays method integration settings.
Manual Integration	Displays manual integration settings.
Peak Labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label to Noise).
Remove Qual Peak	Available only for manually added peaks. Removes the peak displayed in the Peak Chromatogram pane.
Copy to Clipboard	Copies the graphic display to the Clipboard.

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 78. Spectrum pane



Reference spectrum from the library

Actual spectrum data for the

v 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.**

v To display detailed m/z values

- In the spectrum pane, point to the *m/z* value for a peak.

  The application indicates the rounded-off *m/z* value with a red box and displays the complete value in the lower left corner of the display.

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.

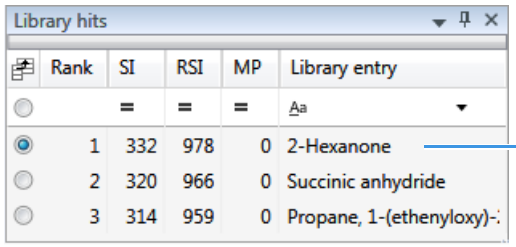
When you select a library entry other than the original entry, the TIC Report and TIC Summary Report indicate this with a "P" flag:

Peak:	Retention Time	Area	Height	Inj Estimate	In-sample Est	Flag
Naphthalene	7.95	13829174	10605061	0.000	0.000	P

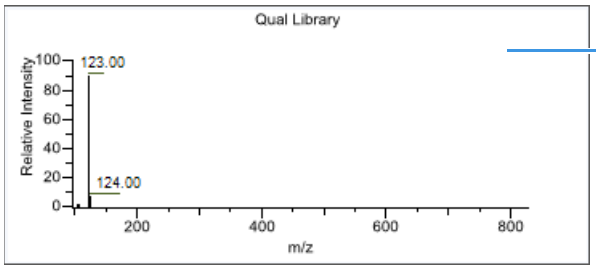
P flag

Change the library entry for a selected peak

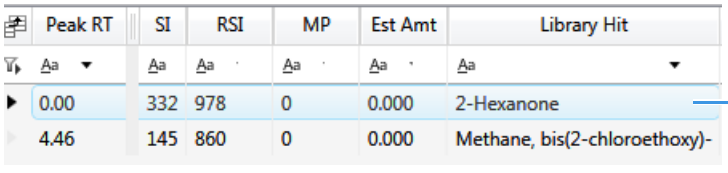
- In the Library Hits pane, select the check box for the library entry that you want to use to identify the selected peak.
  - In the Spectrum pane, the reference spectra change to show the spectra for the selected library entry.
  - In the Peaks pane, the SI, RSI, MP, and Compound values update to reflect the selected library entry.



Selected library entry in the Library Hits pane



Reference spectra for Hexanone



Peak list for Hexanone

Figure 79. Library Hits pane

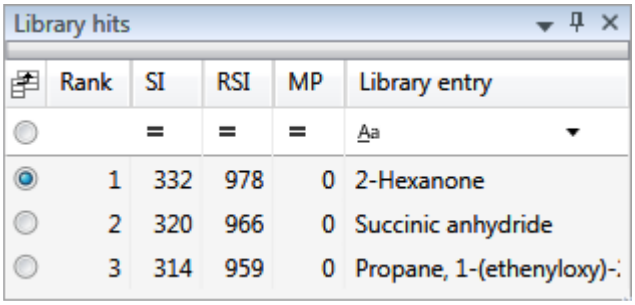


Table 38. Library Hits pane parameters

Parameter	Description
<Check box column>	Indicates selected library entries for the selected peak.
Rank	Indicates the order of best matches between the selected peak and library entries.
SI	(Search index) A method used to search the NIST library.
RSI	(Reverse search index) A method used to search the NIST library. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
MP	Match probability.
Library Entry	Library compound that matches the identified peak.

Column parameters for Compound Results and Sample Results

The Compound Results and Sample Results data review pages use the following parameters and features:

- Common column parameters
- Inactive and Excluded compounds
- Exporting compounds

Common column parameters

Table 39. Common parameters for Compound Results and Sample Results tables (Sheet 1 of 8)

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	Relative standard deviation (RSD) 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. Refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*. 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 Cal Std 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 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.
Actual RT	Actual retention time for the compound. Retention time is the time after injection when a compound elutes and the total time that the compound is retained on the chromatograph column.

Table 39. Common parameters for Compound Results and Sample Results tables (Sheet 2 of 8)

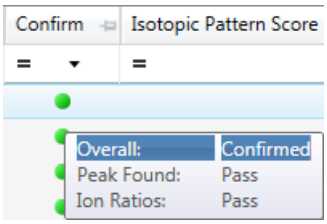
Column	Description
Adduct	The defined adduct for the retention time for a compound.
Area	The area obtained by integrating peak intensities from the start to the end of the peak. When the Response Ratio is specified as Area, this column displays an asterisk (*Area).
Batch Order (Sample Results only)	Sequentially numbers the samples in the batch.
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 the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.
Compound (Compound Results only)	Name of the identified compound.
Comments (Sample Results only)	A user-defined comment for the sample.
Confirm	Specifies that the compound meets all required processing criteria. Refer to the instructions "To display only confirmed peaks" in Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*. To display the confirmation criteria, point to the indicator. 

Table 39. Common parameters for Compound Results and Sample Results tables (Sheet 3 of 8)

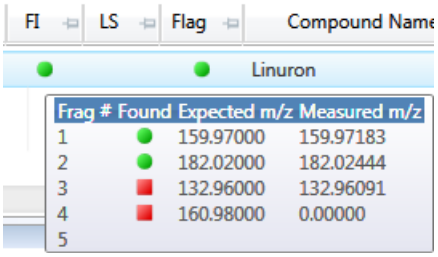
Column	Description
FI	Fragment Ions flag. The application displays one of these indicators: • A green circle (pass) when the measured *m/z* value of any of the fragments is within the mass tolerance specified in the method. • A red square (fail) when the measured *m/z* value of none of the fragments is within the mass tolerance specified in the method. • A blank when there are no fragments detected. To display a list of fragments and their pass/fail status, point to the indicator. 
Filename	A user-defined name that identifies a sample.
Final Units	Specifies the calculated amount. Default: 1
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.
Group (Sample Results only)	Threshold group to which a sample belongs. You can view samples by group in the Comparative View.
Group Average (Compound Results only)	Average of the samples in a threshold group. You can view averaged samples in the Compound View.
Height	Specifies 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	Specifies the integration mode (manual or method). See Quan Peak.

Table 39. Common parameters for Compound Results and Sample Results tables (Sheet 4 of 8)

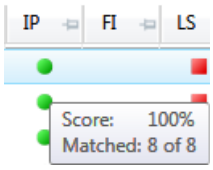
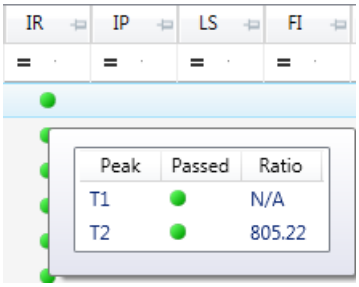
Column	Description
Ion Ratio	Specifies the ratio of the confirming ion's response to the target ion's response.
Ion Type	Specified as **b** or **y** with a numerical designation. Available only for peptide databases.
IP	Isotopic Pattern flag. The application displays one of these indicators: • A green 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, point to 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 To display the ion ratio results, point to the indicator. 
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.
Level (Sample Results only)	The level defined for a calibration sample or quality control sample.

Table 39. Common parameters for Compound Results and Sample Results tables (Sheet 5 of 8)

Column	Description
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 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: • A library score that is higher than or equal to the score threshold meets the criteria, and the values in this column appear in green. • A library score that is lower than the score threshold fails to meet the criteria, and the values in this column appear in red. 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 Probability Percentage	Specifies the probability of the match in the NIST library for forward searches only.

Table 39. Common parameters for Compound Results and Sample Results tables (Sheet 6 of 8)

Column	Description
Library Score (%)	Specifies the score from the library fit. When the application finds a match in the high resolution NIST library or in the mzVault 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: • A library score that is higher than or equal to the score threshold meets the criteria, and the values in this column appear in green. • A library score that is lower than the score threshold fails to meet the criteria, and the values in this column appear in red. 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. Valid range: 1 through 100%
LS	Library Search flag. The application displays one of these flags: • A green circle when the library search passes. • A red square when the library search fails.
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" (not found).
m/z (Delta)	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.
Modification	Specifies the modifications from imported peptide files or from the Peptide Predictor tool. Available only for peptide databases.

Table 39. Common parameters for Compound Results and Sample Results tables (Sheet 7 of 8)

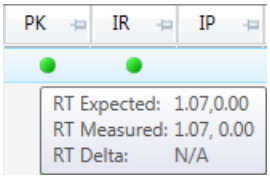
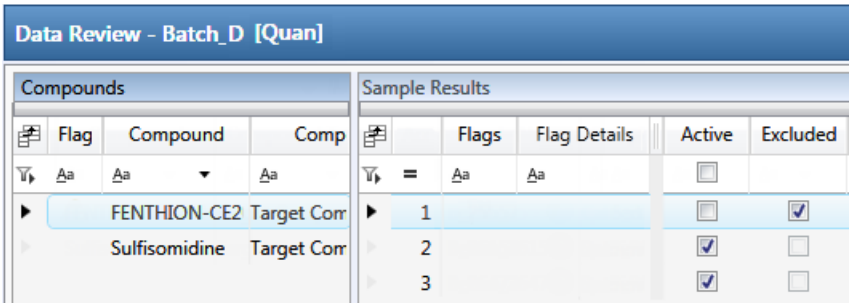
Column	Description
Num Isotopes Matched	The number of isotopes matched in the expected calculated isotope spectra relative to the total number of isotopes used in the score calculation, in the format "x of y", where • x = the number of isotopes matching the elemental composition used for the Isotopic 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.
Peak Label	User-specified label.
Peptide Sequence	Specifies the peptide sequence that the application uses to calculate the *m/z* or precursor *m/z*. Available only for peptide databases.
PK	Specifies if the peak was 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 To display the peak results, point to the indicator. 
Protein Name	Alphanumeric name assigned to the protein.
Relative RT	Specifies the measured retention time relative to the RT Reference values set in the method.
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.
RSI/Rev Dot	Specifies the results of a reverse search of the NIST library. A reverse search compares a library entry to an unknown compound.
RT	Specifies the retention time for the compound.
RT Delta	Specifies the difference between the expected retention time and the measured retention time.
S/N	The signal-to-noise ratio calculated for the found peak.
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.
SI/Dot Product	Specifies the results of a forward search of the NIST library. A forward search compares the mass spectrum of an unknown compound to a mass spectral library entry.

Table 39. Common parameters for Compound Results and Sample Results tables (Sheet 8 of 8)

Column	Description
Sample ID (Sample Results only)	A user-defined, alphanumeric string that identifies a sample.
Sample Name (Sample Results only)	A user-defined name that identifies a sample.
Sample Type (Sample Results only)	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC, or Unknown.
Std Add Amount	Specifies the standard amount added to the sample.
Theoretical Amt	Theoretical amount of the compound expected in the sample.
Type	In the Compound Results pane, specifies Target Compound, Confirming Peak, or Fragment. In the Sample Results pane, specifies Sample, Confirming Peak, or Fragment.

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

v 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 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.

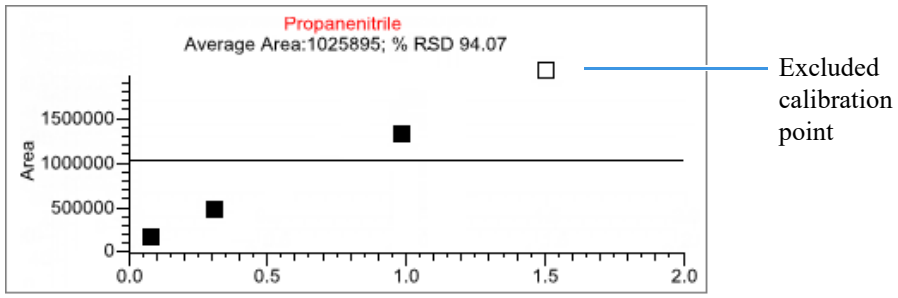
v **To exclude a calibration point**

- In the sample list, select the **Excluded** check box for the sample.

> **Note** Only calibration samples have the Excluded check box available. See Inactive and Excluded compounds.

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.



Exporting compounds

You can export compound data to an Excel spreadsheet or to a CSV file. These export commands are available from the File menu in the Sample View, Compound View, and Comparative View.

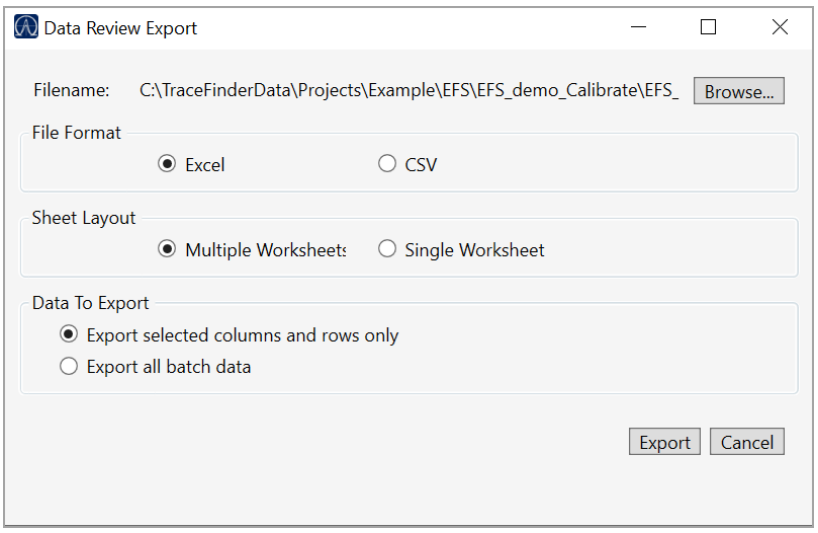
Follow these procedures:

- To export compounds to an Excel spreadsheet
- To export compounds to a CSV file

v 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.

   Note The exported information will be lost when you export the compound data from 5.0 or a higher version of the application to the 3.3 version.

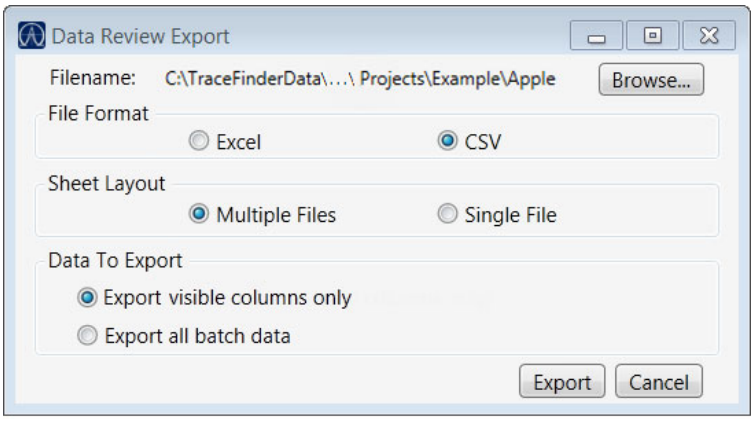
3. Type a file name for the XLSX file and click **Save**.
4. In the File Format area, in the Data Review Export dialog box, select the **Excel** option.
5. In the Sheet Layout area, select one of the following file formats for the spreadsheet.
   - **Multiple Worksheets**: Writes one sample to each Excel worksheet.
   - **Single Worksheet**: Writes all samples to a single Excel worksheet.
6. In the Data to Export area, select one of the following sets of data to export.
   - **Export 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.
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.

v 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 the displayed columns of selected samples to the specified worksheet format.
   - **Export All Batch Data**: Writes all data from all samples in the batch to the specified worksheet format.
7. Click **Export**.

   The application saves the specified compound data to a CSV spreadsheet.

   When you selected to create multiple files, the application opens the folder where you saved the files. The application names each file *Batch_Compound*.csv.

   When you selected to create a single file, the Excel application opens, displaying the exported data for all samples. The application names the file *Batch*.csv.

Working in the Report View for quantitation batches

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

v To open the Report View

- Click **Report View** in the navigation pane.

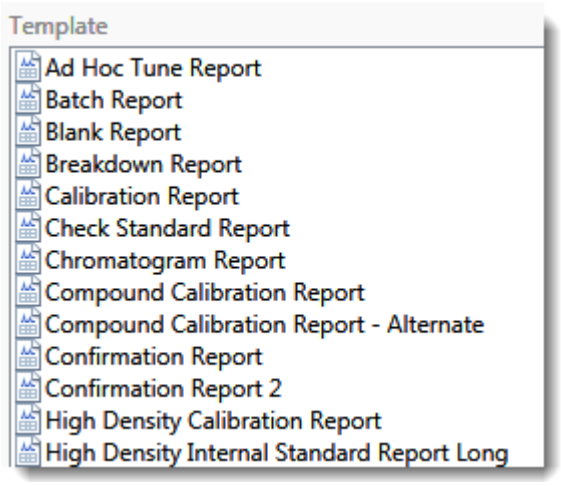
The application opens the Report View.

v To preview a report

1. In the Template pane, select a report template.

   The template list shows all the quantitation report templates that you configured in the Configuration console. Refer to "Specifying the Reports" in Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

   Figure 80. Example of a report template list



2. Click Preview.

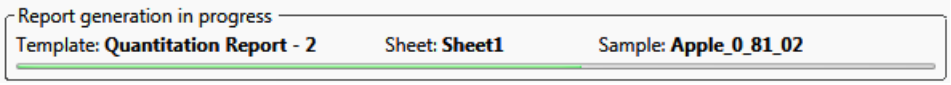
   The application opens a Report Preview, showing the report information for the current batch in the selected report template format.

v To generate a report as a PDF, an Excel, or a CSV file

1. In the Template pane, select a report template.
2. Select the check box for each of the file types that you want to create: **PDF**, **Excel**, or **CSV**.
3. Click Generate.

   The application does the following:

   - Displays a green progress bar as it generates the reports.

   - Creates a report for the current batch as a PDF, an Excel, or a CSV file, using the selected report template format.
   - Adds information about the generated report to the Generated Reports pane.

     For details about the Generated Reports pane, see Report View.
   - Saves the report files to the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

v To print a report

1. In the Template pane, select a report template.
2. Select the check box for the **Print** file format.
3. Click Generate.

   The application does the following:

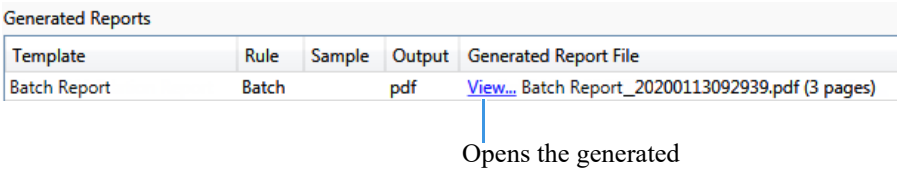
   - Creates a report for the current batch using the selected report template format.
   - Prints the report to your default printer.
   - Adds information about the generated report to the Generated Reports pane.

     For details about the Generated Reports pane, see Report View.
   - Saves the report files to the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

v To display a generated report

- In the Generated Reports pane, click **View** for the report that you want to see.

Figure 81. Generated Reports pane showing a PDF report



The application opens the output file.

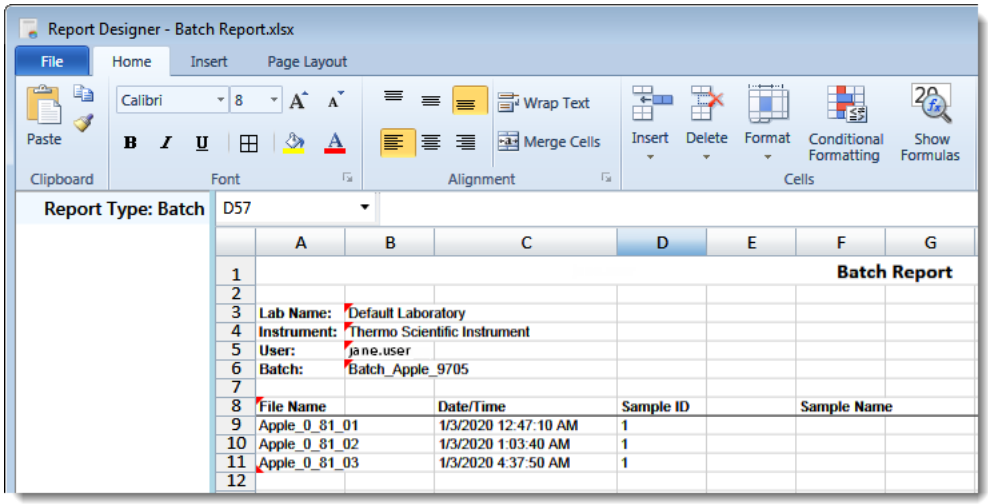
v To edit a report template

You cannot edit report templates that were provided with the TraceFinder application; however, you can open a TraceFinder template, make changes, and save it to a new template name.

1. In the Template pane, select a report template.
2. Click Open.

   The application opens the Report Designer showing the template in an Excel spreadsheet.

   Figure 82. Report Designer showing the template for the selected report



3. Use the features in the Report Designer to edit the template.

   See Chapter 7, "Using the Report Designer."

4. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

v To create a new report template

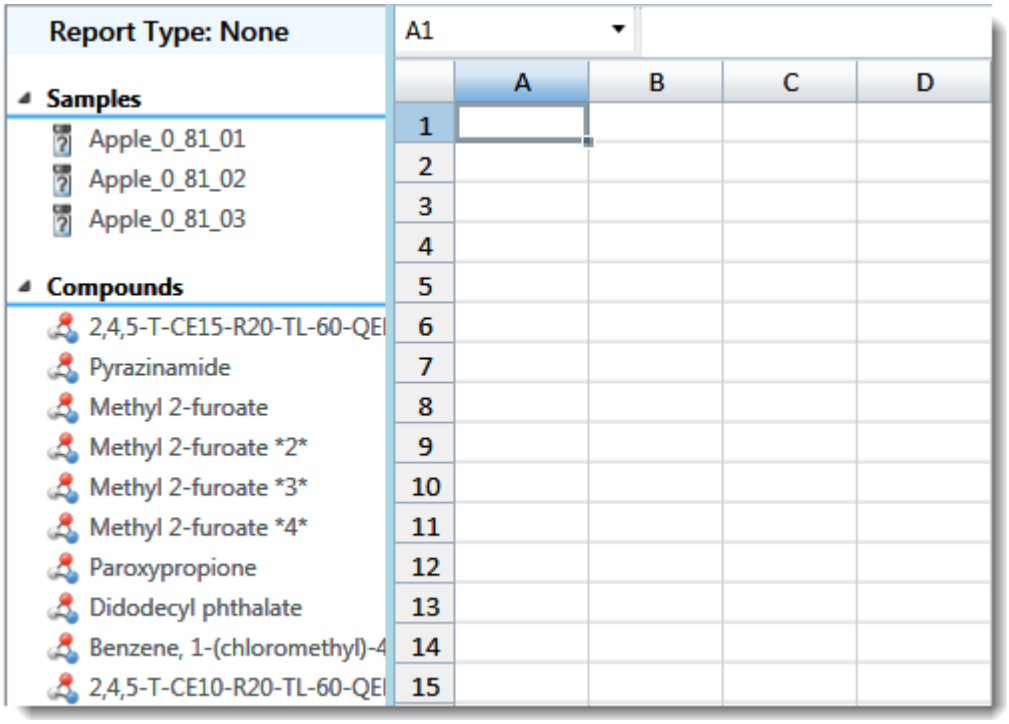
1. Click New.

   The application opens the Report Designer showing a new, 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 83. Report Designer showing a new, empty template

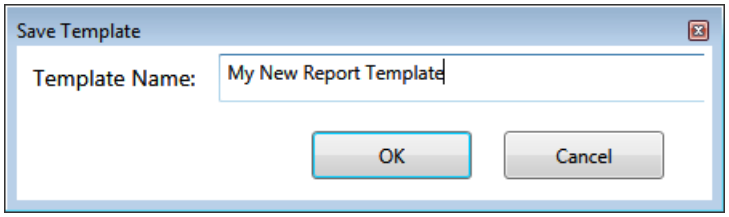


2. Use the features in the Report Designer to create the report template.

   See Chapter 7, "Using the Report Designer."

3. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

   The Save Template dialog box opens.



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 84. Report View

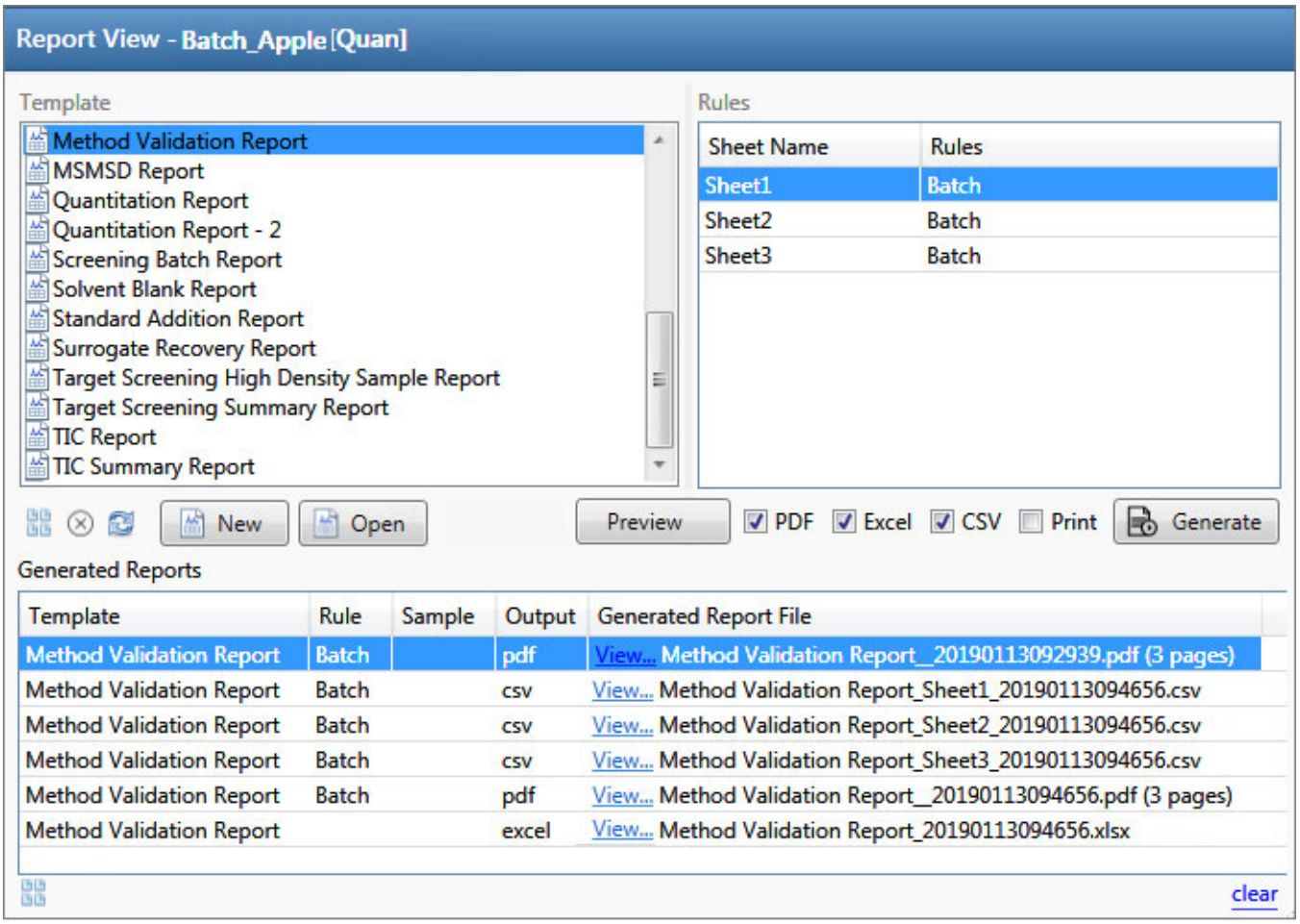


Table 40. Report View parameters (Sheet 1 of 3)

Parameter	Description
Template	
Report list	Displays all report templates.
Rules	
Sheet Name	Specifies each sheet in the report.

Table 40. Report View parameters (Sheet 2 of 3)

Parameter	Description
Rules	Specifies the type of data used in each sheet in the selected report. • Batch • Batch (Calibration Group) • EachSample • SampleType: *SampleType* • CompoundType: *CompoundType* • Compound (Calibration Group) • SampleCustomFormula:
Buttons	
View Report Templates	Displays the …\TraceFinderData\Templates\ReportTemplates folder that contains all report templates.
Open	Opens the selected report template in the Report Designer.
New	Opens a blank report template in the Report Designer.
Preview	Opens the Report Designer showing the report information for the current batch in the selected report template format.
PDF	Writes the generated report to a PDF file in the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.
Excel	Writes the generated report to an Excel file in the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.
CSV	Saves the generated report as a CSV file in the …\TraceFinderData\Projects\…*batch*\ReportOutput folder. When the report contains multiple sheets, the application writes each sheet as a separate CSV file.
Print	Prints the generated report to your default printer.
Generate	Generates the selected type of reports for the current batch using the selected report template.
Generated Reports	
Template	Report template used for the report. See Example of a report template list.
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\Projects\…*batch*\ReportOutput folder.
View	Displays the generated output file.

Table 40. Report View parameters (Sheet 3 of 3)

Parameter	Description
View Generated Reports	Displays the …\TraceFinderData\Projects\…*batch*\ReportOutput folder that contains all report outputs.
Clear	Removes all reports from the Generated Reports display. This does not delete the reports from the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

Working in the Local Method View for quantitation batches

In the Local Method view, you can edit the local method parameters. A local method is a copy of a master method associated with a batch.

You can edit only the local copy of the method, or you can edit the master method and overwrite the local copy with the edited master method. Local methods are named *Batch_MasterMethod*.

v **To open the Local Method View**

1. Click **Analysis** in the navigation pane.
2. Click **Local Method**.

The Local Method view for the currently selected batch opens. See Local Method view.

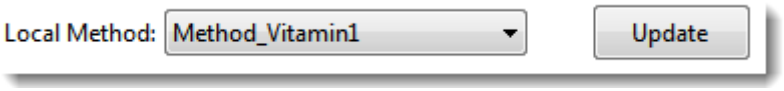
You can edit many of the method parameters in a local method. Editing the local method does not affect parameters in the master method.

For detailed descriptions of method parameters, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

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.

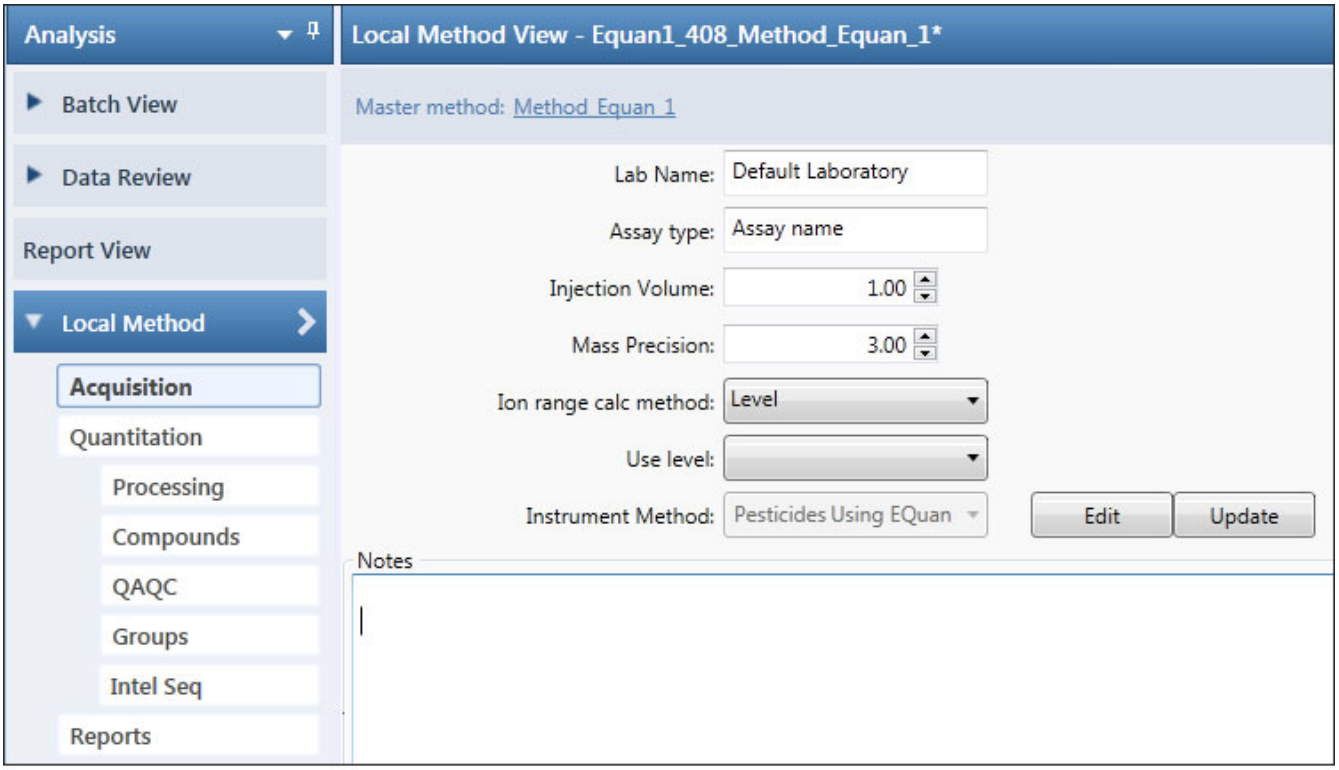
v **To overwrite the local method with the master method in the Batch View**

- In the Batch View, click **Update**.



The application overwrites the local method with the master method of the same name. You can use this feature to overwrite an edited local method with the original master method or to overwrite the local method with an updated master method.

Figure 85. Local Method view



5

Using the Analysis mode for target screening batches

Use the features of the Analysis mode to do the following:

- Create target screening batches.
- Submit target screening batches for acquisition, processing, or report generation.
- Review target screening batches, batch data, reports, and local methods.

Contents

- Working in the Batch View for target screening batches
- Working in Data Review for Target Screening Batches
- Working in the Report View for target screening batches
- Working in the Local Method view for target screening batches

Working in the Batch View for target screening batches

In the Batch View, you can manually create and edit a new target screening batch or open and edit a previously saved batch. When you submit a batch, you can acquire and process data and optionally create reports for the submitted samples.

The Analysis mode includes a toolbar:

Use the Toolbar or the equivalent commands in the Batch View shortcut menu to create the sample list and submit samples for acquisition.

See the following topics:

- Samples page features for target screening batches
- Creating a new target screening batch
- Editing a target screening batch
- Submitting a target screening batch
- Archiving and importing batches

Samples page features for target screening batches

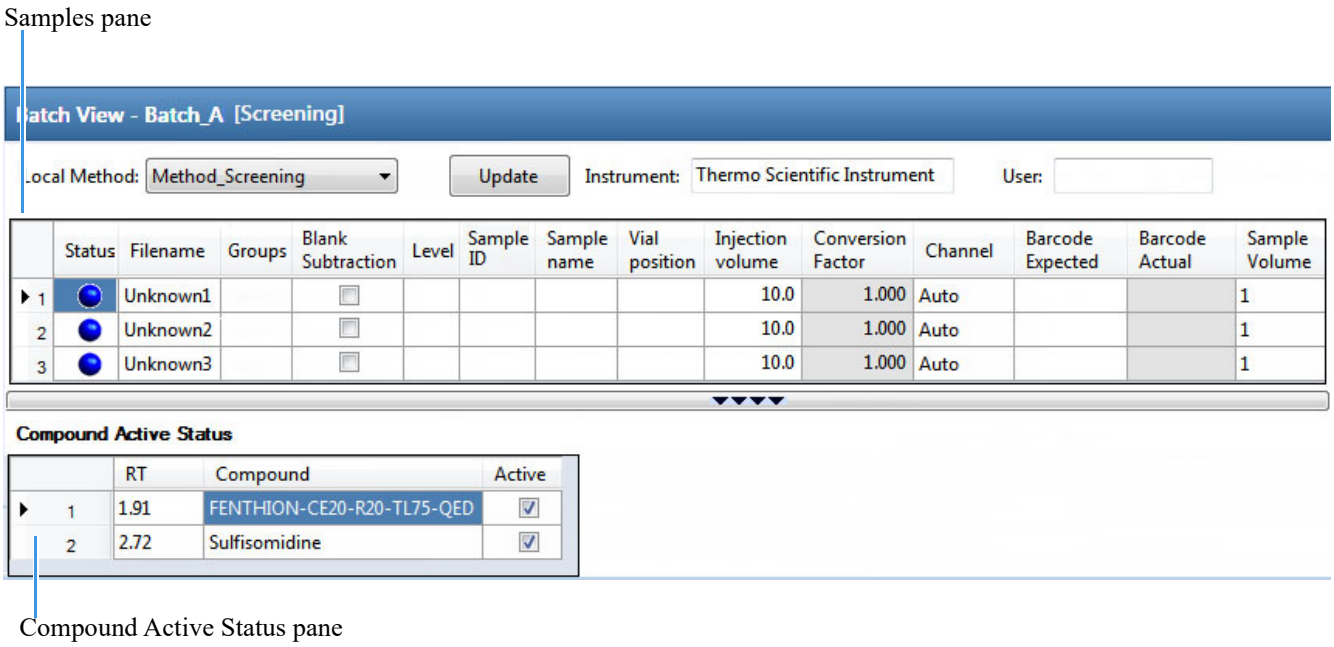
The Samples page is divided into two panes:

- Samples pane

  Use the Samples pane to create a batch.

- Compound Active Status pane

  Use the Compound Active Status pane to make specific compounds active or inactive.



Tip To resize the panes, drag the separators that divide the panes.

Samples pane

The samples pane includes the following features:

- Column display
- Status indicators
- Groups
- Blank Subtraction
- Sample weight calculation
- Instrument methods
- Toolbar
- Batch View sample list
- Batch View shortcut menu for target screening batches

Column display

The sample list contains many columns of information. You can scroll to see all the columns, and you can customize which ones to display and their display order.

v **To scroll the sample list**

Use the horizontal scroll bar at the bottom of the sample list to view all the information.

When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Groups, Blank Subtraction, Level, Sample ID, and Sample Name, while the other columns scroll right and left.

v **To customize the column display**

1. Right-click the sample list and choose **Modify Columns**.

   The Modify Columns dialog box opens. For button descriptions, see Table 41.

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, Groups, Blank Subtraction, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

   a. In the Displayed Columns pane, select a column name.

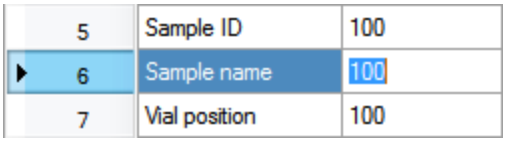
   b. Use **Up** or **Down** to move the selected column up or down in the list.

   The first column in the list represents the leftmost column in the Batch View sample list, and the last column in the list represents the rightmost column in the Batch View sample list.

   Note The following columns are fixed: Status, Filename, Groups, Blank Subtraction, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

   a. In the Displayed Columns pane, select the column width.

   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 86. Modify Columns dialog box

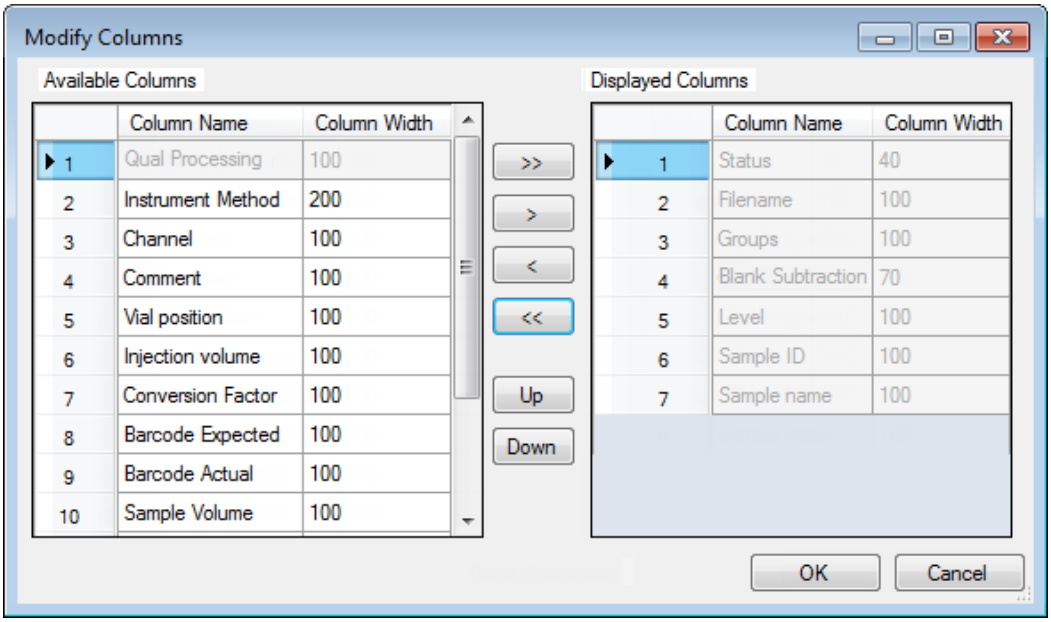


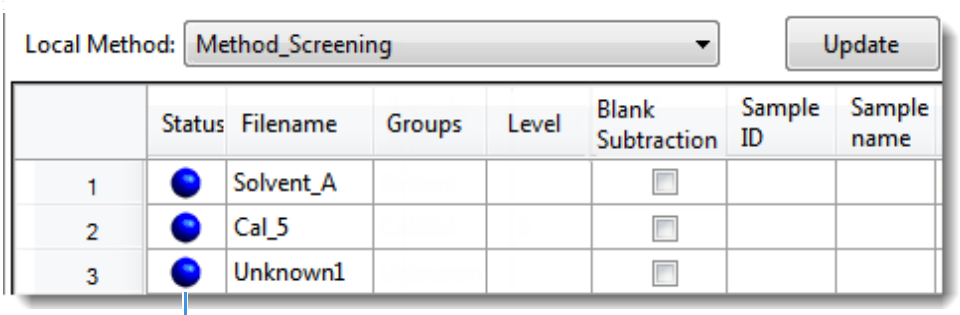
Table 41. Button descriptions for the Modify Columns dialog box

Button	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name.	
<	Moves the selected column to the Available Columns pane.
<<	Moves all columns except fixed columns.
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.

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.



Status indicators

Note When you include unknown screening features in the target screening method and you choose to process with only the target screening criteria, the Samples view shows the Status for the samples as acquired and processed ( ), and the Unknown Screening View shows the Status for the samples as acquired but not processed ( ).

Note When you include unknown screening features in the target screening method and you choose to process with only the unknown screening criteria, both the Samples view and the Unknown Screening View show the Status for the samples as acquired and processed ( ).

Groups

Use the Groups feature to assign samples to a group.

v **To create a group**

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

   Repeat this for each sample that you want to include in a group.

2. Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
	Benzo26473	groupB, groupA
	Benzo25557	groupB
	Benzo26154	groupB, groupA

Blank Subtraction

Use the Blank Subtraction feature to select which matrix blank samples you want to use for peak subtraction. The application subtracts the areas of the peaks in the selected matrix blank samples from the matching areas in the unknown samples.

Status	Filename	Groups	Level	Sample ID	Sample name	Blank Subtraction
	Apple_PosHCD_0_81_01			1		☑
	Apple_PosHCD_0_81_02			1		☐

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

To activate the Blank Subtraction feature, refer to "Editing the Processing page" in Chapter 5, "Using the Method Development Mode for Target Screening Methods," in the *TraceFinder Lab Director User Guide*.

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

v 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**.

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	

v 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.

v 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.

v 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.

v **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**.

      The Modify Columns dialog box opens.

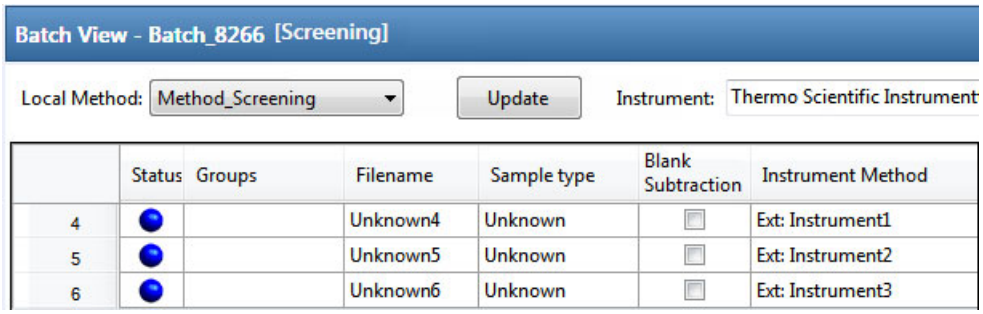
   b. In the Available Columns pane, select **Instrument Method**.
   c. Click > to move the Instrument Method column to the Displayed Columns pane.
   d. Click **OK**.

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

   Local instrument methods:

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

Toolbar

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

Table 42. 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.
	Inserts a new, empty sample or samples above the selected sample. See the instructions To insert samples into the list.
	Removes the selected samples from the sample list. See the instructions To remove samples from the list.
	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.
	Submits only the selected samples for acquisition, processing, or report generation. See the instructions To submit samples in the batch.
	Submits the batch for acquisition, processing, or report generation. See the instructions To submit samples in the batch.
	Submits only the selected samples for processing. See the instructions To submit selected peaks for processing.
	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 Target Screening Batches.
	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.
	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 8, "Confirming audited changes and using the Audit Viewer." Available only when you enable Auditing in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

Batch View sample list

The sample list, a multi-column table, displays all the quantitative data for the samples of a batch.

Status indicators in the Status column indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The sample list includes the following columns of information:

Figure 87. Batch View sample list

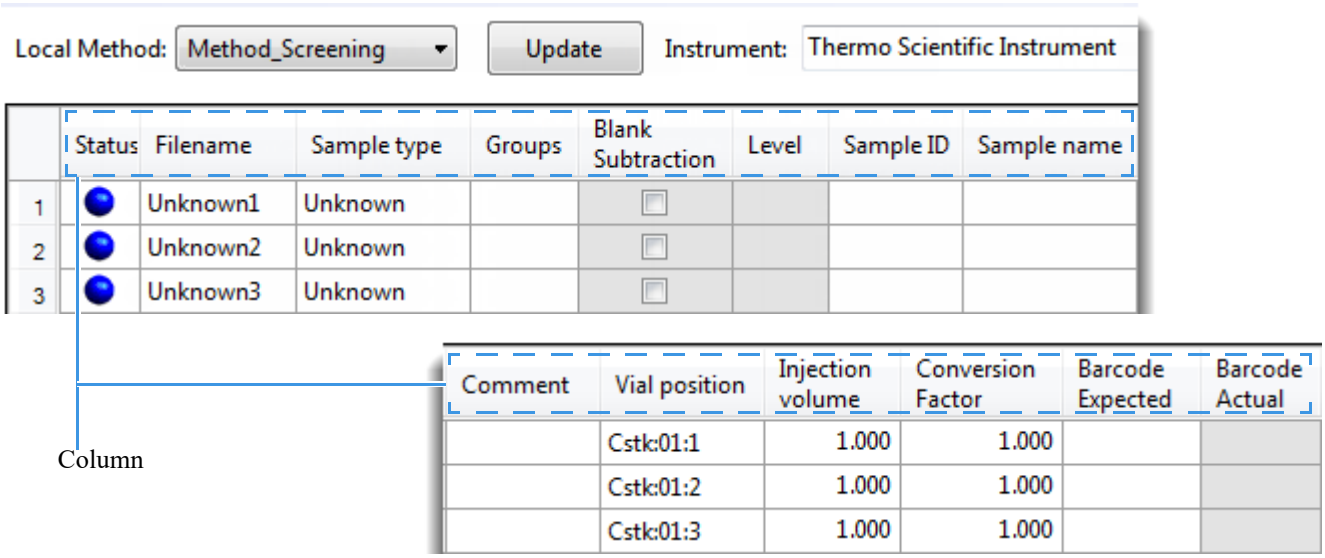


Table 43. Batch View sample list columns (Sheet 1 of 3)

Column	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 Type	Defines how the application processes the sample data. Each sample is classified as either Matrix Blank or Unknown. Default: Unknown
Groups	Threshold group to which a sample belongs.
Blank Subtraction	Enables the Blank Subtraction feature as defined in the method.
Level	Not used in Target Screening processing.

Table 43. Batch View sample list columns (Sheet 2 of 3)

Column	Description
Sample ID	A user-defined, alphanumeric string that identifies a sample.
Sample Name	A user-defined name that identifies a sample.
Comment	A user-defined comment for the sample.
Vial Position	The tray vial number used for an autosampler acquisition.
Injection Volume	The injection volume (in microliters) of the injected sample. When you are using an autosampler, you can set the default injection volume in the Autosampler dialog box in the Instrument View. The minimum and maximum injection volumes that you can use depend on the Autosampler you configure. The usable range depends on the injection mode and might be smaller than the displayed range. The Injection Volume value set in the master method overwrites the value in the instrument method. Valid range: 0.1 through 5000 µL
Calculation Type	Liquid: The application calculates the Conversion Factor as $SampleVolume \div DilutionFactor$ Solid: The application calculates the Conversion Factor as $(SampleVolume \times DilutionFactor) \div SampleWeight$ 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 Instrument methods.

Table 43. Batch View sample list columns (Sheet 3 of 3)

Column	Description
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. The Channel column is available only when you have activated the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.
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.

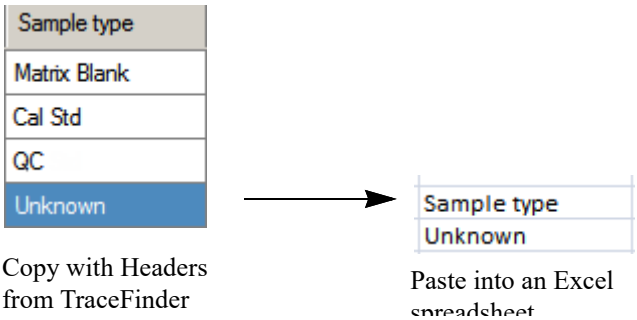
Batch View shortcut menu for target screening batches

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

Table 44. 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.
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.
Hide Sample Weight Calculation	Displays or hides the Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns.

Table 44. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information into a text editor or spreadsheet application. You cannot paste this data back into the Batch View sample list.
Copy with Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information into another text editor or spreadsheet application, for example,  Copy with Headers from TraceFinder Paste into an Excel spreadsheet You cannot paste this data back into the sample list.
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. For detailed information about editing instrument methods, refer to Chapter 3, "Using Instrument Methods in the Method Development Mode," in the *TraceFinder Lab Director User Guide*.
View Sample in Qual Explorer	Displays the selected sample in the qualitative explorer application that you configured as your default in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

Compound Active Status pane

In the Compound Active Status pane, you can choose specific compounds to be active or inactive.

v **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, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

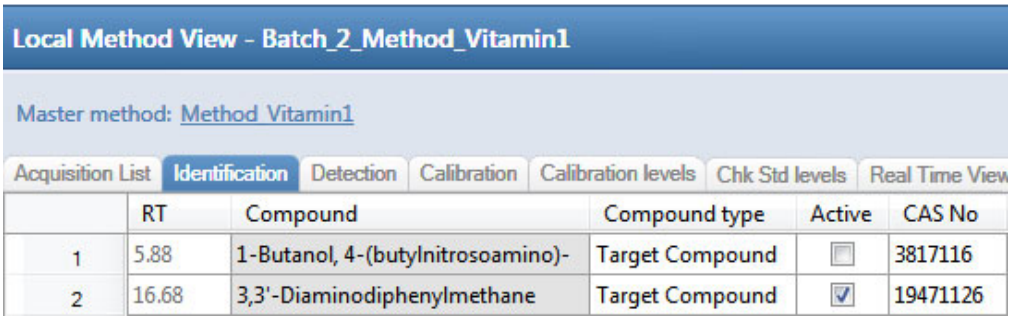
   - To display compounds alphabetically, right-click and choose **Sort by Compound Name**.
   - To display compounds from shorter to longer retention times, right-click and choose **Sort by Retention Time.**

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

Compound active/inactive status

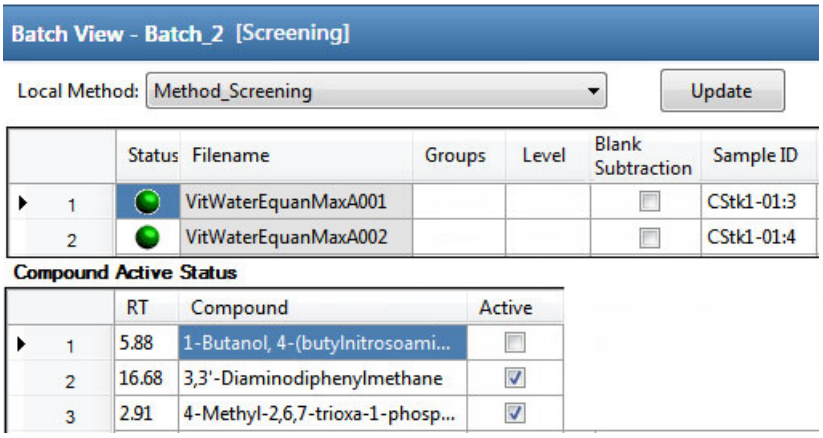
You can specify which compounds are active or inactive in the Local Method View or the Batch View.

Figure 88. Active and inactive compounds in the Local Method View



For details about setting the status on the Identification page, refer to Chapter 4, "Using the Method Development Mode for Quantitation Methods," in the *TraceFinder Lab Director User Guide*.

Figure 89. Active and inactive compounds in the Batch View



For details about setting the status in the Batch View, see Compound Active Status pane.

Creating a new target screening 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

v To create a new batch

1. Choose **File > New > Batch** from the main menu.

   The Create New Batch dialog box opens. See Create New Batch dialog box for target screening batches.

2. Select a repository from the list.

   Tip The application displays all configured and enabled repositories.

   The project list displays all projects, subprojects, and batches in the selected repository.

3. Select the folder where you want to store your batch.

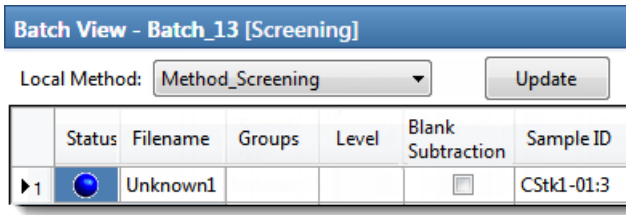
   To create a new folder for the storage location, see Editing folders for batches.

4. Type a batch name in the New Batch box.
5. To select a master method, do the following:
   a. Select **Screening** from the Type list.
   b. Select a repository from the Repository list.
   c. Select a master method from the Name list.

      The Name list displays all methods for the target screening type.
6. Click **Create**.

Tip To activate the Create button, you must enter a unique batch name and select a master method. If the Create button is not activated, you have either entered a batch name that is already used or you have not selected a master method.

A new batch opens with one Unknown sample.



The batch name in the title bar indicates that you are creating a target screening batch.

v To add samples to the list

1. To add a single sample row, right-click the sample list and choose **Add Sample**.
2. To add multiple sample rows, select the number of rows and then click the **Add Sample** icon, .

   The application adds the specified number of new, empty samples to the end of the sample list.

v To insert samples into the list

Select the sample above which you will insert new, Unknown samples, and then do one of the following:

- To insert a single sample row, right-click and choose **Insert Sample**.
- To insert multiple sample rows, select the number of rows and then click the **Insert Sample** icon .

The application inserts the Unknown samples above the selected sample.

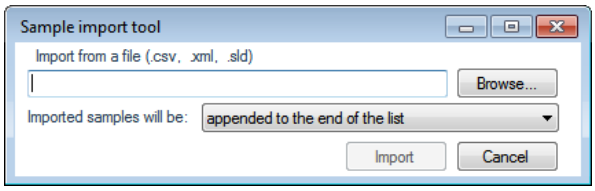
Inserted

	Status	Filename	Groups	Level	Blank Subtraction
1		cal_std_5			
2		Unknown2			
3		Unknown1			
4		cal_std_10			

v **To import samples into the list**

1. Choose **Batch > Import Samples** from the main menu, or click the **Import Samples** icon, .

   The Sample Import Tool dialog box opens.



   From this dialog box, you can import samples from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file that contains the samples to import.

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

4. Click **Import**.

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

   When you import samples from an Xcalibur sequence file (.sld), the application makes the following column name substitutions:

Xcalibur column	TraceFinder column
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conversion Factor

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

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank

5. (Optional) When using the Multi-Channel LC feature, select a channel for each imported sample.

   Imported samples default to Auto.

   Note The Channel column is available only when you have activated the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

v **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**.

v **To copy a sample**

1. Select the sample that you want to copy.
2. Right-click and choose **Insert Copy Sample**.

   The application inserts the copy above the selected sample.

v **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**.

   The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

v **To edit sample values**

1. For each sample, do one of the following:

   - Type a new file name over the current file name.
   - 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**, and then locate a raw data file to use for the sample.

   By default, the application sets the Sample Type to Unknown.

2. For each sample, click the Sample Type column and select a sample type from the list.

Available sample types	
Matrix Blank	Solvent

3. Type a vial position in the Vial Position column for each sample.
4. 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.
5. (Optional) Type or edit the values for the remaining columns.

   Note When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Blank Subtraction, Level, Sample ID, and Sample Name, while the other columns scroll right and left.

   To automatically copy or fill values in these columns, see Appendix B, "Using Copy Down and Fill Down."

v To browse in raw data files

1. Do one of the following:
   - Double-click the Filename column.
   - Right-click and choose **Browse in Raw File.**

   The What Raw File Would You Like to Use dialog box opens.
2. Select a raw data file to use for the sample or use the CTRL key to select multiple files, and then click **Open**.

   The application overwrites the selected, unacquired sample in the batch with the first "browsed in" file and adds any additional browsed in files below the selected sample.

   For all browsed-in raw data files, the application sets the Status to Acquired, , and sets the Sample Type to Unknown.

   Note You cannot overwrite an acquired sample. When you select a sample that is acquired, the application adds all browsed in files below the selected sample.

Create New Batch dialog box for target screening batches

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

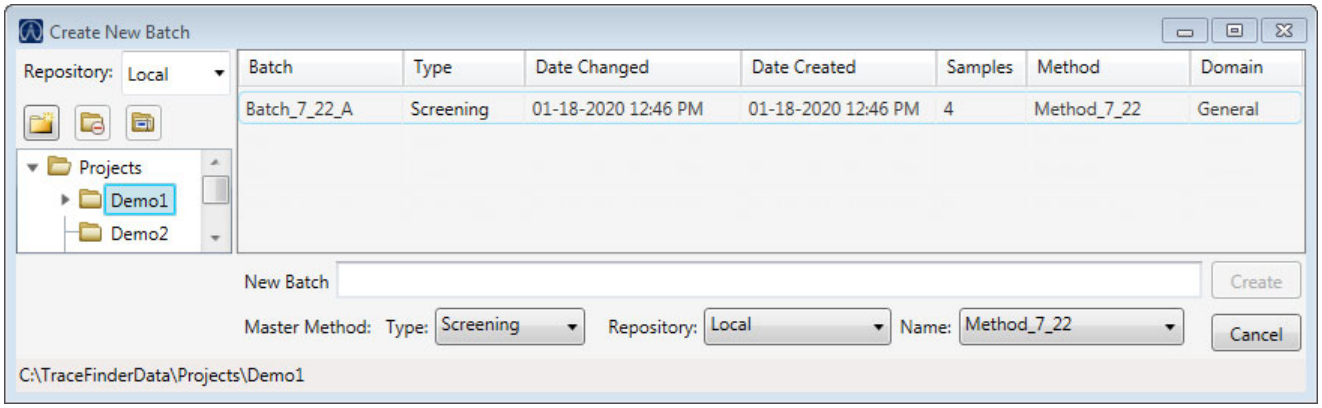


Table 45. Create New Batch dialog box parameters (Sheet 1 of 2)

Parameter	Description
Repository	The default data repository specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.
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, you can right-click and choose Create Folder.
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, you can right-click and choose Delete.
Rename Folder	Renames the selected folder. Or, you can right-click and choose Rename.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.

Table 45. Create New Batch dialog box parameters (Sheet 2 of 2)

Parameter	Description
Batch and Master Method parameters	
New Batch	Name of the new batch to create. **Note** If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Type	Type of batch to create: Quan, Screening, or Unknown Only.
Repository	The repository used to store the new batch.
Name	Method used to create the new batch.
Path	Path to the project in the TraceFinderData\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.

Follow these procedures:

- Create new project folders
- Delete new project folders
- Rename new project folders

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\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.

Delete new 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.

Rename new 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 target screening 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

v **To open a saved batch**

1. Choose **File > Open > Batch** from the main menu.

   The Open Batch dialog box opens.

2. Select a project and a subproject.
3. Select **Screening** or **Any** from the Type list.

   The batch list displays all batches created with Target Screening methods (or when you select Any, all methods of all types).

4. Select a batch from the list.

5. Click **Open**.

   The selected batch opens in the Batch View.

Figure 90. Open Batch dialog box

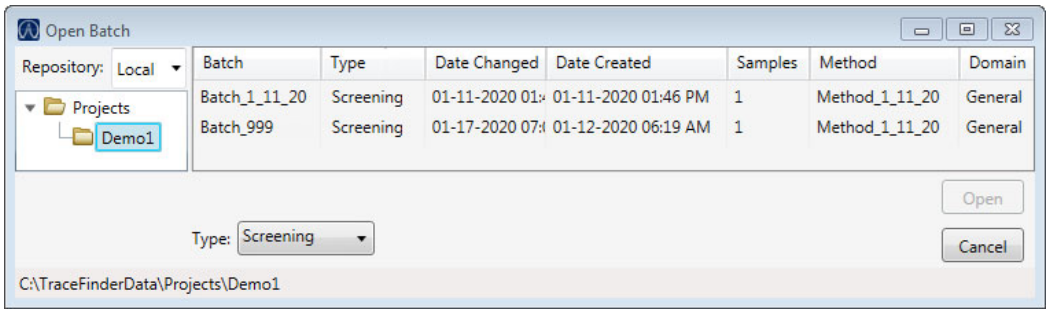
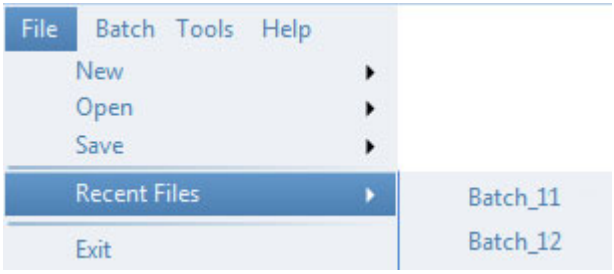


Table 46. Open Batch dialog box parameters

Parameter	Description
Repository	The default data repository specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
Path	Path to the project in the Projects folder where the batch is stored.
Buttons	
Type	Type of batch to display in the Batch list: Quan, Screening, Unknown Only, or Any.
Open	Opens the Batch View for the selected batch.
Cancel	Closes the Open Batch dialog box without opening a batch.

v **To open a recent batch**

- Choose **File > Recent Files >** ***batch*** from the main menu.



The selected batch opens in the Batch View.

v **To edit samples in a batch**

- Use the commands described in Working in the Batch View for target screening batches.

  You can add new samples, edit samples, or delete samples.

v **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**.

   The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

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

	cal_std_50_INJ001	Cal Std	10
	cal_std_50	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

   When you submit all samples in this batch, the application acquires all samples (including previously acquired samples).
3. To save this batch with the new samples for reinjection, choose **File > Save > Batch** from the main menu.

   The batch is saved as a prepared batch that is ready to submit. You can open this batch from the Reinject Samples page in the Acquisition mode and submit the batch. The application acquires only the samples that have not been previously acquired.

Submitting a target screening 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.

For a description of commands in the shortcut menu, see Batch View shortcut menu commands.

Follow these procedures:

- To submit selected peaks for processing
- To submit samples in the batch
- To view the output files

v To submit selected peaks for processing

1. In the Peak List, select the **Selected** check box for the peaks that you want to process.
2. Click the **Submit … for Processing** icon, .

   The application processes the selected peaks and updates the data in the Peak Identifications pane.

v 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.

   Note You can also submit only selected peaks for processing. See To submit selected peaks for processing.
2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.
   - When all submitted samples have been previously acquired, this option is (by default) not selected.
   - When one or more samples in the batch have not been acquired, this option is (by default) selected.

   Tip You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.
3. To process the submitted samples, select the **Process Data** check box.

   The application displays processing options for the Target Screening method.

If the method includes unknown screening features, the application also displays unknown screening options. For specifying processing data for batches that also use unknown screening features, see To submit samples in the batch in Chapter 6, "Using the Analysis mode for unknown screening batches."

4. Select the check box for the options that you want to use.

   Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

   Identify and Confirm: Performs both identification and confirmation.

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

6. (Optional with the Multi-Channel LC feature activated) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.

7. (Optional without the Multi-Channel LC feature activated) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   - **Next Available Batch** places the batch immediately after the currently acquiring batch.
   - **Next Available Sample** places the batch immediately after the currently acquiring sample.

   Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.
   a. Select the **Use** check box for the device that you want to use for this acquisition.
   b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

      This is usually the autosampler.

   c. Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

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

   d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.

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

The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Analysis mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT When your batch also uses unknown screening features, after the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages for the unknown screening features (refer to Chapter 5, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*) and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Figure 91. Submit Options dialog box

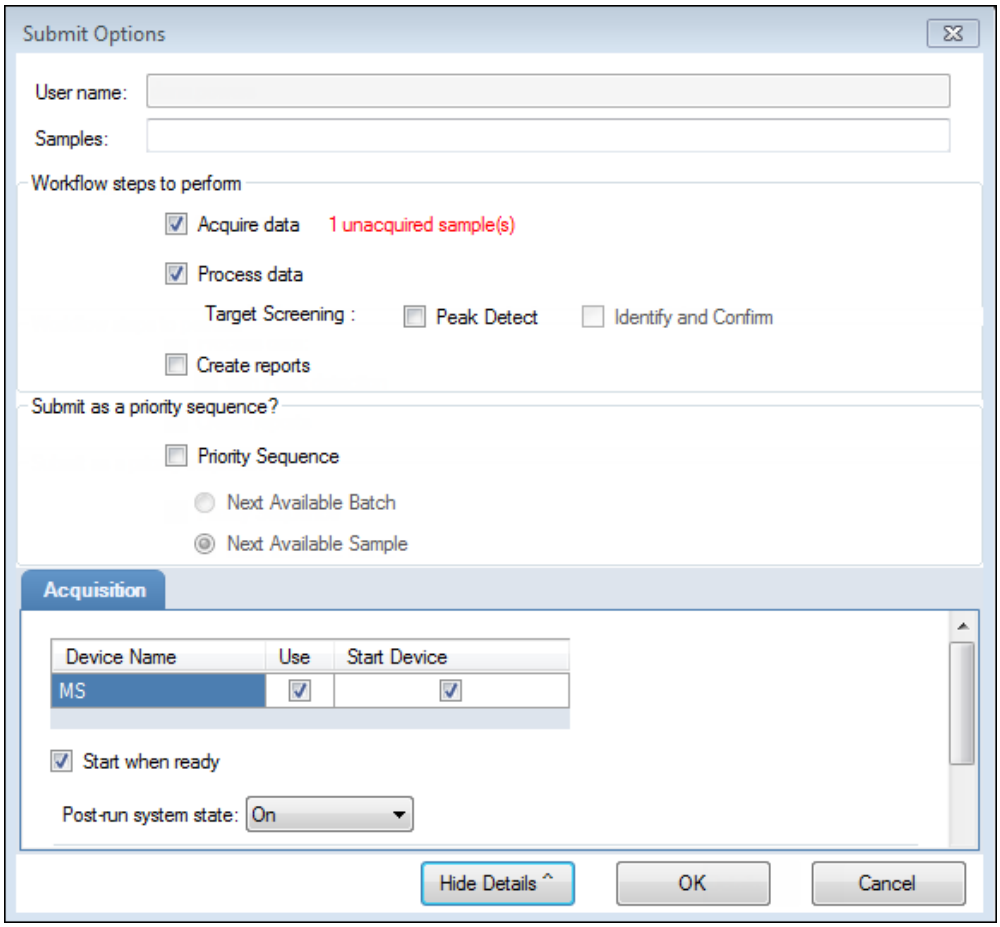


Table 47. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Workflow Steps to Perform	
Acquire Data	Submits the current batch to acquisition. • When all submitted samples have been previously acquired, this option is (by default) not selected. • When one or more samples in the batch have not been acquired, this option is (by default) selected.
Process Data	Processes the data for the current batch using any of the following options: Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples. Identify and Confirm: Performs both identification and confirmation. **Note** Target Screening methods can include unknown screening features. For specifying processing data for batches that also use unknown screening features, see To submit samples in the batch.
Create Reports	Creates reports for the current batch.
Submit as a Priority Sequence?	
Priority Sequence	With the Multi-Channel LC feature activated, places the batch immediately after the currently acquiring batch. Without the Multi-Channel LC feature 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.

Table 47. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
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 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.
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.

v **To view the output files**

- Locate the files to view from the following directories:

  The application writes saved batches to the project folder:

  …\TraceFinderData\Projects\…

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

  …\TraceFinderData\Projects\…*batch*\Data

  The application saves method information to the batch Methods folder:

  …\TraceFinderData\Projects\…*batch*\Methods

  The application writes the reports to the batch ReportOutput folder:

  …\TraceFinderData\Projects\…*batch*\ReportOutput

Saving a quantitation batch to a new location

You can move the current batch to a different project folder, or you can make a copy of the current batch and save the copy to a different project folder.

Follow these procedures:

- To save a batch to another project folder
- To move a batch to another folder
- To create a new project folder
- To delete project folders
- To rename project folders

v To save a batch to another project folder

1. Choose **File > Save > Save Batch As** from the Batch View main menu in the Analysis mode.

   The Save Batch As dialog box opens.

2. (Optional) Select a different repository.

   The default data repository is specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

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.

v To move a batch to another folder

1. Choose **File > Save > Move Batch** from the Batch View main menu in the Analysis mode.

   The Move Batch dialog box opens.

2. (Optional) Select a different repository.

   The default data repository is specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

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.

v **To create a new project folder**

1. In the Save Batch As dialog box, select the folder for which you will create a new lower-level folder.
   - You can select the main TraceFinderData\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.

v **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.

v **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 and Move Batch dialog box for target screening batches

Use the features in the Save Batch As dialog box to save a batch to a new name, or use the features in the Move Batch dialog box to move a batch to a different project folder. The features in the two dialog boxes are virtually identical.

Figure 92. Save Batch As dialog box

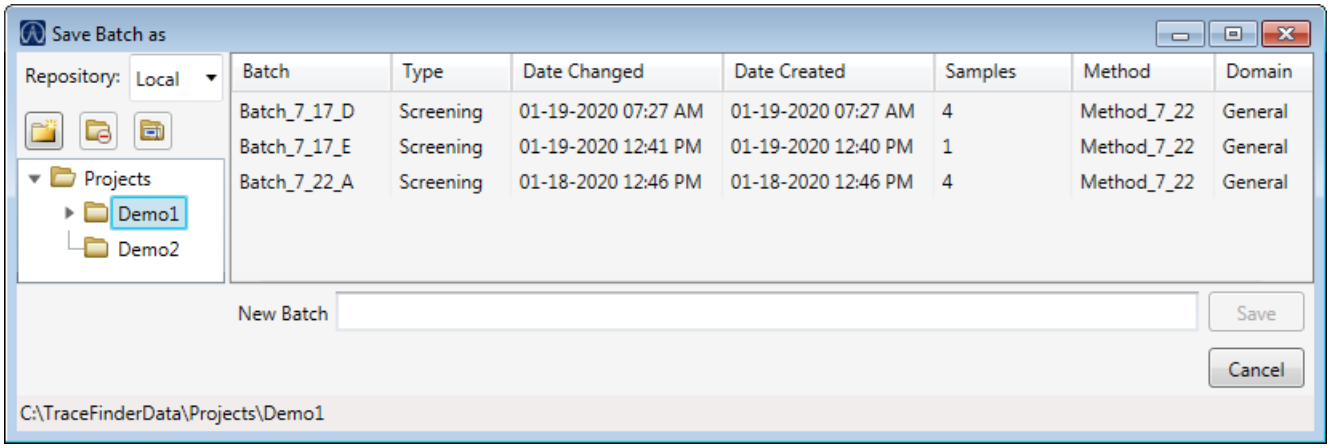


Figure 93. Move Batch dialog box

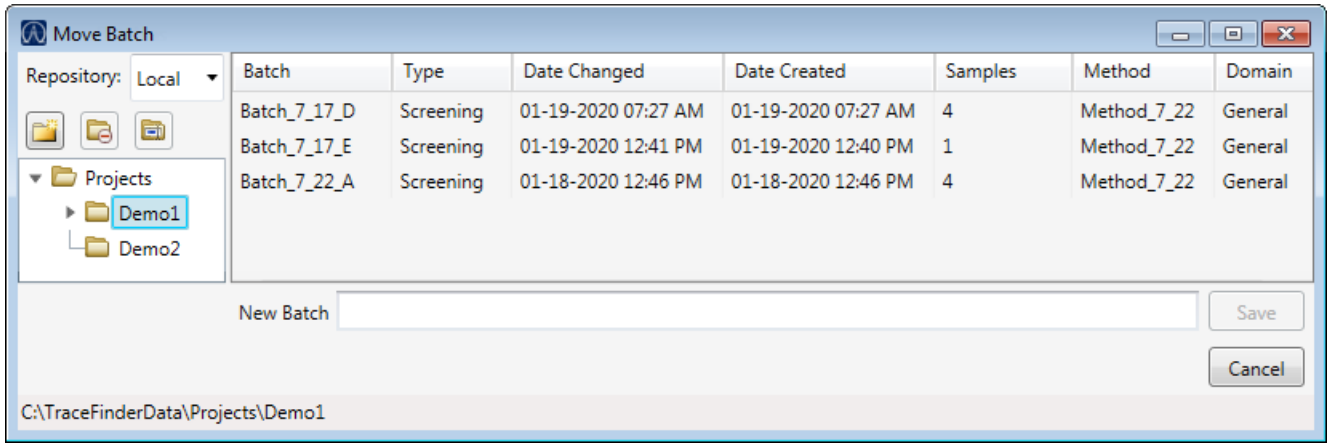


Table 48. Save Batch As dialog box and Move Batch dialog box parameters (Sheet 1 of 3)

Parameter	Description
Repository	The data repository where you want to store the batch.
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, you can right-click and choose Create Folder.

Table 48. Save Batch As dialog box and Move Batch dialog box parameters (Sheet 2 of 3)

Parameter	Description
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, you can right-click and choose Delete.
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, you can right-click and choose Rename.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
New batch parameters	
New Batch	Name of the new batch to create. **Note** If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Path	Path to the project in the TraceFinderData\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.

Table 48. Save Batch As dialog box and Move Batch dialog box parameters (Sheet 3 of 3)

Parameter	Description
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.

Archiving and importing batches

From any page in the Batch View, you can archive batches or import batches that have been archived.

v **To import a batch**

1. Choose **File > Import Batch** from the main menu.

   The Import Batch dialog box opens.

2. Select a project for the imported batch.
3. Click **Browse** and select a zipped batch file (.zBatch) that contains the batch to import.
4. Type a name for the new batch in the New Batch box.
5. Click **Import**.

   The application extracts the batch from the zipped file in the specified project folder and opens the batch in the Batch View.

v **To archive the current batch**

1. Choose **File > Archive Batch** from the main menu.

   Note You must have an open batch.

   The Browse for Folder dialog box opens.

2. Locate the folder where you want to store the archived batch, and click **OK**.

   The application zips the current batch and moves it to the specified archive folder.

   IMPORTANT The batch is no longer available from its original location. To access the batch, you must import it to your repository. See To import a batch.

   The zipped file includes the processed results, compound database, local method, results, raw data files, report templates, generated reports, and audit logs for the batch.

Working in Data Review for Target Screening Batches

The Data Review view displays the data generated by the master method. Use Data Review to verify the data for a compound before you generate reports.

Follow these procedures:

- To open the Data Review page
- To display or hide a pane
- To restore the default layout

v To open the Data Review page

1. Click **Analysis** in the navigation pane.

   The Analysis navigation pane opens.

2. Click **Data Review**.

Panes on the Data Review page show the following:

- A list of all samples in the current batch
- The compound results for all compounds in the method
- Chromatogram and spectrum plots for all compounds found in the currently selected sample

v To display or hide a pane

- From the View menu, choose to display—indicated with a check mark—or hide the following panes:

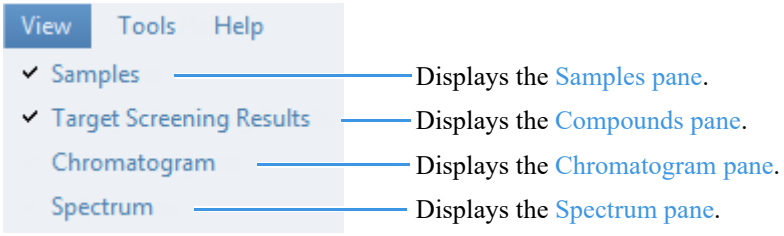
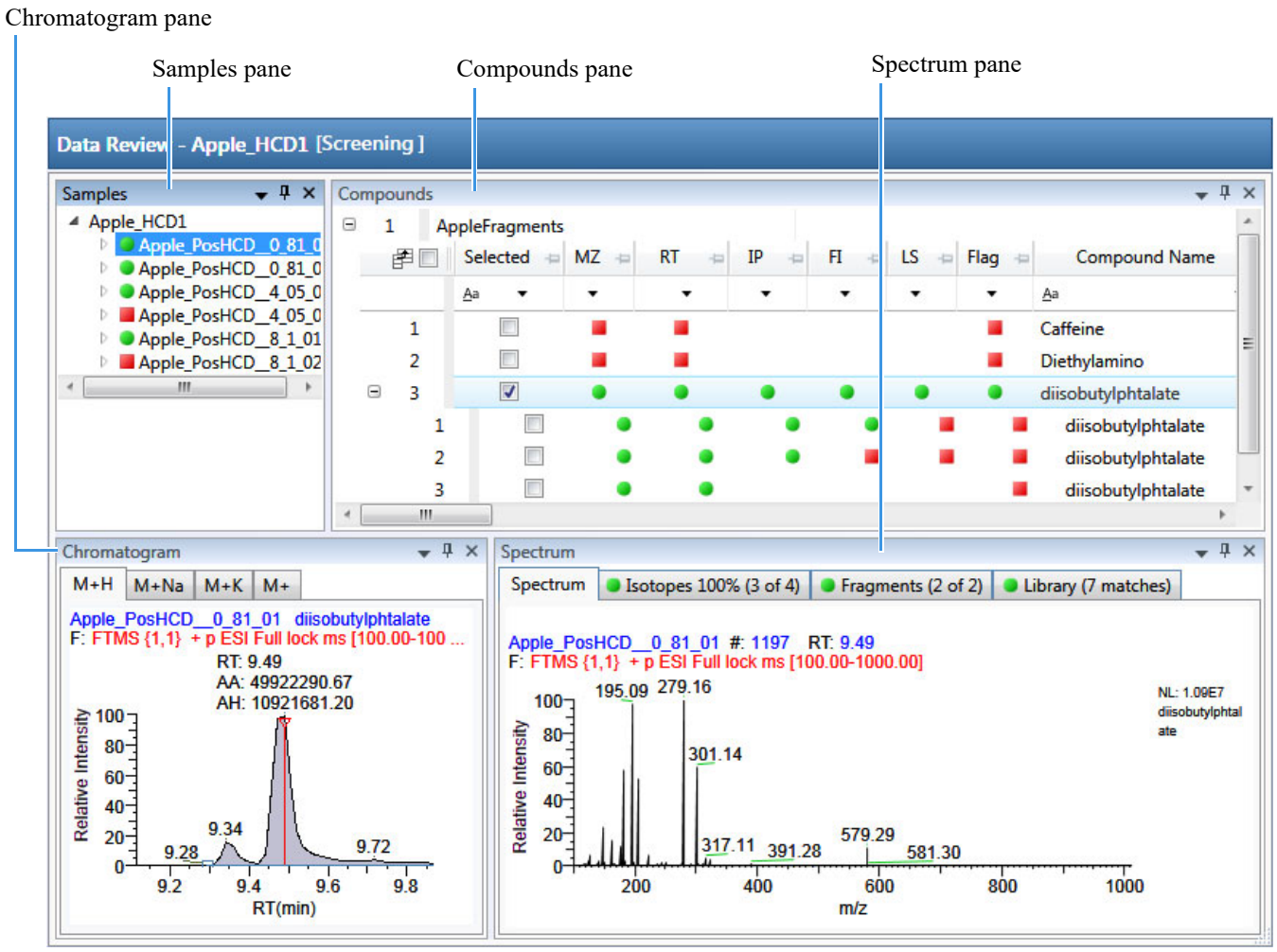


Figure 94. Data Review panes



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.

v **To restore the default layout**

- Choose **View > Restore Default Layout**.

  The Target Screening view displays the default panes in their default locations.

The Target Screening view 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 means that the sample/compound/peak combination is identified and fully confirmed.

A yellow triangle means that the sample/compound/peak combination is identified but not fully confirmed.

A red square means that the sample/compound/peak combination is not identified.

Figure 95. Samples pane

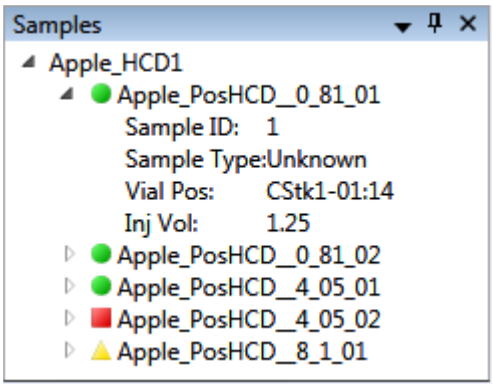


Table 49. Samples pane shortcut menu commands

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.

Use the following Compounds pane features:

- Color coding for measured or calculated values
- Displaying multiple adducts
- Exporting compounds
- Compounds pane columns

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 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 commands in the File menu to export data to an Excel spreadsheet, a CSV file, a compound database, or a new quantitation method.

Follow these procedures:

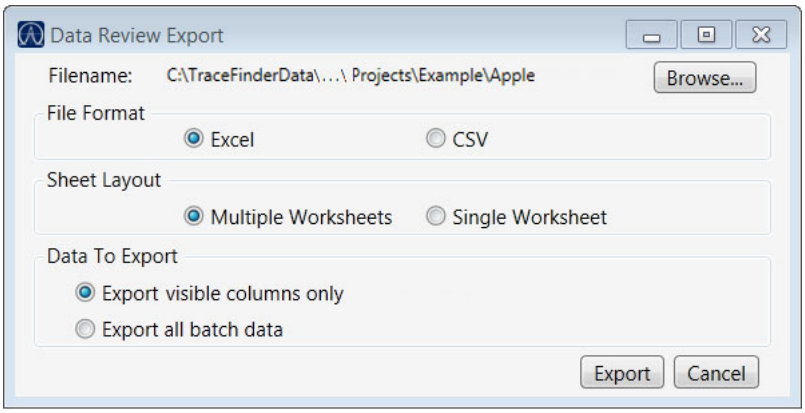
- To export compounds to an Excel spreadsheet
- To export compounds to a CSV file
- To export compounds to a compound database
- To export selected compounds to mass list
- To create a new quantitation method with the selected compounds
- To create a new quantitation method and update the compound database

v 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.



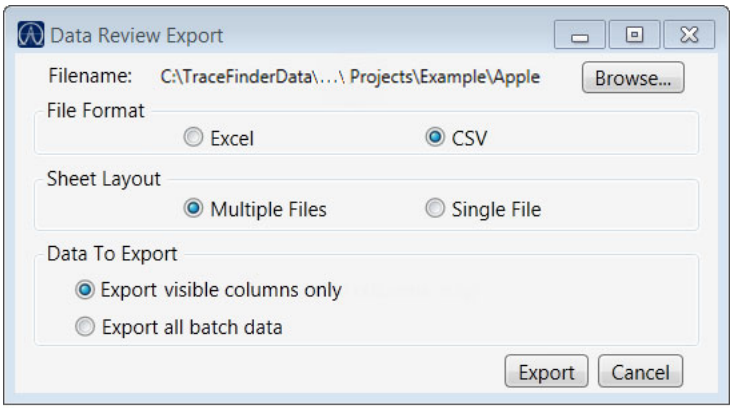
3. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.
4. Type a file name for the XLSX file and click **Save**.
5. In the File Format area, select the **Excel** option.
6. In the Sheet Layout area, select one of the following file formats for the spreadsheet.
   - **Multiple Worksheets**: Writes one sample to each Excel worksheet.
   - **Single Worksheet**: Writes all samples to a single Excel worksheet.
7. In the Data to Export area, select one of the following sets of data to export.
   - **Export 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.

v 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.



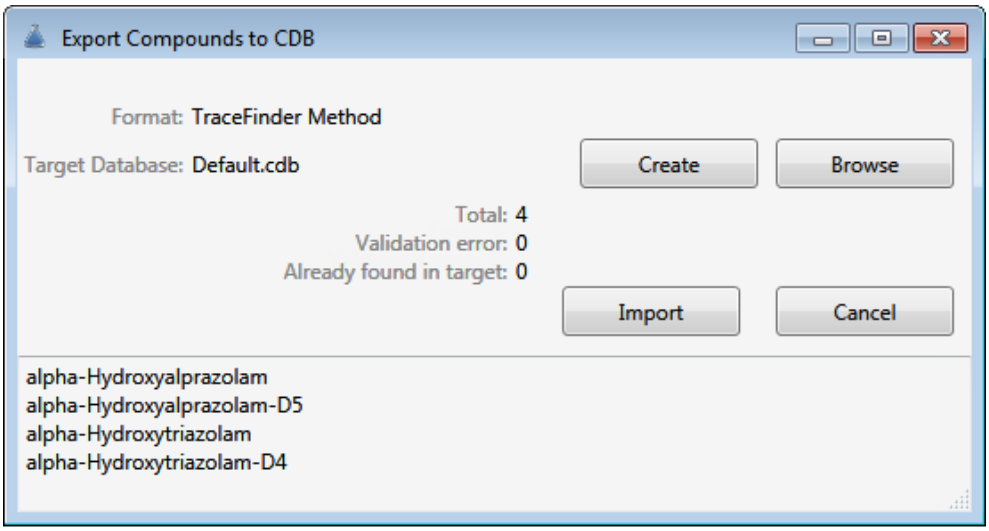
3. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.
4. Type a file name for the CSV file and click **Save**.
5. In the File Format area, select the **CSV** option.
6. In the Sheet Layout area, select one of the following file formats for 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 Visible Columns Only**: Writes data from the displayed columns of selected samples 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.

v 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 does the following:
   - Uses the measured retention time value for the compound in the updated or new compound database.
   - Uses the expected *m/z* value for the compound in the updated or new compound database.
   - Exports all found fragments to the updated or new compound database.

v **To export selected compounds to mass list**

The application writes the mass data to the specified .xml format file and you can use the data in the instrument method editors of the associated applications. The application exports only the following compound parameters to the XML file:

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

1. Choose **File > Open Compound Database** from the main menu.

   The Open compound database dialog box opens.

2. Select the Compound database and click Open.

   The compound database opens.

3. Select the compounds from the compound database.

4. Select **Compound Database > Export selected compounds to mass list** from the drop-down menu

   The mass list is selected for export.

5. Import the mass list to the Exploris method editor.

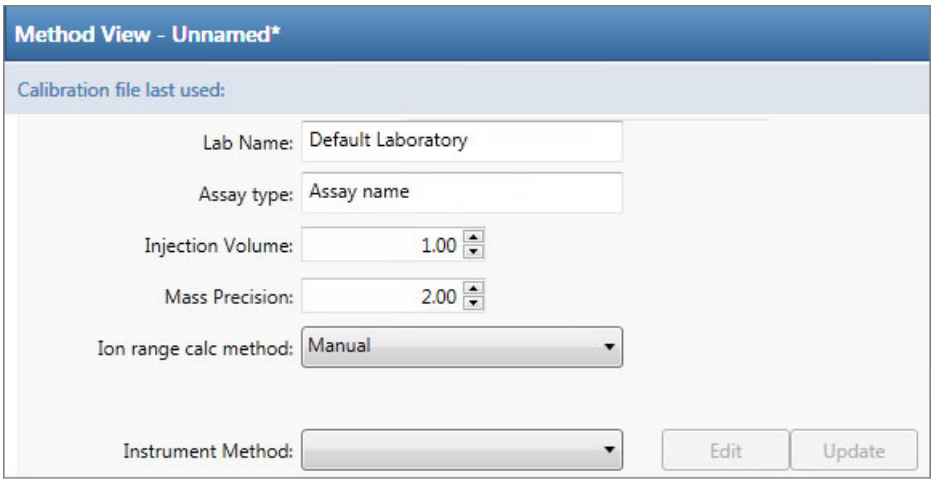
   Compare the imported information in the method editor to the exported csv file. The data should match.

v **To create a new quantitation method with the selected compounds**

1. For each compound that you want to export to a new quantitation method, select the check box in the Selected column including any adducts that you want to export.

2. Choose **File > Export Data To > New Quantitation Method** from the main menu.

   The Acquisition page of a new quantitation method opens.



3. From the Instrument Method list, select a method (.meth) file to use for acquiring the data.
4. Choose **File > Save** from the main menu.
5. In the Save Master Method dialog box, type a name for the method and click **OK**.
6. Click **Compounds** in the Method View navigation pane.

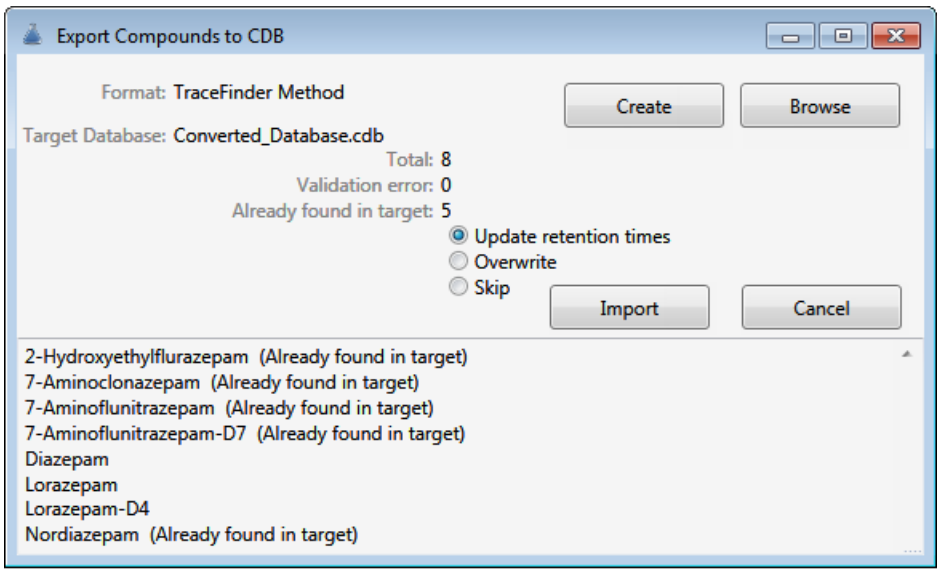
   The application exports the selected compounds from the target screening method to the new quantitation method and uses data from the selected compounds as follows:

   - Exports quantitation peaks in the order of intensity.
   - Exports measured retention time value for the compounds in the new method.
   - Exports expected *m/z* value for the compounds in the new method.
   - Exports all found fragments to the new method.
   - Adds a filter for both quantitative peaks and confirming ions.

v 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.

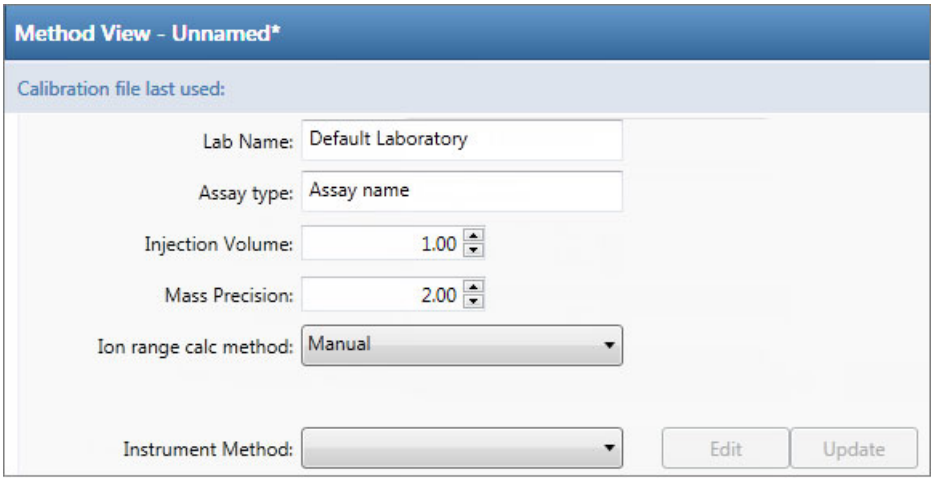
3. Do one of the following:
   - Accept the default target database.
   - Click **Create** and type the name for a new target database.
   - Click **Browse** and select from the list of compound databases.

   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.

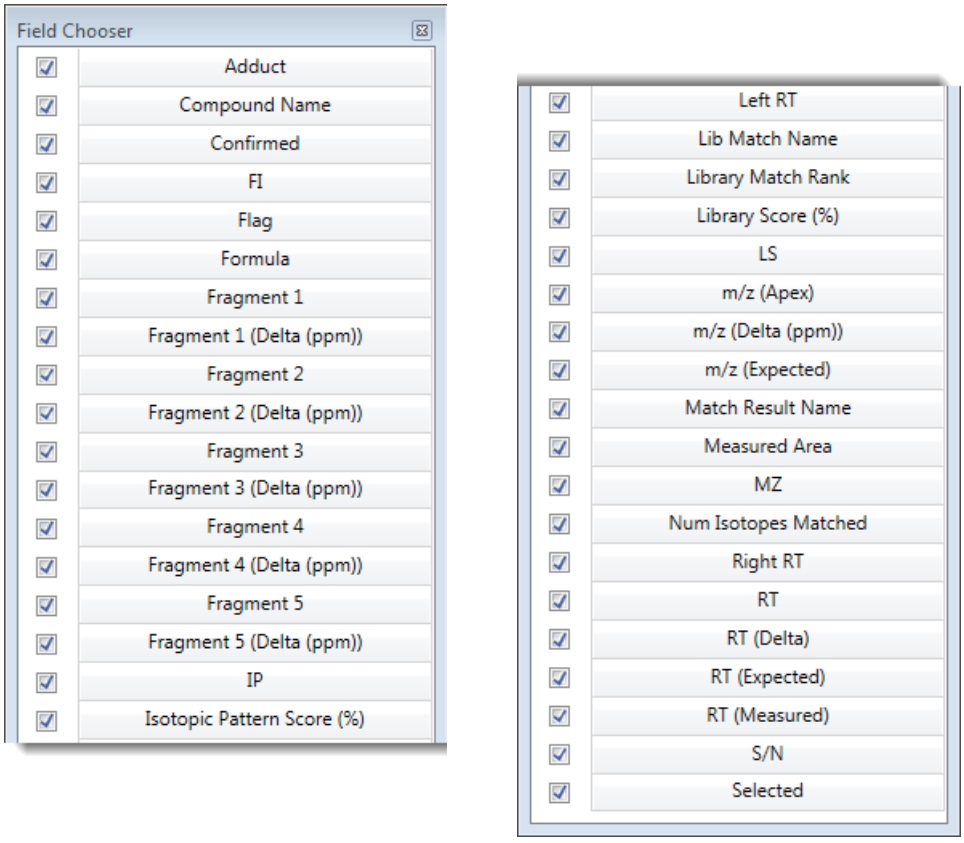
   The application exports the selected compounds (with the specified options) from the target screening method to the new quantitation method.

Compounds pane columns

The columns of data in the Compounds pane display all parameter values associated with each compound in the selected sample. See Compounds pane parameters for target screening batches.

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, close the Field Chooser.

Compounds pane parameters for target screening batches

The Compounds pane displays all parameter values associated with each compound in the selected sample.

Figure 96. Compounds pane

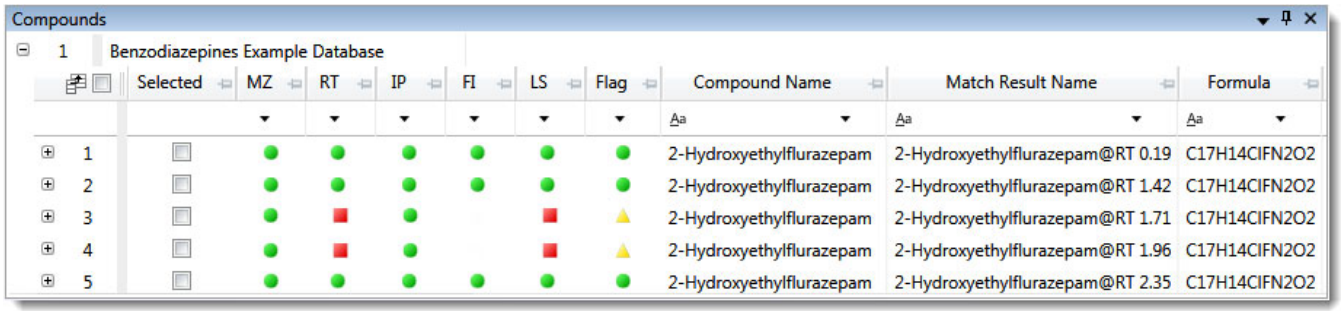


Table 50. Compounds pane parameters (Sheet 1 of 5)

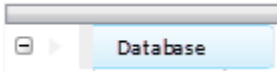
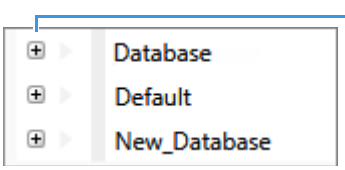
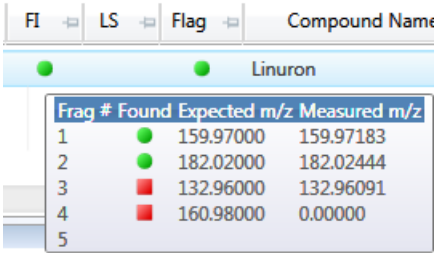
Column	Description
	Displays the current compound database. When you have multiple screening databases, the application lists the results for each database separately.  Expand the list of found compounds in the screening database.
Adduct	The most intense adduct for the retention time for a compound.
Compound Name	The compound name match in the compound database.
Confirmed	The number of criteria confirmed out of the total number specified in the method.
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. • A red square (fail) when the measured *m/z* value of none of the fragments is within the mass tolerance specified in the method. • A blank when there are no fragments detected. To display a list of fragments and their pass/fail status, point to the indicator. 

Table 50. Compounds pane parameters (Sheet 2 of 5)

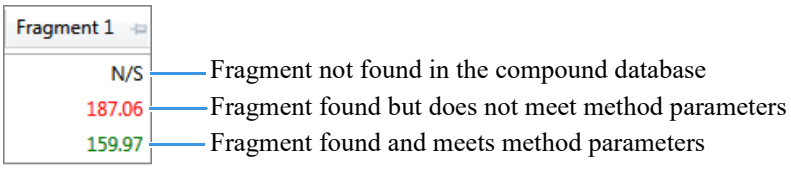
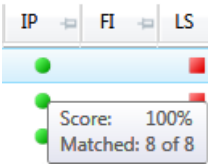
Column	Description
Flag	Indicates the status of the identification and confirmation criteria. • A green circle when the sample/compound/peak combination is identified and fully confirmed. • A yellow triangle when the sample/compound/peak combination is identified but not fully confirmed. • A red square when the sample/compound/peak combination is not identified.
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.
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, point to the indicator. 
Isotopic Pattern Score (%)	The percentage of the number of total isotopes to the number of matched isotopes.
Left RT	The time point of the left leading edge of the integrated peak.

Table 50. Compounds pane parameters (Sheet 3 of 5)

Column	Description
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 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: • A library score that is higher than or equal to the score threshold meets the criteria, and the values in this column appear in green. • A library score that is lower than the score threshold fails to meet the criteria, and the values in this column appear in red. 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: • A library score that is higher than or equal to the score threshold meets the criteria, and the values in this column appear in green. • A library score that is lower than the score threshold fails to meet the criteria, and the values in this column appear in red. 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. Valid range: 1 through 100%

Table 50. Compounds pane parameters (Sheet 4 of 5)

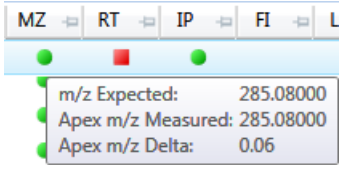
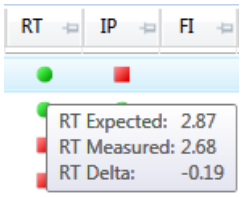
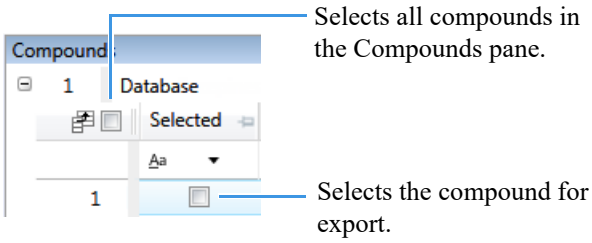
Column	Description
LS	Library Search flag. The application displays one of these flags: • A green circle when the library search passes. • A red square when the library search fails.
m/z (Apex)	Mass-to-charge ratio found in the spectra for the peak. Assumes the charge is 1. When the application successfully 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" (not found).
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)).
m/z (Expected)	Mass-to-charge ratio from the compound database. Assumes the charge is 1.
Match Result Name	The compound name match in the compound database and the retention time.
Measured Area	The AA value from the chromatogram pane.
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*, point to the indicator. 
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.
Right RT	The time point of the right trailing edge of the integrated peak.

Table 50. Compounds pane parameters (Sheet 5 of 5)

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 on the Processing page in the method. Refer to Chapter 5, "Using the Method Development Mode for Target Screening Methods," in the *TraceFinder Lab Director User Guide*. To display the expected, measured, and delta retention times, point to the indicator. 
RT (Delta)	Difference between the expected and measured retention time for the peak.
RT (Expected)	The retention time for the peak as specified in the compound database.
RT (Measured)	The found retention time for the peak apex.
S/N	The signal-to-noise ratio calculated for the found peak.
Selected	Identifies individual compounds for export. To select all compounds for export, select the check box in the first column. 

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.

Figure 97. Chromatogram pane

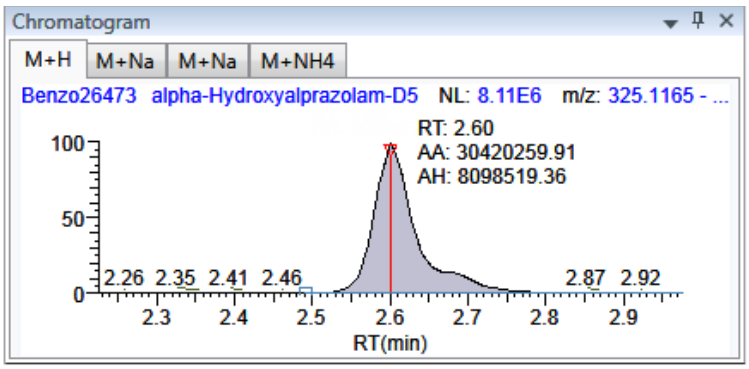


Table 51. Chromatogram pane shortcut menu commands

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. Refer to “Editing the Processing page” in Chapter 5, “Using the Method Development Mode for Target Screening Methods,” in the *TraceFinder Lab Director User Guide*.

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.

Follow these procedures:

- To zoom in on a peak
- To copy a plot to another format
- To customize the labels in a small molecule or peptide spectrum

v To zoom in on a peak

1. On the Spectrum page, 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 page and choose **Reset Scaling.**

v To copy a plot to another format

1. In the data spectrum or the reference spectrum, right-click and choose **Copy to Clipboard.**

   The application copies the specified plot graphic to the Clipboard.

   Note The application copies only the indicated data spectrum or the reference spectrum. It does not copy the entire Spectrum page.

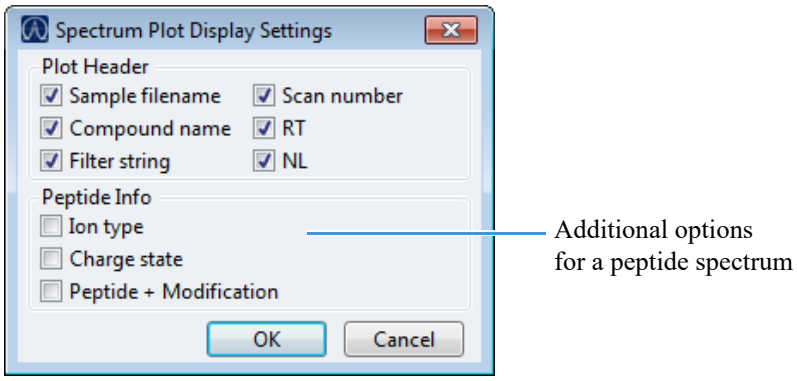
2. In the source format (for example, an Excel spreadsheet or email window), right-click and choose **Paste**.

   The application pastes the graphic into the new format.

v To customize the labels in a small molecule or peptide spectrum

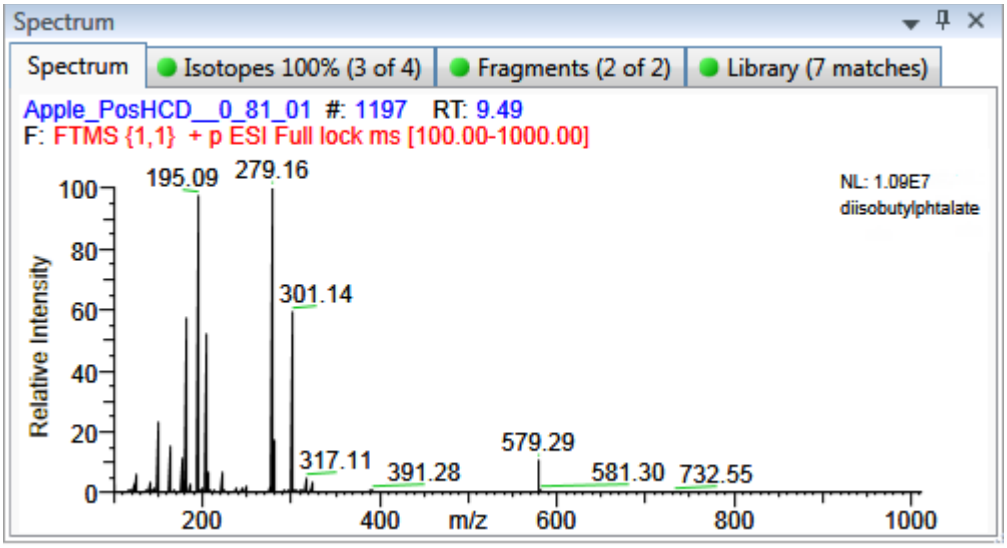
1. Right-click the Spectrum page and choose **Display Settings.**

   The Spectrum Plot Display Settings dialog box opens.



2. Select the check box for each label that you want to display and click **OK**.

Figure 98. Spectrum page



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, refer to "Editing the Processing page" in Chapter 5, "Using the Method Development Mode for Target Screening Methods," in the *TraceFinder Lab Director User Guide*.

The Isotopes page displays the isotopes in one of three ways:

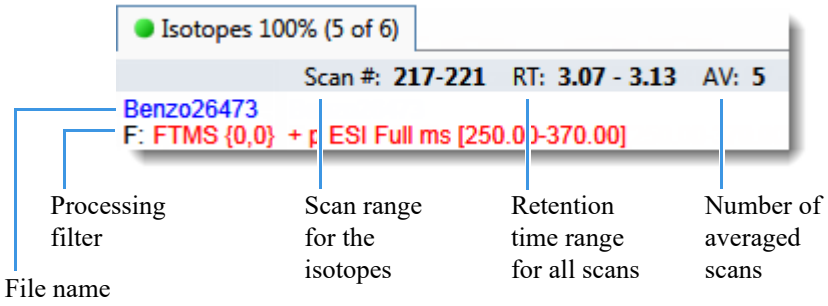
- All Isotopes
- Multi-Isotopes
- Individual isotopes

All isotopes pages use a shortcut menu so that you can specify how to display the data. See Isotopes page shortcut menu.

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:



You can display all isotopes as either stacked spectra or overlaid spectra.

Figure 99. Isotopes page with stacked spectra for all isotopes

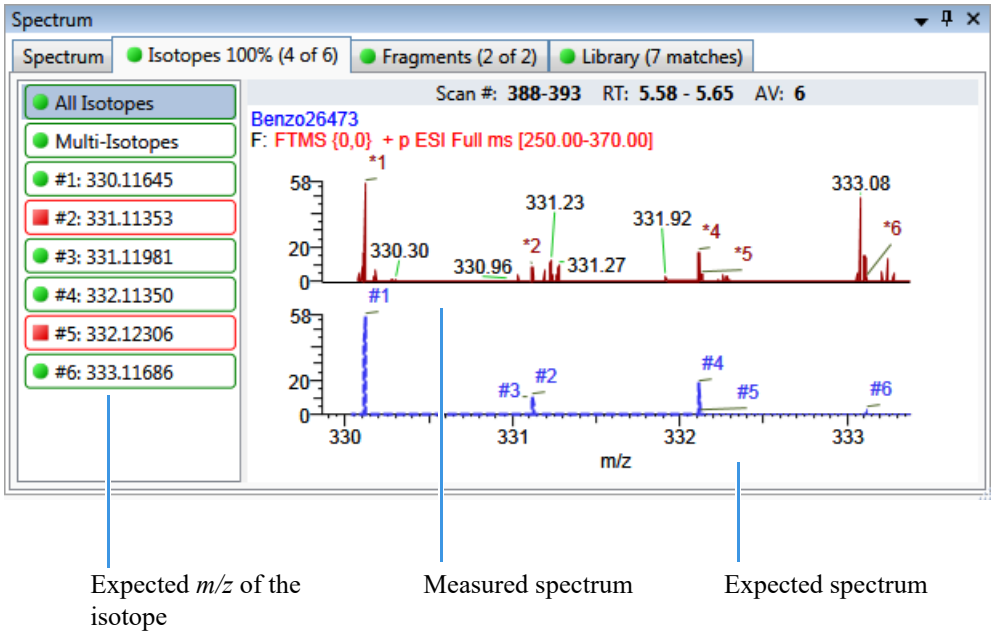
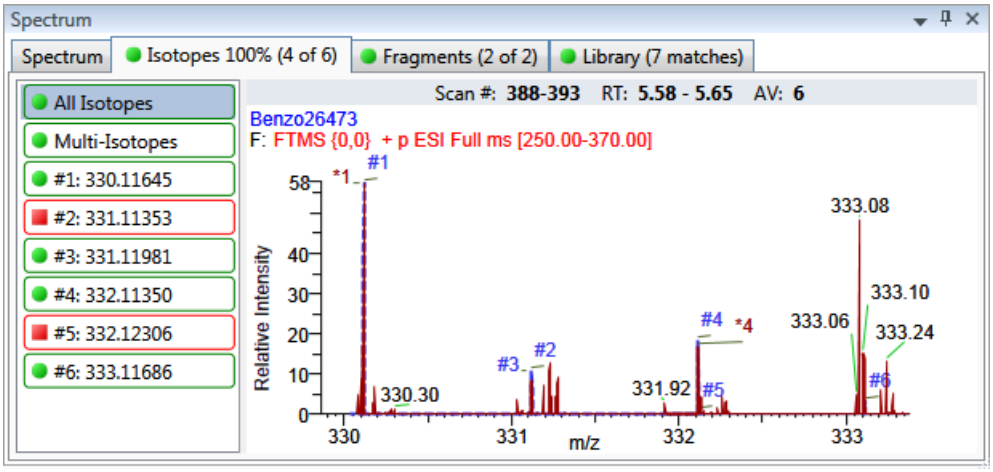


Figure 100. Isotopes page with overlaid spectra for all isotopes

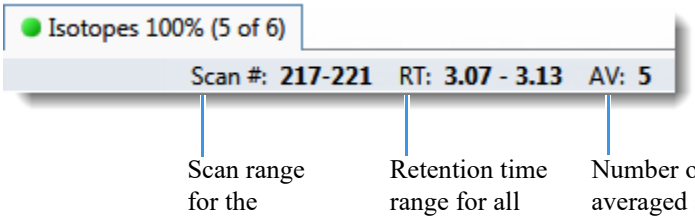


Expected spectrum in blue Measured spectrum in red

Multi-Isotopes

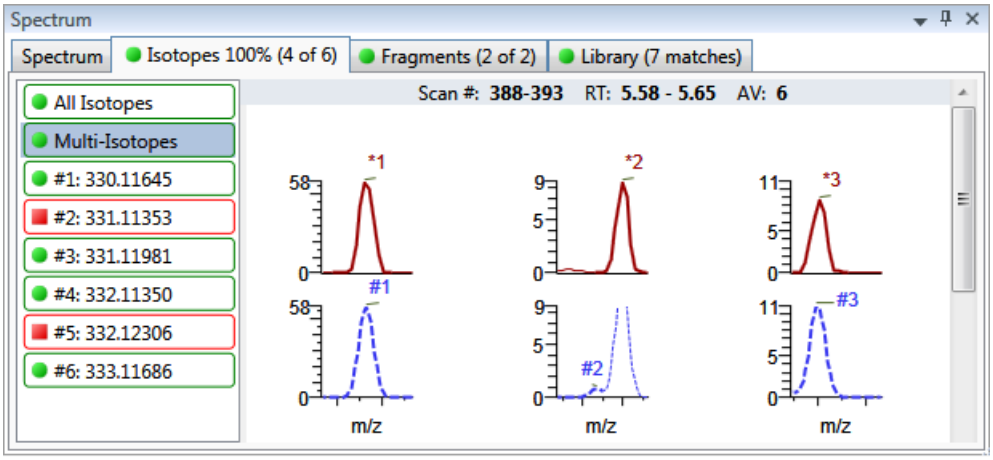
The Multi-Isotopes view displays individual plots for each isotope.

The application displays these headers for the Multi-Isotopes view:



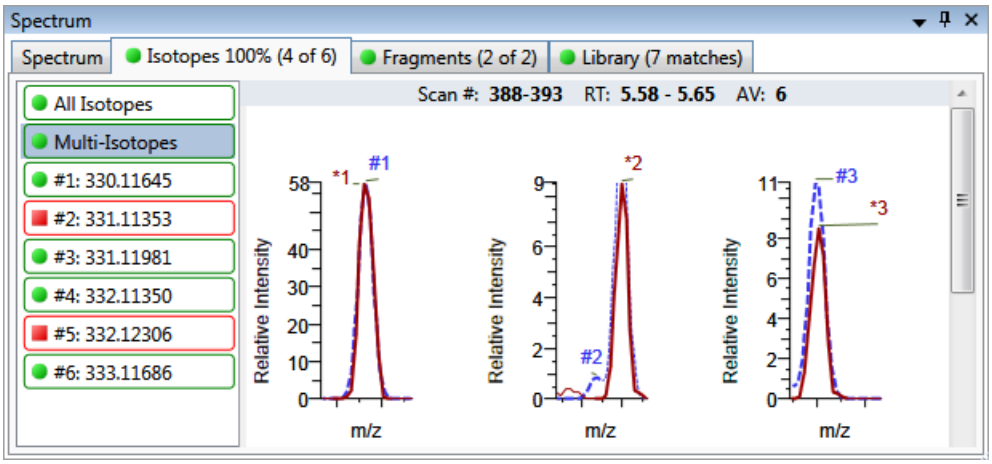
You can display the isotopes as stacked spectra, overlaid spectra, or both stacked and overlaid spectra.

Figure 101. Isotopes page with stacked spectra for multi-isotopes



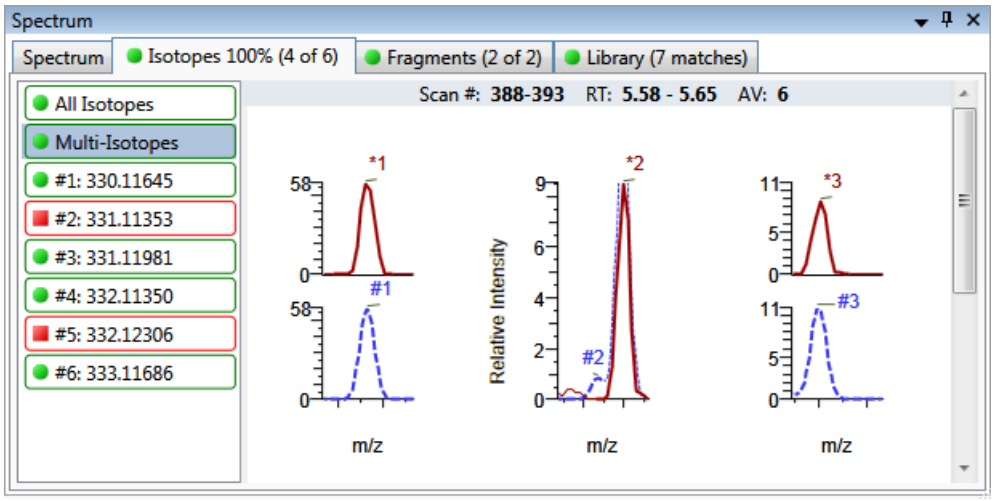
Expected spectrum in blue Measured spectrum in red

Figure 102. Isotopes page with overlaid spectra for multi-isotopes



Expected spectrum in blue Measured spectrum in red

Figure 103. Isotopes page with stacked and overlaid spectra for multi-isotopes

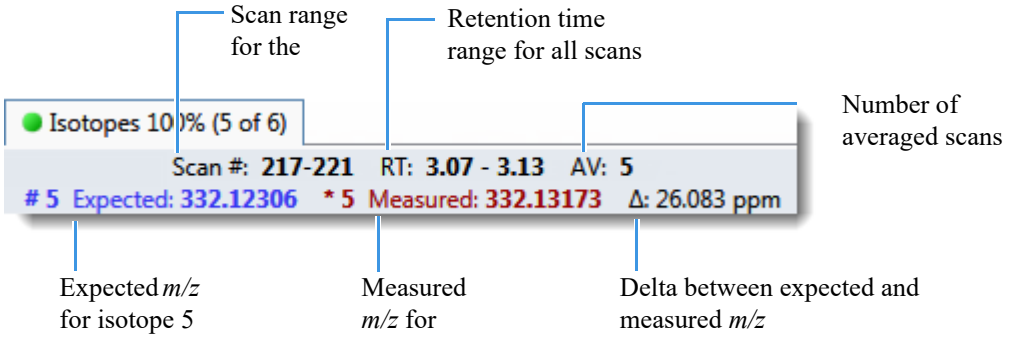


Expected spectrum in blue Measured spectrum in red

Individual isotopes

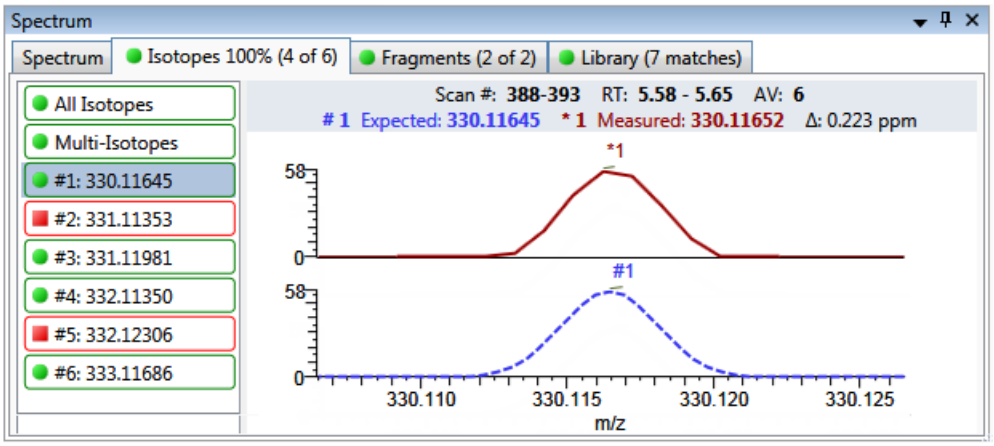
The individual isotopes view displays the expected and measured peaks for a single isotope.

The application displays these headers for the individual isotopes view:



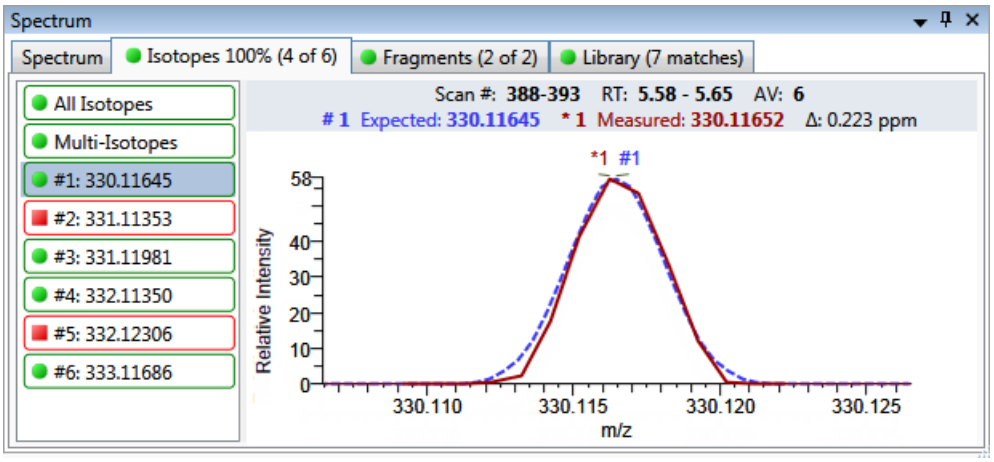
You can display the isotope as either stacked spectra or overlaid spectra.

Figure 104. Isotopes page with stacked spectra for a single isotope



Expected spectrum in blue Measured spectrum in red

Figure 105. Isotopes page with overlaid spectra for a single isotope



Expected spectrum in blue Measured spectrum in red

Isotopes page shortcut menu

Use the commands in the shortcut menu to specify how you want the data displayed.

Table 52. 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 peak apex spectrum over the simulated 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. Refer to "Editing the Processing page" in Chapter 5, "Using the Method Development Mode for Target Screening Methods," in the *TraceFinder Lab Director User Guide*.

If there are no fragments defined in the screening library for the compound, you can add fragments to the screening library. Refer to the instructions "To add a fragment to a target peak" in Chapter 2, "Using Compound Databases in the Method Development Mode," in the *TraceFinder Lab Director User Guide*.

The Fragments page displays the fragments in one of two ways:

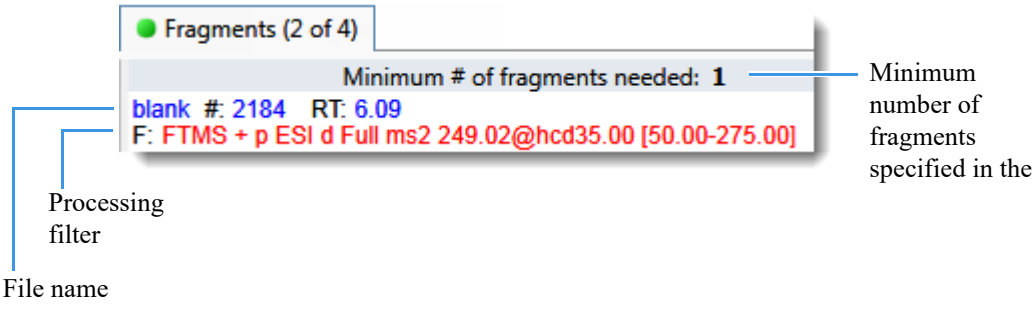
- All Fragments
- Individual fragments

All fragments pages use a shortcut menu so that you can specify how to display the data. See Fragments page shortcut menu.

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:



You can display the fragments as either stacked spectra or overlaid spectra.

Figure 106. Fragments page with stacked spectra for all fragments

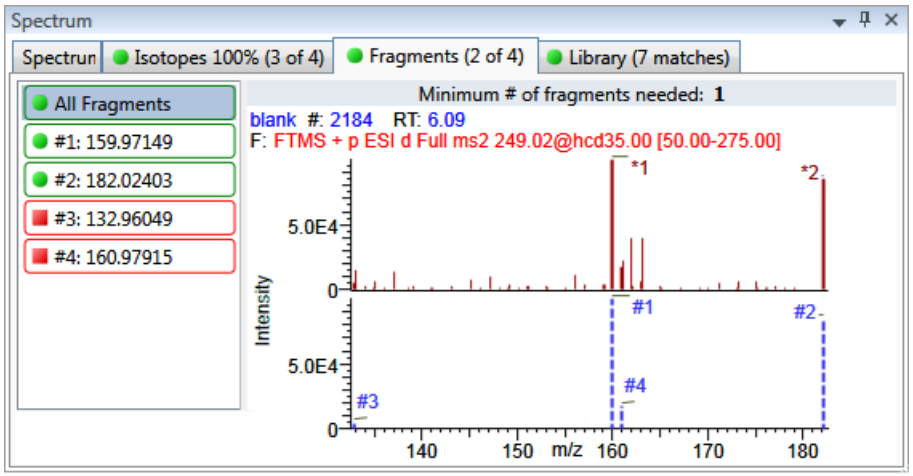
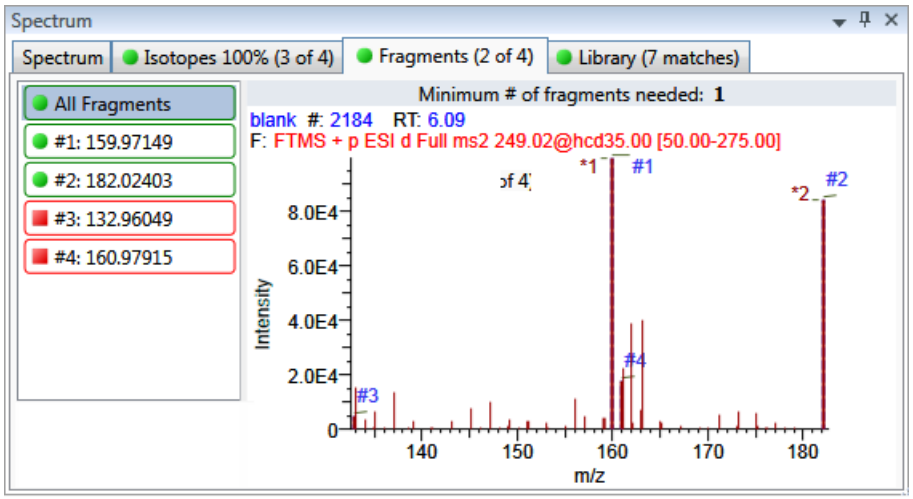


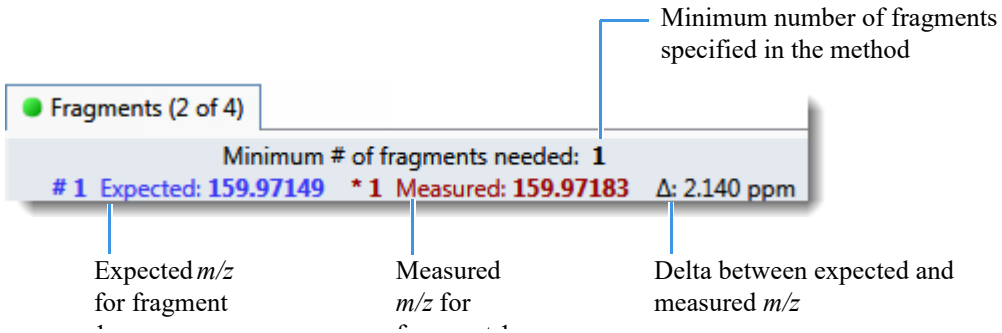
Figure 107. Fragments page with overlaid spectra for all fragments



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:



You can display the fragment as either stacked spectra or overlaid spectra.

Figure 108. Fragments page with stacked spectra for a single fragment

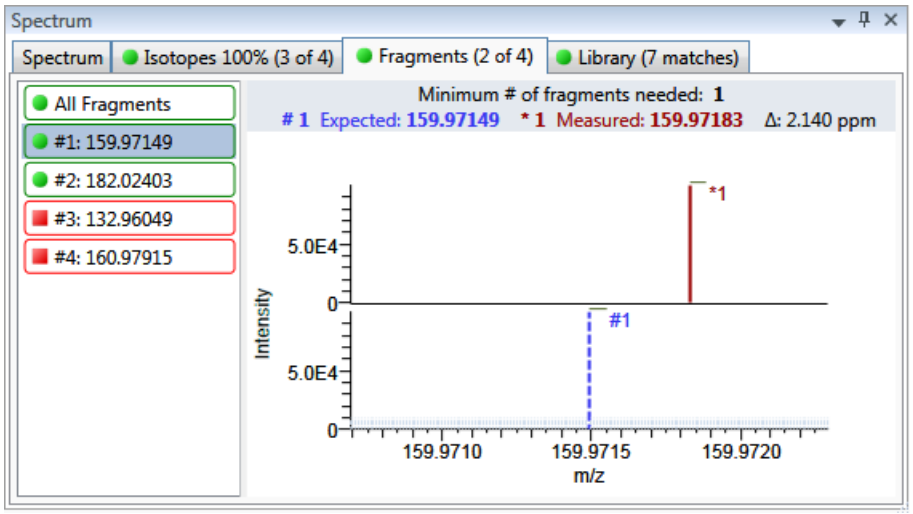
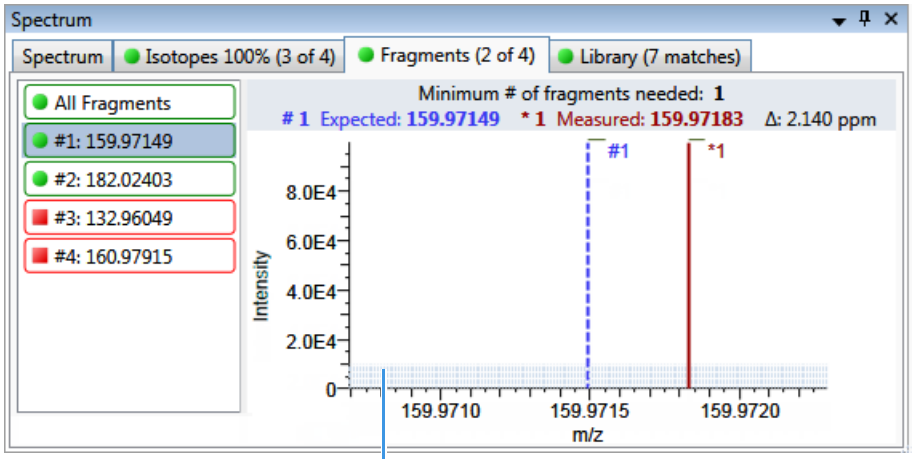


Figure 109. Fragments page with overlaid spectra for a single fragment



Intensity threshold specified in the

Fragments page shortcut menu

Use the commands in the shortcut menu to specify how you want the data displayed.

Table 53. Fragments page shortcut menu commands

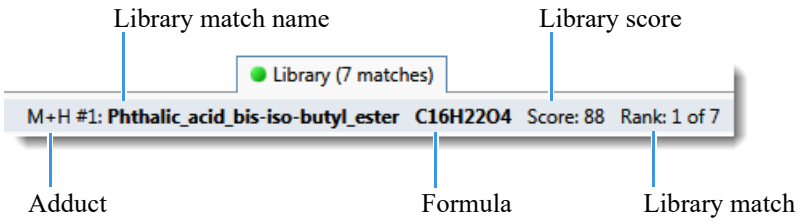
Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.

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. Refer to "Editing the Processing page" in Chapter 5, "Using the Method Development Mode for Target Screening Methods," in the *TraceFinder Lab Director User Guide*.

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 side of the plot.

The application displays these headers for the individual adducts:



You can display the library matches as either stacked spectra or overlaid spectra.

Figure 110. Library page with stacked spectra

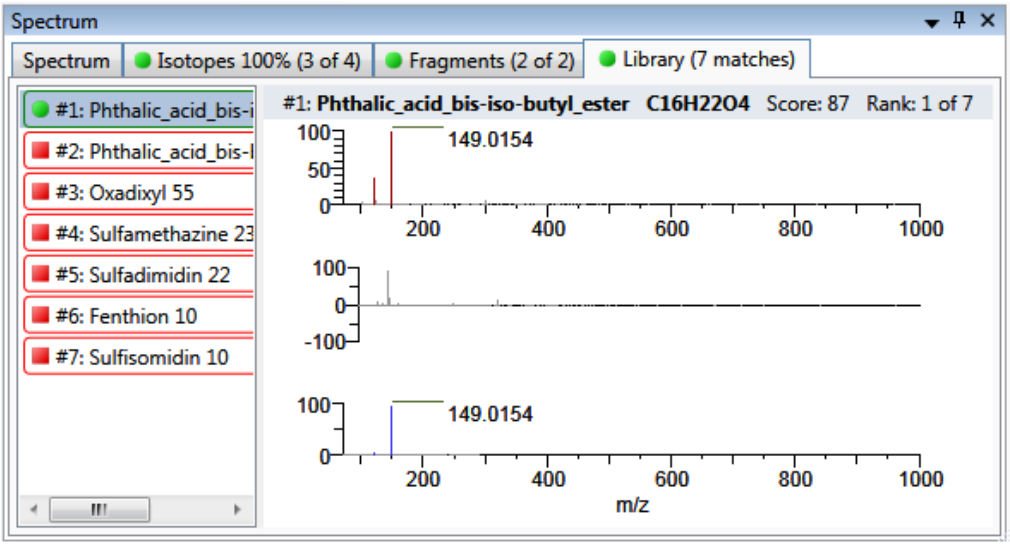
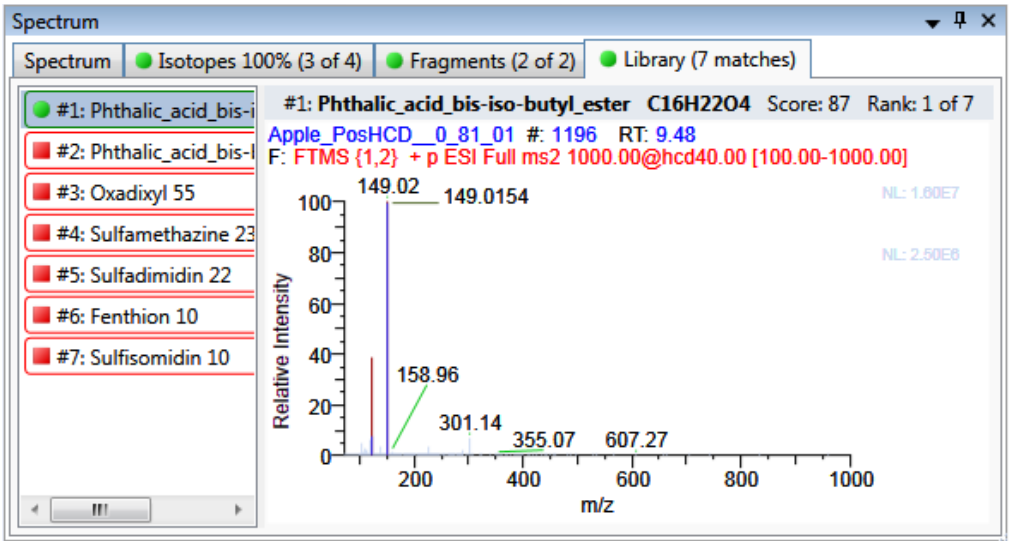


Figure 111. Library page with overlaid spectra



Library page shortcut menu

Use the commands in the shortcut menu to specify how you want the data displayed.

Table 54. 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 Report View for target screening batches

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:

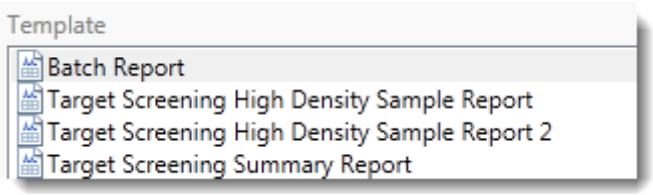
- To preview a report
- To generate a report as a PDF, an Excel, or a CSV file
- To print a report
- To display a generated report
- To edit a report template
- To create a new report template

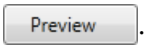
v To preview a report

1. In the Template pane, select a report template.

   The template list shows all the report templates that you configured in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

   Figure 112. Example of a report template list

2. Click **Preview**, 

   .

   The application opens the Report Designer, showing the report information for the current batch in the selected report template format.

   For details about using the Report Designer, see Chapter 7, "Using the Report Designer."

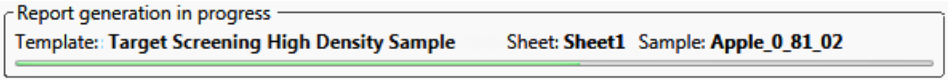
v To generate a report as a PDF, an Excel, or a CSV file

1. In the Template pane, select a report template.
2. Select the check box for each of the file types that you want to create: **PDF**, **Excel**, or **CSV**.
3. Click **Generate**,

   .

The application does the following:

- Displays a green progress bar as it generates the reports.



- Creates a report for the current batch as a PDF, an Excel, or a CSV file, using the selected report template format.
- Adds information about the generated report to the Generated Reports pane.

  For details about the Generated Reports pane, see Report View.
- Saves the report files to the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

v To print a report

1. In the Template pane, select a report template.
2. Select the check box for the **Print** file format.
3. Click **Generate**,

.

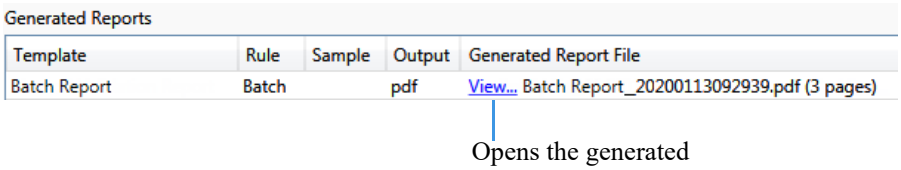
   The application does the following:

   - Creates a report for the current batch using the selected report template format.
   - Prints the report to your default printer.
   - Adds information about the generated report to the Generated Reports pane.

     For details about the Generated Reports pane, see Report View.
   - Saves the report files to the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

v To display a generated report

- In the Generated Reports pane, click **View** for the report that you want to see.



The application opens the output file.

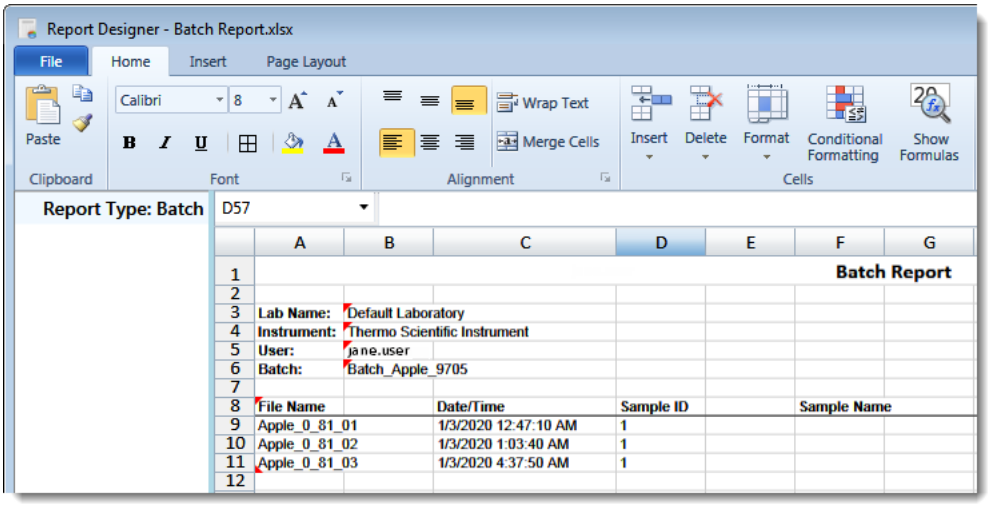
v To edit a report template

You cannot edit report templates that were provided with the TraceFinder application; however, you can open a TraceFinder template, make changes, and save it to a new template name.

1. In the Template pane, select a report template.
2. Click **Open**, Open.

   The application opens the Report Designer showing the template in an Excel spreadsheet.

   Figure 113. Report Designer showing the template for the selected report



3. Use the features in the Report Designer to edit the template.

   For details about using the Report Designer, see Chapter 7, "Using the Report Designer."

4. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

v To create a new report template

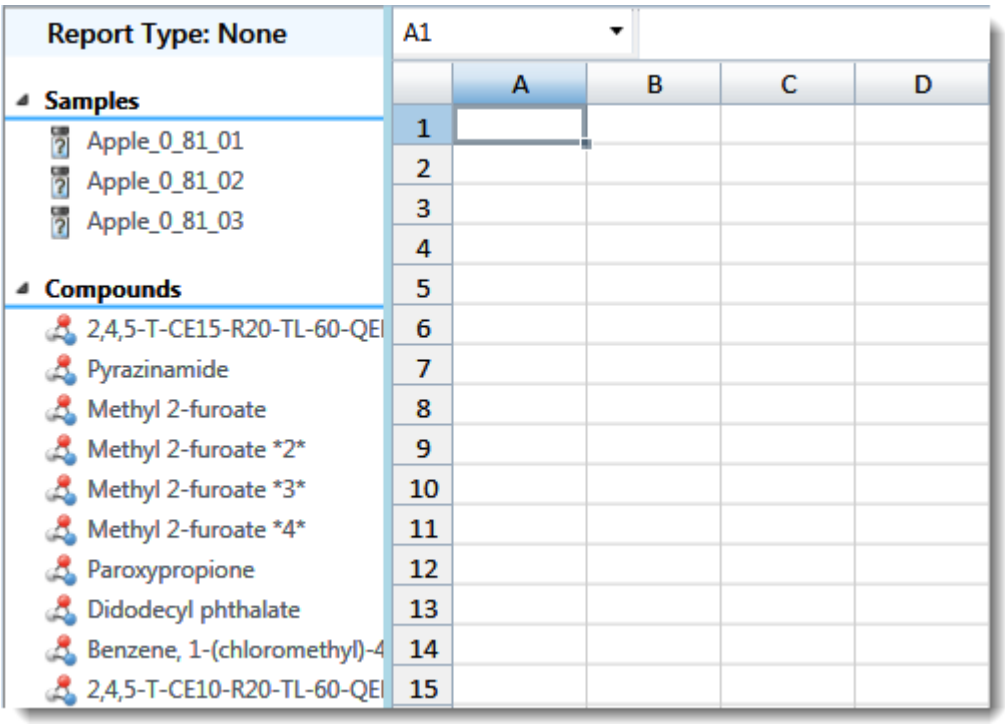
1. Click **New**, New.

   The application opens the Report Designer showing an empty template in an Excel spreadsheet. See Report Designer showing a new, empty template.

   The Report Type is None.

   In the left pane, the spreadsheet lists all samples in the current batch and all compounds in the method used for the batch.

Figure 114. Report Designer showing a new, empty template



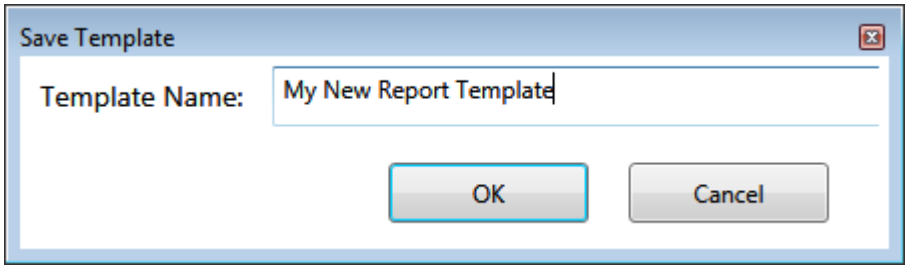
2. Use the features in the Report Designer to create the report template.

   For details about using the Report Designer, see Chapter 7, "Using the Report Designer."

3. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

   The Save Template dialog box opens.

   Figure 115. 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 116. Report View

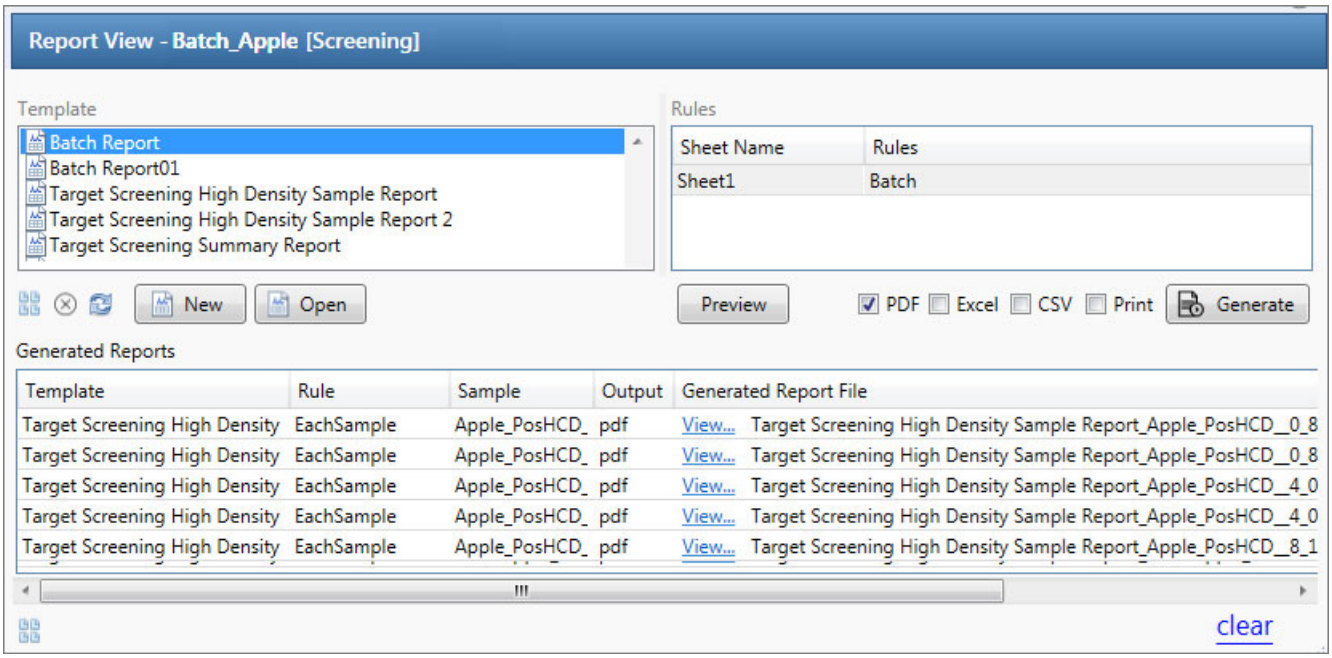


Table 55. Report View parameters (Sheet 1 of 2)

Parameter	Description
Template	
	Displays all report templates.
Rules	
Sheet Name	Specifies each sheet in the report.
Rules	Specifies the type of data used in each sheet in the selected report. • Batch • EachSample • SampleType: *SampleType* • CompoundType: *CompoundType* • SampleCustomFormula:
Buttons	
View Report Templates	Displays the …\TraceFinderData\Templates\ReportTemplates folder that contains all report templates.
Open	Opens the selected report template in the Report Designer.
New	Opens a blank report template in the Report Designer.

Table 55. Report View parameters (Sheet 2 of 2)

Parameter	Description
Preview	Opens the Report Designer showing the report information for the current batch in the selected report template format.
PDF	Writes the generated report to a PDF file in the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.
Excel	Writes the generated report to a PDF file in the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.
CSV	Saves the generated report as a PDF file in the …\TraceFinderData\Projects\…*batch*\ReportOutput folder. When the report contains multiple sheets, the application writes each sheet as a separate CSV file.
Print	Prints the generated report to your default printer.
Generate	Generates the selected type of reports for the current batch using the selected report template.
Generated Reports	
Template	Report template used for the report. See Example of a report template list.
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\Projects\…*batch*\ReportOutput folder.
View	Displays the generated output file.
View Generated Reports	Displays the …\TraceFinderData\Projects\…*batch*\ReportOutput folder that contains all report outputs.
Clear	Removes all reports from the Generated Reports display. This does not delete the reports from the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

Working in the Local Method view for target screening batches

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*.

v **To open the Local Method View**

1. Click **Analysis** in the navigation pane.
2. Click **Local Method**.

The Local Method View for the currently selected batch opens.

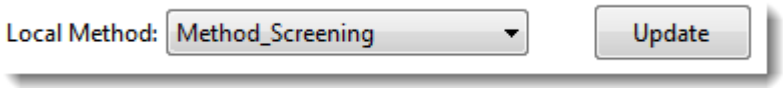
You can edit many of the method parameters in a local method. Editing the local method does not affect parameters in the master method.

For detailed descriptions of method parameters, refer to "Editing a Master Method" in Chapter 5, "Using the Method Development Mode for Target Screening Methods," in the *TraceFinder Lab Director User Guide*.

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.

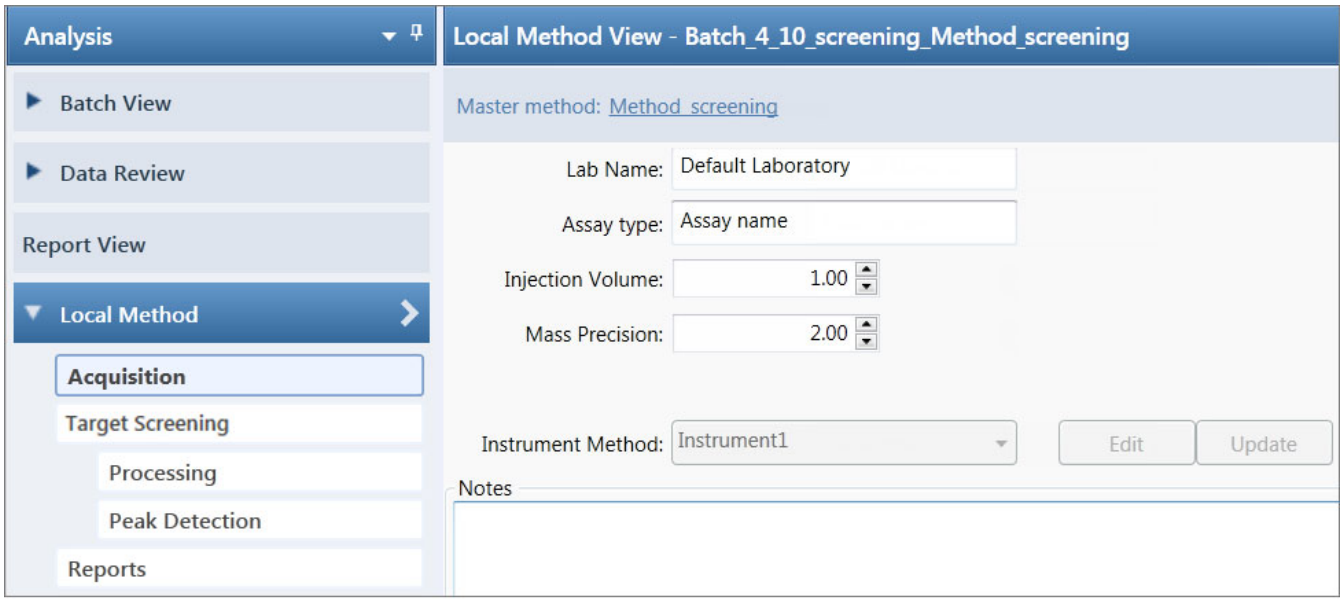
v **To overwrite the local method with the master method in the Batch View**

- 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 117. Local Method View



6

Using the Analysis mode for unknown screening batches

Use the features of the Analysis mode to do the following:

- Create unknown screening batches.
- Submit unknown screening batches for acquisition, processing, or report generation.
- Review unknown screening batches, batch data, reports, and local methods.

Contents

- Working in the Batch View for unknown screening batches
- Working in Data Review for unknown screening batches
- Working in the Report View for unknown screening batches
- Working in the Local Method View for unknown screening batches

Working in the Batch View for unknown screening batches

In the Batch View, you can manually create and edit a new unknown screening batch or open and edit a previously saved batch. When you submit a batch, you can acquire and process data and optionally create reports for the submitted samples.

The Analysis mode includes a toolbar:

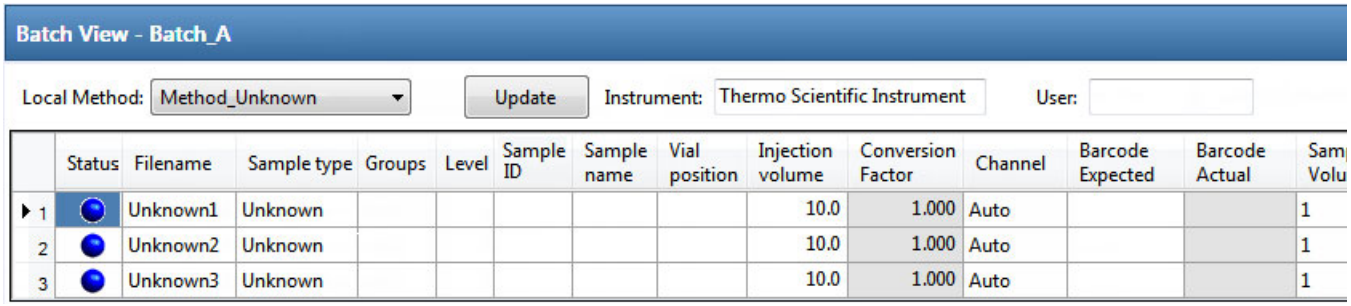
Use the Toolbar or the equivalent commands in the Batch View Shortcut Menu to create the sample list and submit samples for acquisition.

See the following topics:

- Samples page features
- Creating a new batch
- Editing a batch
- Submitting a batch
- Archiving and importing batches

Samples page features

Use the Samples page to create a batch.



Samples page

The Samples page includes the following features:

- Column display
- Status indicators
- Groups
- Sample weight calculation
- Instrument Methods
- Toolbar for unknown screening batches
- Batch View sample list
- Batch View shortcut menu for unknown screening batches

Column display

The sample list contains many columns of information. You can scroll to see all the columns, and you can customize which ones to display and their display order.

v To scroll the sample list

Use the horizontal scroll bar at the bottom of the sample list to view all the information.

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

v To customize the column display

1. Right-click the sample list and choose **Modify Columns**.

   The Modify Columns dialog box opens.

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

   These columns appear after the Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

   a. In the Displayed Columns pane, select a column name.

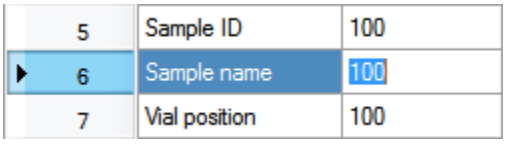
   b. Use **Up** or **Down** to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Batch View sample list, and the last column in the list represents the rightmost column in the Batch View sample list.

      Note The following columns are fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:

   a. In the Displayed Columns pane, select the column width.

   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 118. Modify Columns dialog box

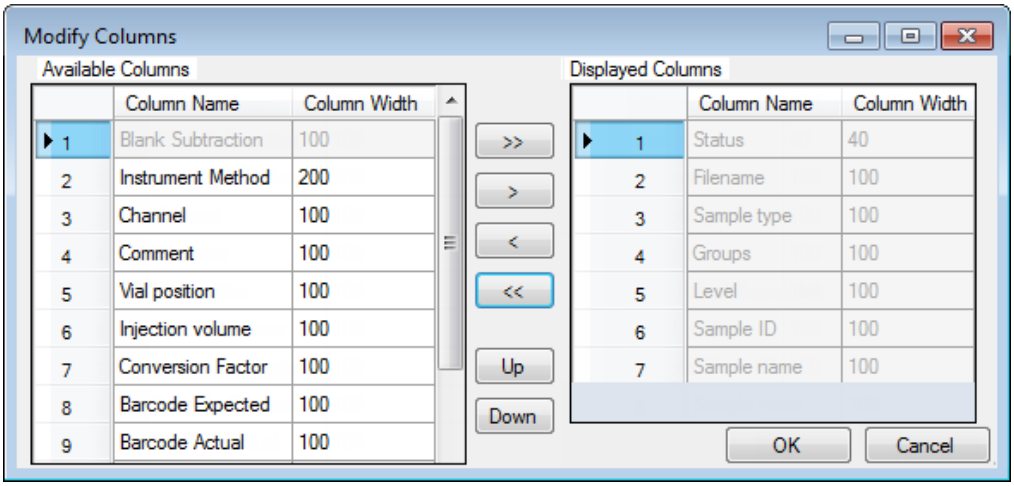


Table 56. Button descriptions for the Modify Columns dialog box

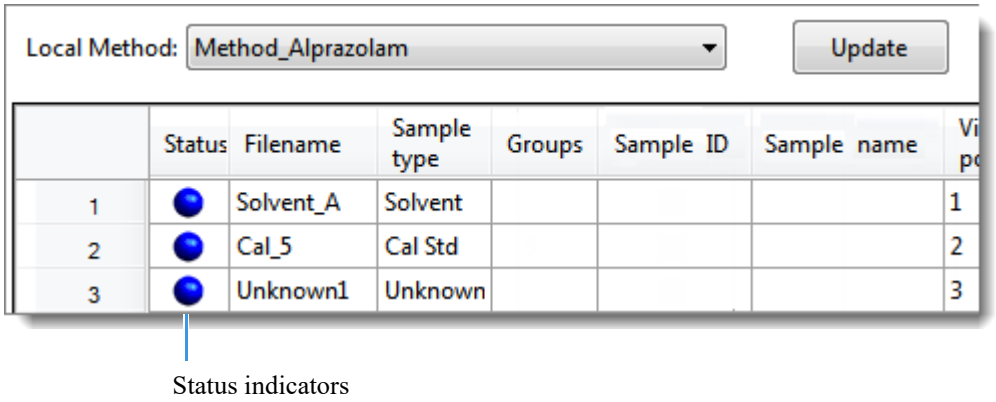
Button	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name.	
<	Moves the selected column to the Available Columns pane.
<<	Moves all columns except fixed columns.
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.

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.

Figure 119. Status indicators



Groups

Use the Groups feature to assign samples to a group.

v **To create a group**

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

   Repeat this for each sample that you want to include in a group.

2. Create as many groups as you want.

Note To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
	Benzo26473	groupB, groupA
	Benzo25557	groupB
	Benzo26154	groupB, groupA

The application uses the first group listed for the Maximum Fold analysis and in the Group Averages pane.

You can create a control group (specify the group name as Control) to use for group averages in Data Review.

For information about group averages, see Group Averages pane. For information about maximum fold analysis, see Cross Sample Peak List pane.

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*

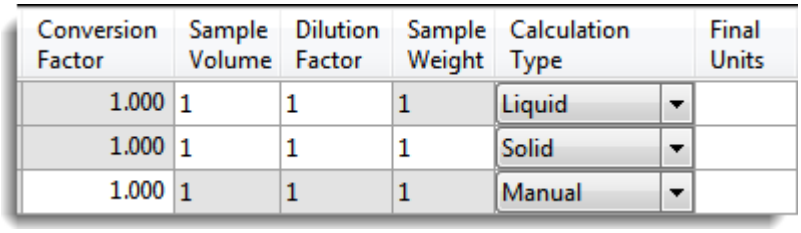
Manual: The application does not calculate the Conversion Factor. Instead, you can enter the Conversion Factor value.

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

v 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**.



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	

v 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.

v 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.

v **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.

v **To specify instrument methods for samples**

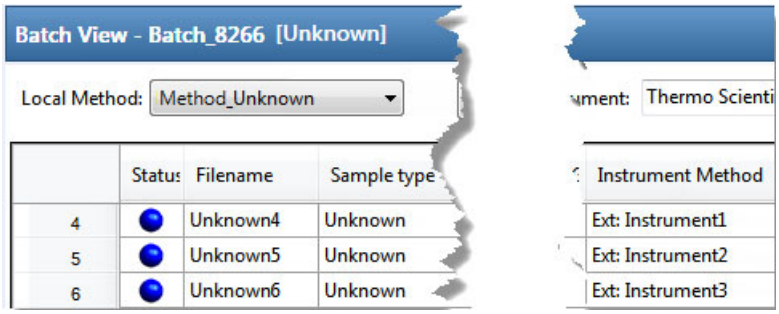
1. Display the Instrument Method column in the sample list:
   a. Right-click the sample list and choose **Modify Columns**.

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

Local instrument methods:

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

Toolbar for unknown screening batches

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

Table 57. Toolbar icons (Sheet 1 of 2)

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.
	Inserts a new, empty sample or samples above the selected sample. See the instructions To insert samples into the list.
	Removes the selected samples from the sample list. See the instructions To remove samples from the list.
	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.
	Submits only the selected samples for acquisition, processing, or report generation. See the instructions To submit samples in the batch.
	Submits the batch for acquisition, processing, or report generation. See the instructions To submit samples in the batch.

Table 57. Toolbar icons (Sheet 2 of 2)

Icon	Description
	Submits only the selected samples for processing. See the instructions To submit selected peaks for processing.
	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 unknown screening batches.
	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.
	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 8, "Confirming audited changes and using the Audit Viewer." Available only when you enable Auditing in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

Batch View sample list

The sample list, a multi-column table, displays all the quantitative data for the samples of a batch. Status indicators in the Status column indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The sample list includes the following columns of information.

Figure 120. Batch View sample list

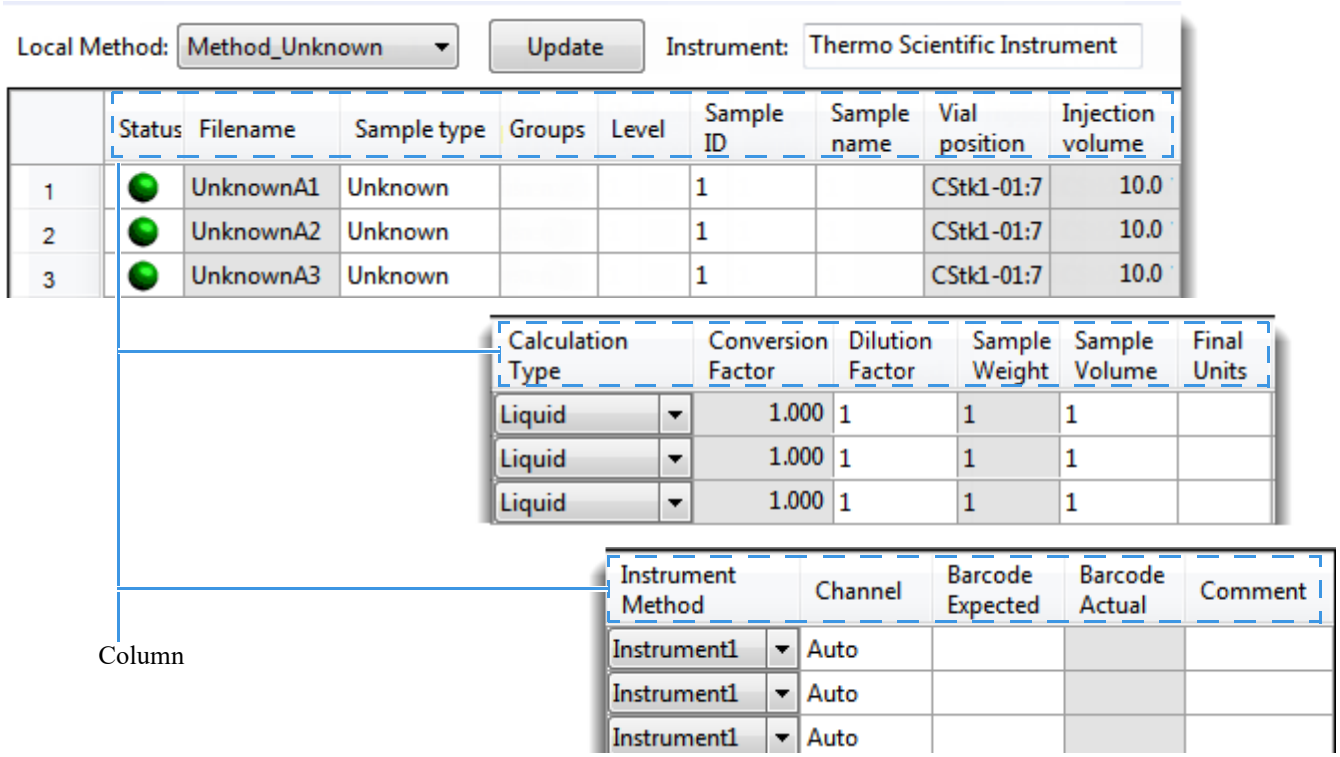


Table 58. Batch View sample list columns (Sheet 1 of 3)

Column	Description
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.
	Note When you include unknown screening features in a quantitation method and you choose to process with only the unknown screening criteria, both the Sample View and the Unknown Screening View show the Status for the samples as acquired and processed ( ).
	Note When you include unknown screening features in a target screening method and you choose to process with only the unknown screening criteria, both the Samples view and the Unknown Screening View show the Status for the samples as acquired and processed ( ).

Table 58. Batch View sample list columns (Sheet 2 of 3)

Column	Description
Filename	Name of the raw data file that contains the sample data.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, QC, or Unknown. Default: Unknown
	Note Unknown Screening does not use calibration sample types ().
Groups	Threshold group to which a sample belongs.
Level	Not used in Unknown Screening processing.
Sample ID	A user-defined, alphanumeric string that identifies a sample.
Sample Name	A user-defined name that identifies a sample.
Vial Position	The tray vial number used for an autosampler acquisition.
Injection Volume	The injection volume (in microliters) of the injected sample. When you are using an autosampler, you can set the default injection volume in the Autosampler dialog box in the Instrument View. The minimum and maximum injection volumes that you can use depend on the Autosampler you configure. The usable range depends on the injection mode and might be smaller than the displayed range. The Injection Volume value set in the master method overwrites the value in the instrument method. Valid range: 0.1 through 5000 µL
Calculation Type	Liquid: Calculates the Conversion Factor as $SampleVolume \div DilutionFactor$ Solid: Calculates the Conversion Factor as $(SampleVolume \times DilutionFactor) \div SampleWeight$ 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

Table 58. Batch View sample list columns (Sheet 3 of 3)

Column	Description
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 Instrument Methods.
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 the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.
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.

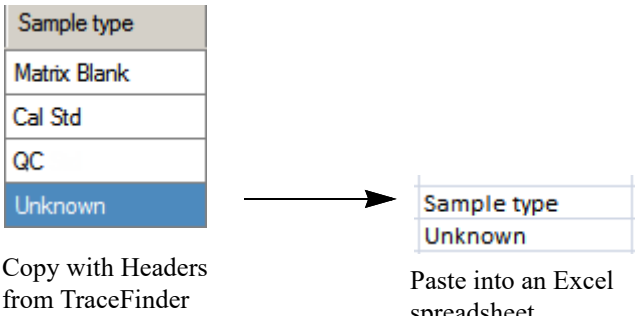
Batch View shortcut menu for unknown screening batches

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

Table 59. 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.
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.

Table 59. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
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.
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.
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, for example,  Copy with Headers from TraceFinder Paste into an Excel spreadsheet You cannot paste this data back into the sample list.
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. For detailed information about editing instrument methods, refer to Chapter 3, "Using Instrument Methods in the Method Development Mode," in the *TraceFinder Lab Director User Guide*.

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 edit sample values
- To browse in raw data files
- To customize the column display

v **To create a new batch**

1. Choose **File > New > Batch** from the main menu.

   The Create New Batch dialog box opens. See Create New Batch dialog box for unknown screening batches.

2. Select a repository from the list.

   Tip The application displays all configured and enabled repositories.

   The project list displays all projects, subprojects, and batches in the selected repository.

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.

4. Type a batch name in the New Batch box.

5. To select a master method, do the following:

   a. Select **Unknown Only** from the Type list.

   b. Select a repository from the Repository list.

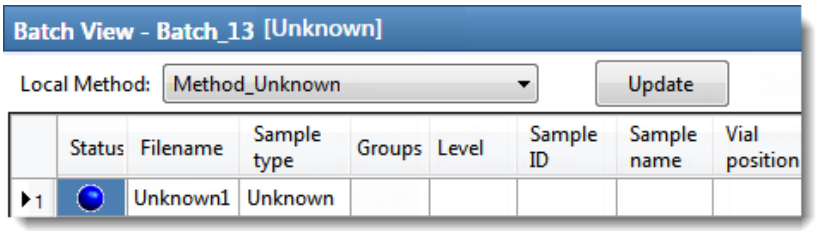
   c. Select a master method from the Name list.

      The Name list displays all methods for the target screening type.

6. Click **Create**.

Tip To activate the Create button, you must enter a unique batch name and select a master method. If the Create button is not activated, you have either entered a batch name that is already used or you have not selected a master method.

A new batch opens with one Unknown sample.



The batch name in the title bar indicates that you are creating an unknown screening batch.

v To add samples to the list

1. To add a single sample row, right-click the sample list and choose **Add Sample**.
2. To add multiple sample rows, select the number of rows and then click the **Add Sample** icon, .

   The application adds the specified number of new, empty samples to the end of the sample list.

v To insert samples into the list

- Select the sample above which you will insert new, Unknown samples, and then do one of the following:

  – To insert a single sample row, right-click and choose **Insert Sample**.

  –or–

  – To insert multiple sample rows, select the number of rows and then click the **Insert Sample** icon .

The application inserts the Unknown samples above the selected sample.

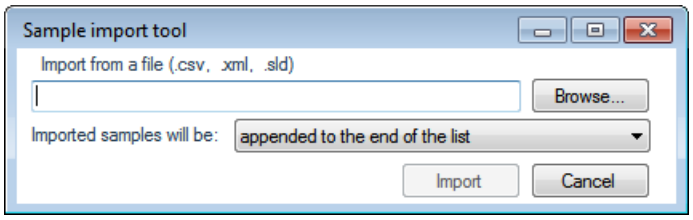
Inserted

	Status	Filename	Sample type	Groups	Level
1		cal_std_5	Cal Std		
2		Unknown2	Unknown		
3		Unknown1	Unknown		
4		cal_std_10	Cal Std		

v To import samples into the list

1. Choose **Batch > Import Samples** from the main menu, or click the **Import Samples** icon, .

   The Sample Import Tool dialog box opens.



   From this dialog box, you can import samples from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file that contains the samples to import.

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

4. Click **Import**.

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

   When you import samples from an Xcalibur sequence file (.sld), the application makes the following column name substitutions:

Xcalibur column	TraceFinder column
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conversion Factor

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

Xcalibur sample type	TraceFinder sample type
Blank	Matrix Blank
QC	QC
Std Bracket	

5. (Optional) When using the Multi-Channel LC feature, select a channel for each imported sample.

   Imported samples default to Auto.

   Note The Channel column is available only when you have activated the Multi-Channel LC feature in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

v 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**.

v To copy a sample

1. Select the sample that you want to copy.
2. Right-click and choose **Insert Copy Sample**.

   The application inserts the copy above the selected sample.

v 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**.

   The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

v To edit sample values

1. For each sample, do one of the following:

   - Type a new file name over the current file name.
   - 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**, and then locate a raw data file to use for the sample.

   By default, the application sets the Sample Type to Unknown.

2. For each sample, click the Sample Type column and select a sample type from the list.

Available sample types			
Matrix Blank	Solvent	QC	Unknown

3. Type a vial position in the Vial Position column for each sample.
4. 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.

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

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

   To automatically copy or fill values in these columns, see Appendix B, "Using Copy Down and Fill Down."

v **To browse in raw data files**

1. Do one of the following:

   - Double-click the Filename column.
   - Right-click and choose **Browse in Raw File.**

   The What Raw File Would You Like to Use dialog box opens.

2. Select a raw data file to use for the sample or use the CTRL key to select multiple files, and then click **Open**.

   The application overwrites the selected, unacquired sample in the batch with the first "browsed in" file and adds any additional browsed in files below the selected sample.

   For all browsed-in raw data files, the application sets the Status to Acquired, , and sets the Sample Type to Unknown.

   Note You cannot overwrite an acquired sample. When you select a sample that is acquired, the application adds all browsed in files below the selected sample.

v **To customize the column display**

1. Right-click the Batch View sample list and choose **Modify Columns**.

   The Modify Columns dialog box opens.

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

   All the columns you select appear after the Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name columns.

3. To arrange the order of the columns, do the following:

   a. In the Displayed Columns pane, select a column name.

   b. Use **Up** or **Down** to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Batch View sample list, and the last column in the list represents the rightmost column in the Batch View sample list.

      Note The following columns are fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name.

4. To change the width of a column, do the following:
   a. In the Displayed Columns pane, select the column width.

7	Vial position	69
8	Injection volume	100
9	Calculation Type	100

   b. Type a new value for the width.
5. When you have completed your changes, click **OK**.

   The columns in the sample list immediately reflect your changes. The application uses these settings for all sample lists in the Batch View.

Figure 121. Modify Columns dialog box

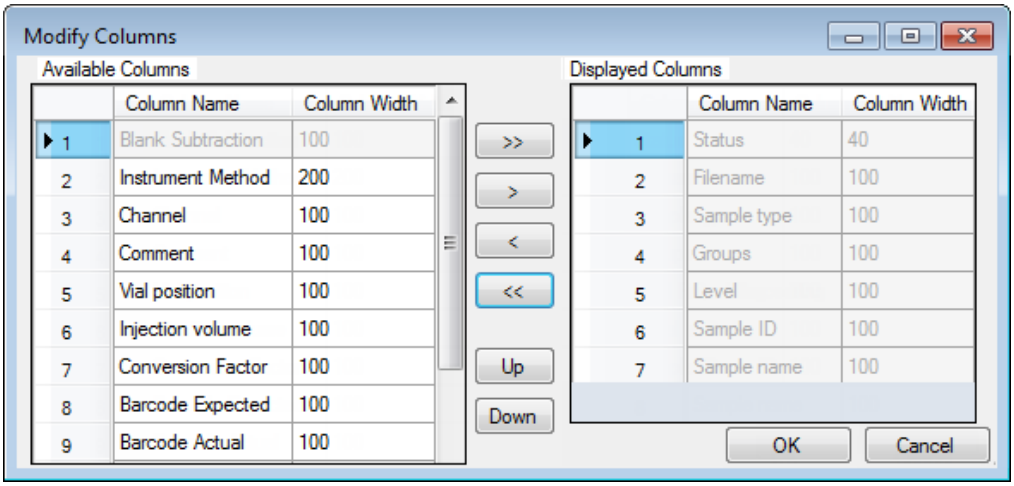


Table 60. Button descriptions for the Modify Columns dialog box

Button	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
The following buttons apply to all columns, except for those that are fixed: Status, Filename, Sample Type, Groups, Level, Sample ID, and Sample Name.	
<	Moves the selected column to the Available Columns pane.
<<	Moves all columns except those that are fixed.
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.

Create New Batch dialog box for unknown screening batches

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

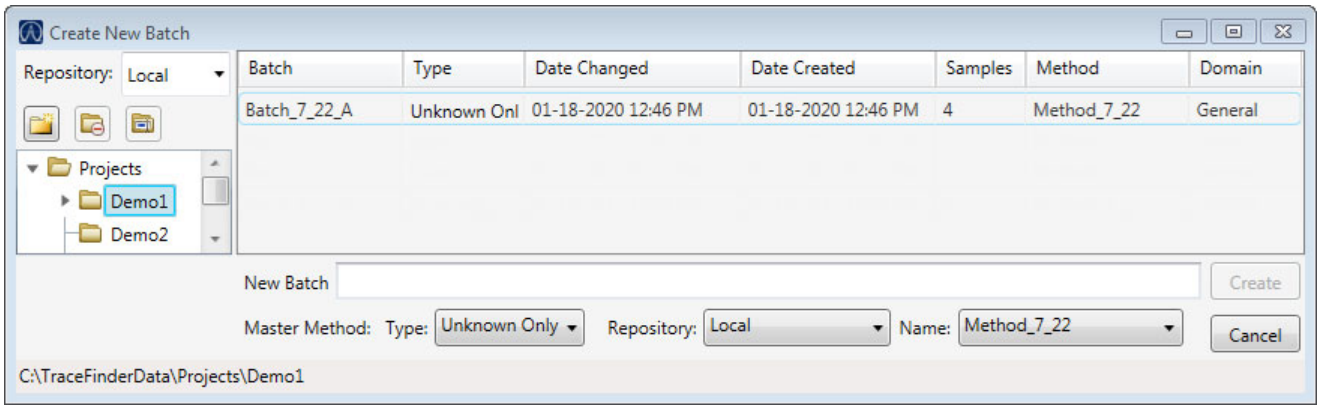


Table 61. Create New Batch dialog box parameters (Sheet 1 of 2)

Parameter	Description
Repository	The default data repository specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.
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, you can right-click and choose Create Folder.
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, you can right-click and choose Delete.
Rename Folder	Renames the selected folder. Or, you can right-click and choose Rename.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.

Table 61. Create New Batch dialog box parameters (Sheet 2 of 2)

Parameter	Description
Batch and Master Method parameters	
New Batch	Name of the new batch to create. **Note** If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Type	Type of batch to create: Quan, Screening, or Unknown Only.
Repository	The repository used to store the new batch.
Name	Method used to create the new batch.
Path	Path to the project in the TraceFinderData\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.

Follow these procedures:

- To create new project folders
- To delete project folders
- To rename project folders

v 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\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.

v **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.

v **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

v **To open a saved batch**

1. Choose **File > Open > Batch** from the main menu.

   The Open Batch dialog box opens.

2. Select a project and a subproject.
3. Select **Unknown Only** or **Any** from the Type list.

   The batch list displays all batches created with Unknown methods (or all methods of all types when you select Any).

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

   The selected batch opens in the Batch View.

Figure 122. Open Batch dialog box

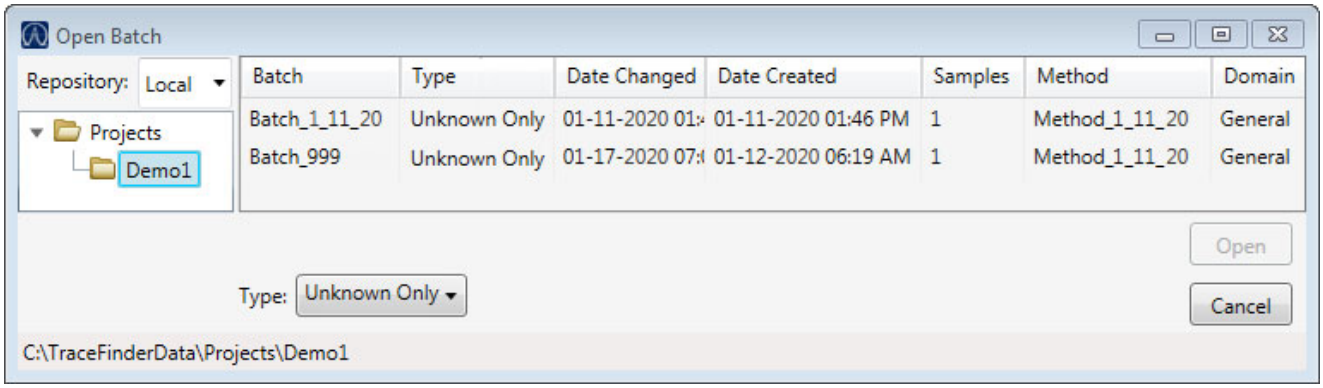
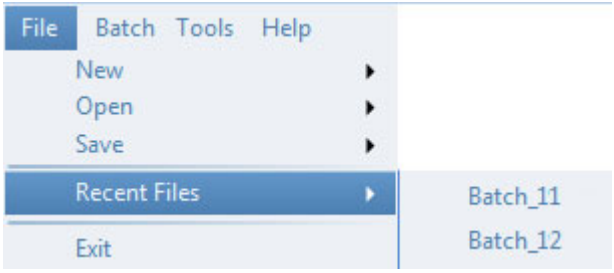


Table 62. Open Batch dialog box parameters

Parameter	Description
Repository	The default data repository specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.
Path	Path to the project in the Projects folder where the batch is stored.
Buttons	
Type	Type of batch to display in the Batch list: Quan, Screening, Unknown Only, or Any.
Open	Opens the Batch View for the selected batch.
Cancel	Closes the Open Batch dialog box without opening a batch.

v **To open a recent batch**

- Choose **File > Recent Files >** ***batch*** from the main menu.



The selected batch opens in the Batch View.

v **To edit samples in a batch**

- Use the commands described in Working in the Batch View for unknown screening batches.

  You can add new samples, edit samples, or delete samples.

v **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**.

   The application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the sample are numbered INJ002, INJ003, and so forth. The application copies all parameter values from the original sample.

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

	cal_std_50_INJ001	Cal Std	10
	cal_std_50	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

   When you submit all samples in this batch, the application acquires all samples (including previously acquired samples).
3. To save this batch with the new samples for reinjection, choose **File > Save > Batch** from the main menu.

   The batch is saved as a prepared batch that is ready to submit. You can open this batch from the Reinject Samples page in the Acquisition mode and submit the batch. The application acquires only the samples that have not been previously acquired.

Submitting a batch

In the Batch View, you can submit an entire batch or only selected samples in the batch. When you submit a batch for acquisition and processing, you can choose to create reports for the submitted samples. See Submit Options dialog box.

For a description of commands in the shortcut menu, see Batch View shortcut menu commands.

Follow these procedures:

- To submit selected peaks for processing
- To submit samples in the batch
- To view the output files

v To submit selected peaks for processing

1. In the Peak List, select the **Selected** check box for the peaks that you want to process.
2. Click the **Submit … for Processing** icon, .

   The application processes the selected peaks and updates the data in the Peak Identifications pane.

v 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.

   Note You can also submit only selected peaks for processing. See To submit selected peaks for processing.
2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.
   - When all submitted samples have been previously acquired, this option is (by default) not selected.
   - When one or more samples in the batch have not been acquired, this option is (by default) selected.

   Tip You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.
3. To process the submitted samples, select the **Process Data** check box.

   The application displays processing options for the Unknown Screening method.
4. Select the check box for the unknown screening options that you want to use.

   Peak Detect: Performs peak detection. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

   Identify: Performs identification. This produces the peak identification data in the Unknown Screening View.

   With RT Alignment: Performs retention time alignment. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.
5. (Optional) Select the **Create Reports** check box.

6. (Optional with the Multi-Channel LC feature activated) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.

7. (Optional without the Multi-Channel LC feature activated) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   - **Next Available Batch** places the batch immediately after the currently acquiring batch.
   - **Next Available Sample** places the batch immediately after the currently acquiring sample.

   Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.
   a. Select the **Use** check box for the device that you want to use for this acquisition.
   b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

      This is usually the autosampler.

   c. Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

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

   d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.

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

   The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Analysis mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT After the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages in the method (refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*) and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Figure 123. Submit Options dialog box

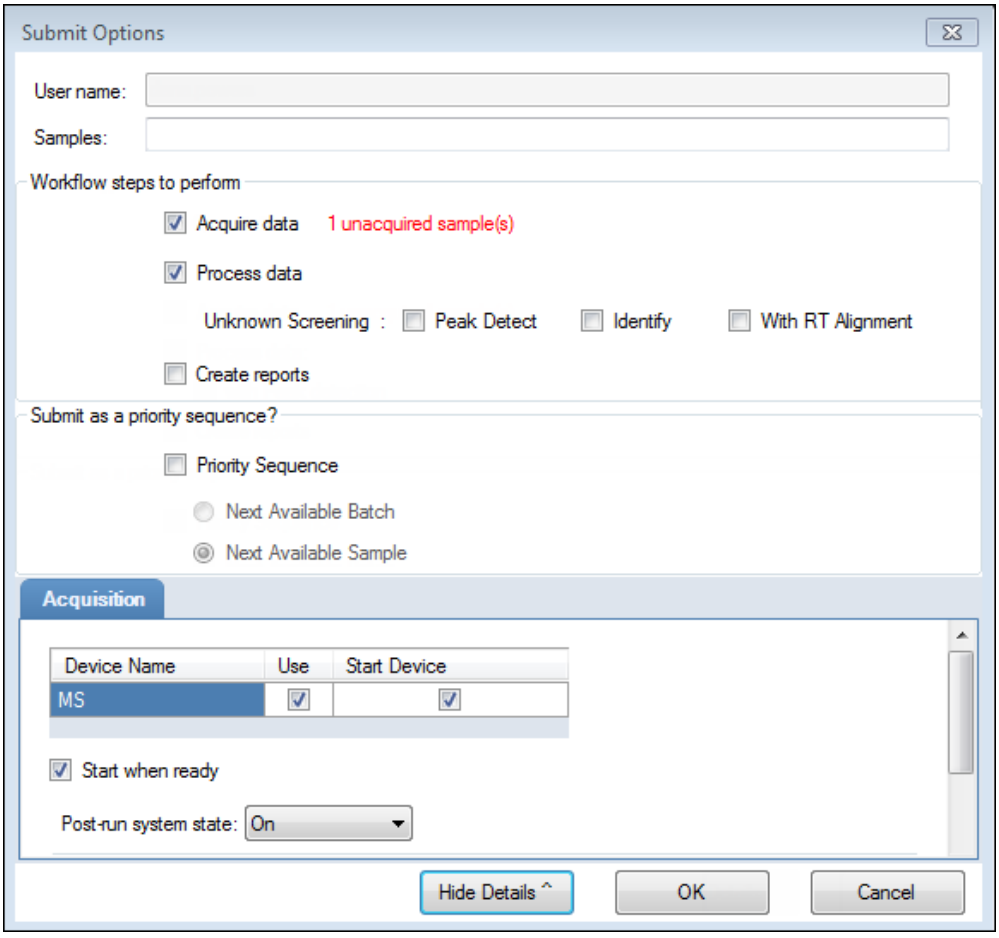


Table 63. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Workflow Steps to Perform	
Acquire Data	Submits the current batch to acquisition. • When all submitted samples have been previously acquired, this option is (by default) not selected. • When one or more samples in the batch have not been acquired, this option is (by default) selected.
Process Data	Processes the data for the current batch using any of the following options: Peak Detect: Performs peak detection for all method types. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples. Identify: Performs identification for unknown screening methods. With RT Alignment: Performs retention time alignment for unknown screening methods. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.
	Note You can use unknown screening features in conjunction with quantitation or target screening methods. For specifying processing data for batches that also use quantitation methods, see To submit samples in the batch. For specifying processing data for batches that also use target screening methods, see To submit samples in the batch.
Create Reports	Creates reports for the current batch.

Table 63. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
Submit as a Priority Sequence?	
Priority Sequence	With the Multi-Channel LC feature activated, places the batch immediately after the currently acquiring batch. Without the Multi-Channel LC feature 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 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.
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.

v **To view the output files**

- Locate the files to view from the following directories:

  The application writes saved batches to the project folder:

  …\TraceFinderData\Projects\…

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

  …\TraceFinderData\Projects\…*batch*\Data

  The application saves method information to the batch Methods folder:

  …\TraceFinderData\Projects\…*batch*\Methods

  The application writes the reports to the batch ReportOutput folder:

  …\TraceFinderData\Projects\…*batch*\ReportOutput

Saving a batch to a new location

You can move the current batch to a different project folder, or you can make a copy of the current batch and save the copy to a different project folder.

Follow these procedures:

- To save a batch to another project folder
- To move a batch to another folder
- To create new project folder
- To delete project folders
- To rename project folders

v **To save a batch to another project folder**

1. Choose **File > Save > Save Batch As** from the Batch View main menu in the Analysis mode.

   The Save Batch As dialog box opens.

2. (Optional) Select a different repository.

   The default data repository is specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

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.

v To move a batch to another folder

1. Choose **File > Save > Move Batch** from the Batch View main menu in the Analysis mode.

   The Move Batch dialog box opens.

2. (Optional) Select a different repository.

   The default data repository is specified in the Administrator Console. Refer to the instructions in the *TraceFinder Administrator Console User Guide*.

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.

v To create new project folder

1. In the Save Batch As dialog box, select the folder for which you will create a new lower-level folder.

   - You can select the main TraceFinderData\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.

v **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.

v **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 and Move Batch dialog box for unknown only batches

Use the features in the Save Batch As dialog box to save a batch to a new name, or use the features in the Move Batch dialog box to move a batch to a different project folder. The features in the two dialog boxes are virtually identical.

Figure 124. Save Batch As dialog box

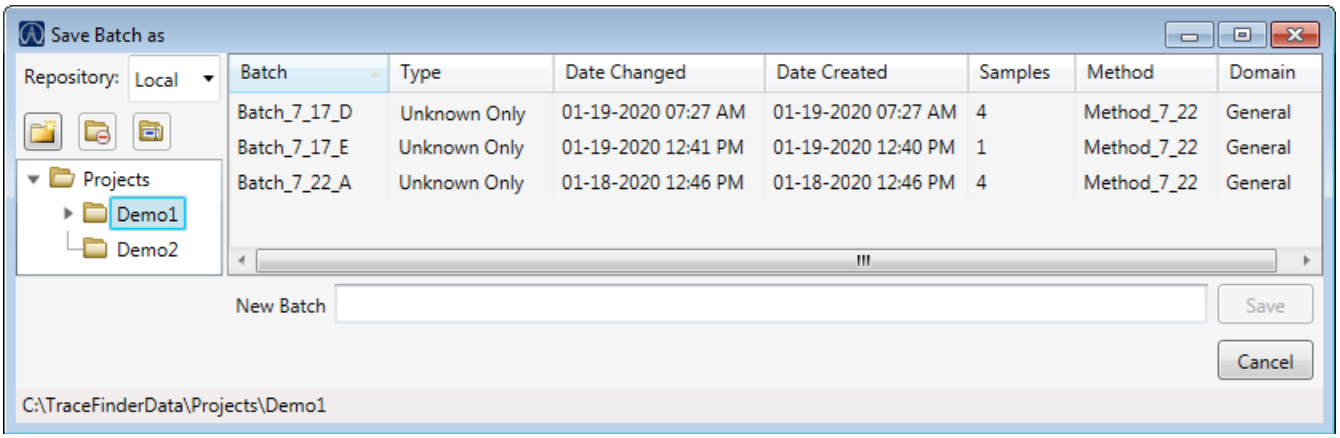


Figure 125. Move Batch dialog box

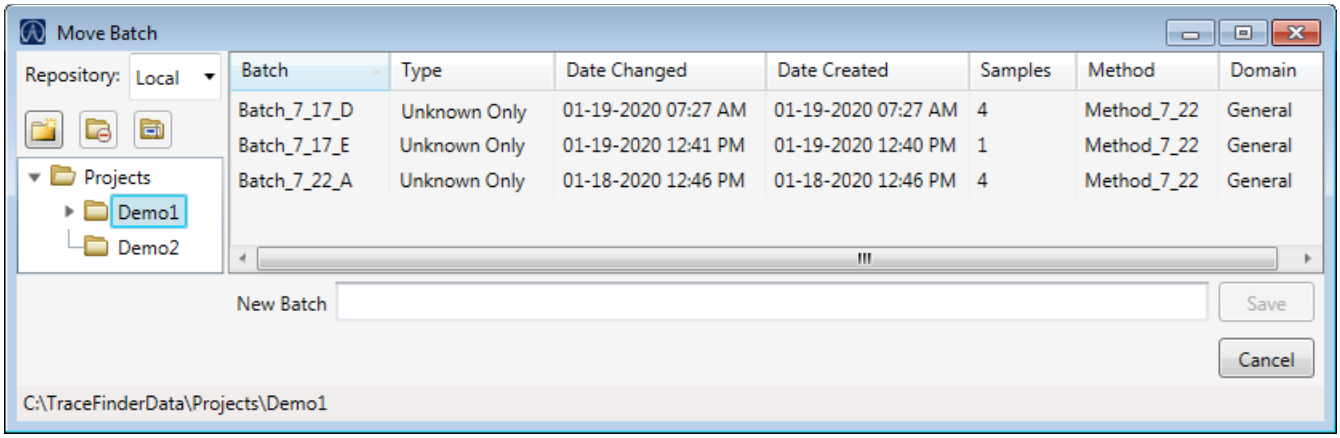


Table 64. Save Batch As dialog box and Move Batch dialog box parameters (Sheet 1 of 2)

Parameter	Description
Repository	The data repository where you want to store the batch.
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, you can right-click and choose Create Folder.
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, you can right-click and choose Delete.
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, you can right-click and choose Rename.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan, Screening, or Unknown Only.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created.

Table 64. Save Batch As dialog box and Move 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.
Path	Path to the project in the TraceFinderData\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.

Archiving and importing batches

From any page in the Batch View, you can archive batches or import batches that have been archived.

v **To import a batch**

1. Choose **File > Import Batch** from the main menu.

   The Import Batch dialog box opens.

2. Select a project for the imported batch.
3. Click **Browse** and select a zipped batch file (.zBatch) that contains the batch to import.
4. Type a name for the new batch in the New Batch box.

5. Click **Import**.

   The application extracts the batch from the zipped file in the specified project folder and opens the batch in the Batch View.

v To archive the current batch

1. Choose **File > Archive Batch** from the main menu.

   Note You must have an open batch.

   The Browse for Folder dialog box opens.

2. Locate the folder where you want to store the archived batch, and click **OK**.

   The application zips the current batch and moves it to the specified archive folder.

   IMPORTANT The batch is no longer available from its original location. To access the batch, you must import it to your repository. See To import a batch.

   The zipped file includes the processed results, compound database, local method, results, raw data files, report templates, generated reports, and audit logs for the batch.

Working in Data Review for unknown screening batches

The Data Review view displays the data generated by the master method. Use Data Review to verify the data for identified peaks before you generate reports.

When you run samples in an experiment, you can check for peaks that are not already identified in either an associated target screening or quantitation method and take appropriate steps when the application finds these peaks and proposes whether they match one or more compounds using various identification sources.

IMPORTANT When unknown screening features are associated with a quantitation or target screening method, the unknown screening results do not include any compounds (other than internal standards) that were identified by the quantitation or target screening methods.

Follow these procedures:

- To open the Data Review view
- To display or hide a pane on the Unknown Screening View page
- To restore the default layout

v 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 view opens.

   IMPORTANT In the Data Review view, you might be restricted to the Survey Mode display (refer to the *TraceFinder Administrator Console User Guide*).

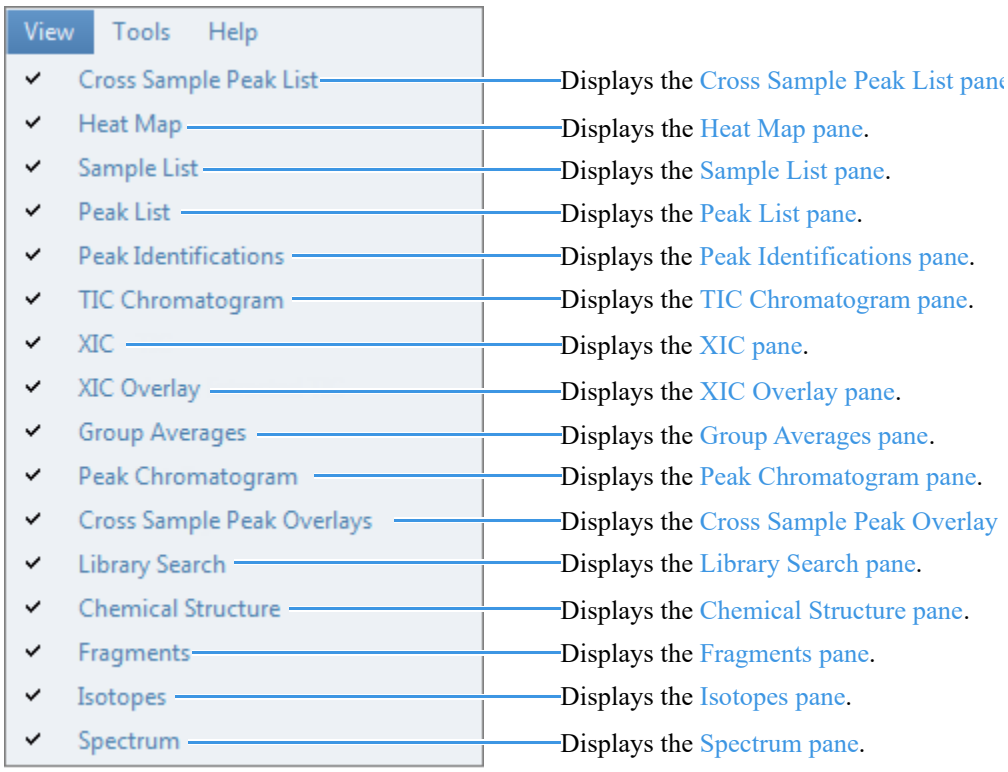
   When you are assigned strict Survey View permission, the Data Review header shows **Survey Mode** and only Cal Std and QC sample types are displayed during processing.

   When you are assigned loose Survey View permission, the Data Review header shows **Survey Mode – Loose Restrictions** and only Cal Std and QC sample types are displayed during processing. But after processing is completed, all sample types are available.

v To display or hide a pane on the Unknown Screening View page

- From the View menu, choose to display or hide any of the following panes.

  A check mark indicates a displayed pane.



v **To restore the default layout**

Choose **View > Restore Default Layout**.

The Unknown Screening View displays the default panes in their default locations.

The unknown screening view includes the following features:

- Cross Sample Peak List pane
- Heat Map pane
- Sample List pane
- Peak List pane
- Peak Identifications pane
- TIC Chromatogram pane
- XIC pane
- XIC Overlay pane
- Group Averages pane
- Peak Chromatogram pane
- Cross Sample Peak Overlay pane

- Library Search pane
- Chemical Structure pane
- Fragments pane
- Isotopes pane
- Spectrum pane

Cross Sample Peak List pane

Use the Cross Sample Peak List pane to compare peak values across all samples in a batch.

v **To use the Cross Sample Peak List pane**

1. In the Peak List pane, select a peak.

   The application scrolls the Cross Sample Peak List pane to the specified peak and selects the peak.

2. Use the scroll bar at the bottom of the pane to scroll across the values for the selected peak in all samples and groups in the batch.

Figure 126. Cross Sample Peak List pane

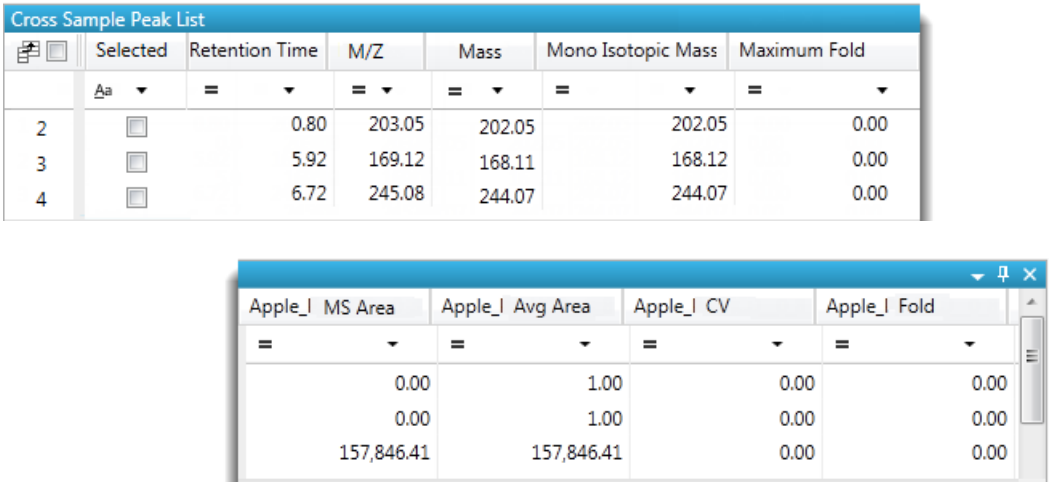


Table 65. Cross Sample Peak List pane columns (Sheet 1 of 2)

Column	Description
Selected	Identifies peaks to display when you select the Selected option in the XIC Overlay pane, or identifies which peaks to process when you click the Submit … for Processing icon, . Do not confuse a check mark in the Selected column with the currently selected peak. The row for a currently selected peak is highlighted in blue.
Retention Time	The time after injection when the compound elutes. The total time that the compound is retained on the column.
M/Z	Mass-to-charge ratio found in the spectra for the peak. Assumes that the charge is 1.
Mass	The uncharged mass found in the spectra for the peak.
Monoisotopic Mass	The most abundant mass in the spectra for the peak.
Maximum Fold	The maximum difference of the group average response from the control average response.
Compound Name	Displays the compound name found in the library or compound database. This column is displayed only when the peaks are aligned and you have performed a simple search. Refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*.
Sample n MS Area	The MS peak area for each sample.
Default Average Area	The averaged response of all peak occurrences in the sample.
Default % CV	The coefficient of variance for each sample. The coefficient of variance is calculated as the standard deviation of the multiple samples of one level, multiplied by 100, and divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.
Default Fold	The maximum difference of the sample average response from the control average response.
Group n Average Area	The averaged response of all peak occurrences in the group. The minimum value is 1, even when the peak never occurs in the group.

Table 65. Cross Sample Peak List pane columns (Sheet 2 of 2)

Column	Description
Group n % CV	The coefficient of variance for each sample. The coefficient of variance is calculated as the standard deviation of the multiple samples of one level, multiplied by 100, and divided by the average of the multiple samples of that level. This calculation is based on the areas of all the peaks in the group of samples.
Group n Fold	The maximum difference of the average response of all samples in a group from the control average response.

Heat Map pane

Use the Heat Map pane to display the response of each peak occurrence in the batch. The Heat Map pane displays all MS Area values for all peaks in all samples in the batch that are above the peak threshold value specified in the method. When you select a peak in the Heat Map pane, the application displays the associated results for the selected peak in all panes of the Unknown Screening view.

The Heat Map pane is available only when you select the Alignment and Gap Filling option in the method (refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*) or select the RT Alignment option when you submit the batch (see Submitting a batch).

Follow these procedures:

- To use the Heat Map pane
- To use the Heat Map pane with the TIC Chromatogram pane
- To use the Heat Map pane with the XIC chromatogram pane

v To use the Heat Map pane

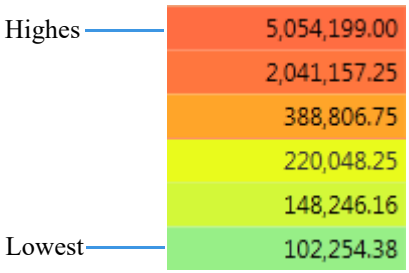
1. Click the **Heat Map** tab to display the pane.

   For detailed descriptions of all parameters in the Heat Map pane, see Heat Map pane columns.

2. In the Peak List pane, select a peak.

   The application scrolls the Heat Map pane to the specified peak and selects the peak.

   For each found peak in the batch, the application assigns a color code indicating the relative MS area value from highest (orange) to lowest (green).



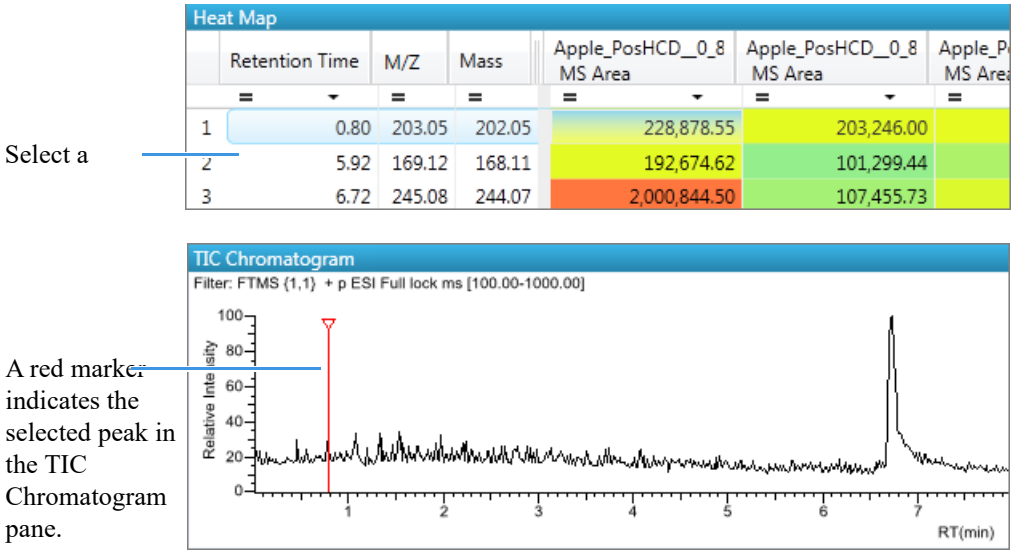
v To use the Heat Map pane with the TIC Chromatogram pane

1. Click the **TIC Chromatogram** tab to display the pane.

   The total ion current (TIC) chromatogram pane displays the relative intensity of all found peaks in the batch.

2. In the Heat Map pane, select a peak.

   The application identifies the selected peak in the TIC Chromatogram pane and indicates it with a red marker.



   Or, you can select a peak in the TIC Chromatogram pane, and the application scrolls the heat map to the selected peak.

v To use the Heat Map pane with the XIC chromatogram pane

1. Click the **XIC** tab to display the pane.

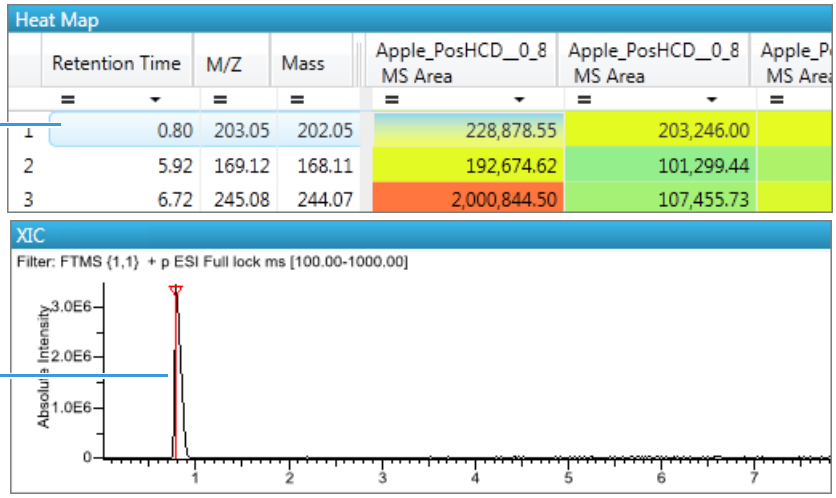
   The extracted ion chromatogram (XIC) pane displays the absolute intensity of the selected peak.

2. In the Heat Map pane, select a peak.

   The application identifies the selected peak in the XIC, scales the chromatogram's *y* axis to fit the peak, and indicates it with a red marker.

Select a

A red marker indicates the selected peak in the XIC



Or, you can select a peak in the XIC pane, and the application scales the chromatogram to fit the peak, indicates it with a red marker, and scrolls the heat map to the selected peak.

Figure 127. Heat Map pane

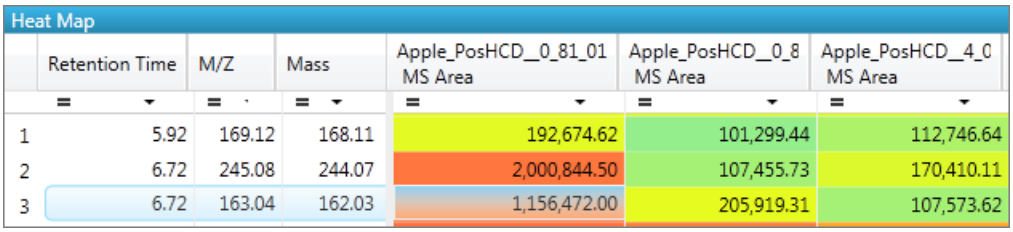


Table 66. Heat Map pane columns

Column	Description
Retention Time	The time after injection when the compound elutes. The total time that the compound is retained on the column.
M/Z	Mass-to-charge ratio found in the spectra for the peak. Assumes that the charge is 1.
Mass	The uncharged mass found in the spectra for the peak.
Sample n MS Area	The MS peak area for each sample.

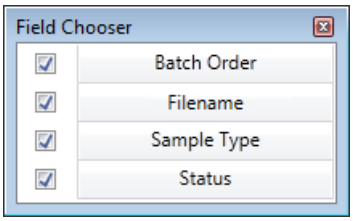
Sample List pane

Use the Sample List pane to select a sample of interest. The application displays the associated results for the selected sample in all panes of the Unknown Screening view.

v **To hide or display columnsin the Sample List pane**

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

   The Field Chooser displays all available columns of data for the Sample List pane.



2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   The application immediately displays or hides the column in the Sample List pane.

3. When you are finished modifying the column display, click to close the Field Chooser.

Figure 128. Sample List pane

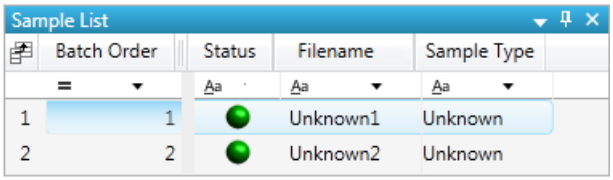


Table 67. Sample List pane columns

Column	Description
Batch Order	The order in which the samples were acquired.
Filename	A user-defined name that identifies a sample.
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, QC, or Unknown. Default: Unknown
Status	Sample is not acquired. Sample is acquired but not processed. Sample is acquired and processed. Sample is currently acquiring.

Peak List pane

Use the Peak List pane to select a specific peak found in the selected sample. The Peak List displays each peak that the application identified in the sample.

v **To display information for a peak**

In the Peak List, click anywhere in the peak row.

The application displays information for the selected peak in the other Data Review panes.

Note Do not confuse a check mark in the Selected column with the currently selected peak. The row for the current, selected peak is highlighted in blue. A selected check box in the Selected column does not indicate the current, selected peak (see Selected).

Figure 129. Peak List pane

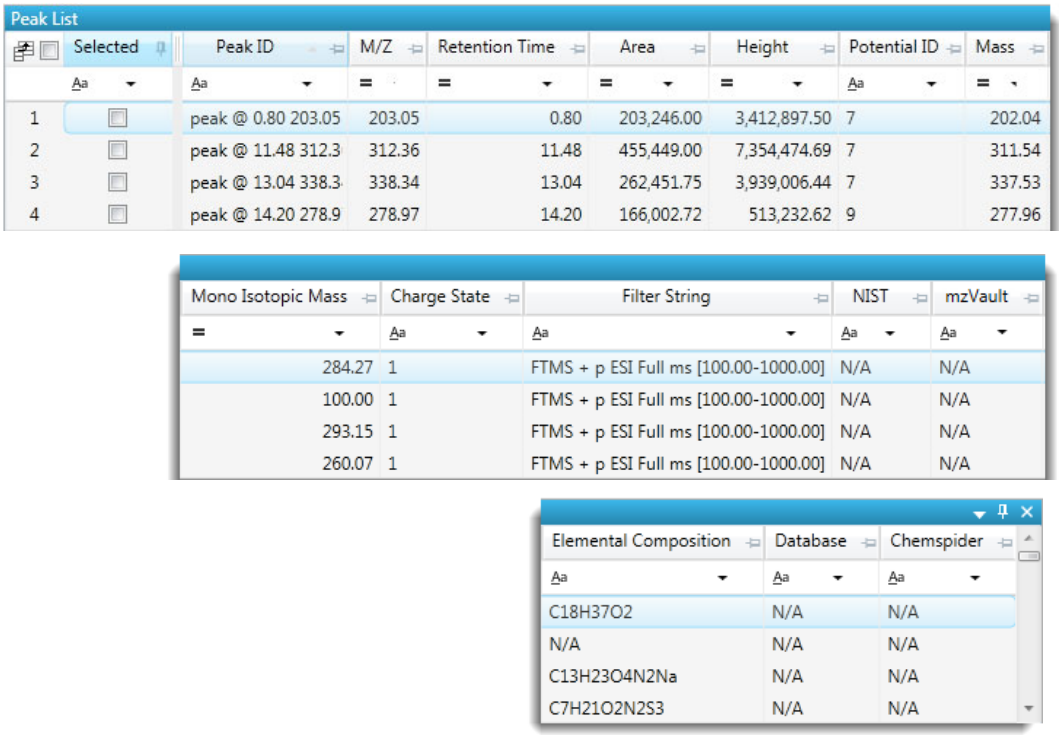


Table 68. Peak List pane columns (Sheet 1 of 2)

Column	Description
Selected	Identifies peaks to display when you select the Selected option in the XIC Overlay pane, or identifies which peaks to process when you click the Submit … for Processing icon, . Do not confuse a check mark in the Selected column with the currently selected peak. The row for the current, selected peak is highlighted in blue.
Peak ID	Identifies the peak as "peak @ *retention time m/z.*" Example: peak @ 0.80 203.05
m/z	Mass-to-charge ratio found in the spectra for the peak. Assumes the charge is 1.
Retention Time	The time after injection when the compound elutes. The total time (in minutes) that the compound is retained on the column.

Table 68. Peak List pane columns (Sheet 2 of 2)

Column	Description
Area	The area obtained by integrating peak intensities from the start to the end of the peak.
Height	The distance from the peak maximum to the peak base, measured perpendicular to the ordinate.
Potential ID	The number of returned peak IDs.
Mass	The uncharged mass found in the spectra for the peak.
Monoisotopic Mass	The sum of the masses of the most abundant isotope.
Charge State	The charge state of the ion (the *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 range: 1 through 10 Default: 1
Filter String	Filter used to identify the peak. Specified in the raw data file or the master method.
NIST	The NIST match result name for the identified peak. If there is no match or if the Library search was not specified in the method, this shows as “N/A”.
mzVault	The library match result name for the identified peak. If there is no match or if the Library Search was not specified in the method, this shows as “N/A”.
Elemental Composition	The chemical formula for the identified peak. If there is no match or the Elemental Composition search was not specified in the method, this shows as “N/A”.
Database	The compound database match result name for the identified peak. If there is no match or the Database Search was not specified in the method, this shows as “N/A”.
ChemSpider	The ChemSpider database match result name for the identified peak. If there is no match or the ChemSpider Search was not specified in the method, this shows as “N/A”.

Peak Identifications pane

Use the Peak Identifications pane to display the name and formula for identified peaks and the source of the identification.

Figure 130. Peak Identifications pane

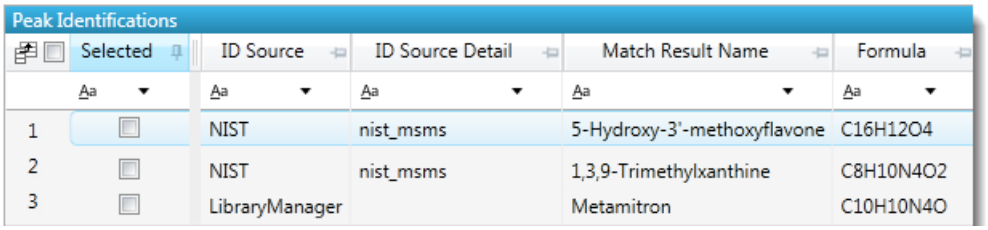


Table 69. Peak Identifications pane columns (Sheet 1 of 2)

Column	Description
Selected	Identifies peaks to display when you select the Selected option in the XIC Overlay pane, or identifies which peaks to process when you click the Submit … for Processing icon, . Do not confuse a check mark in the Selected column with the currently selected peak. The row for a currently selected peak is highlighted in blue.
ID Source	Specifies the search type used to identify the peak (Database Search, Library Search [NIST or mzVault], Elemental Composition, or ChemSpider Search). Refer to the instructions "To specify the search options" in Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*.
ID Source Detail	Specifies the name of the library, the compound database, or the ChemSpider hyperlink where the peak was identified.
Match Result Name	Specifies the compound name that was found in the library, in the compound database, or in the ChemSpider hyperlink.
Formula	Specifies the chemical formula that was found in the library, in the compound database, in the elemental composition, or in the ChemSpider hyperlink.
Isotope Pattern Score %	Specifies the percentage of matched isotopes in the total number of isotopes.
Number of Isotopes Matched	Specifies the number of isotopes matched in the calculated isotope spectra relative to the total number of isotopes used in the score calculation, in the format "x of y", where • x = the number of isotopes matching the elemental composition used for the Isotope Pattern Score calculation. • y = the total number of isotopes considered in the Isotope Pattern Score calculation. This is the number of isotope peaks expected to be above the spectral noise.

Table 69. Peak Identifications pane columns (Sheet 2 of 2)

Column	Description
Score	Specifies the score from the library fit. When the application finds a match in the library, in the compound database, or through the ChemSpider hyperlink, this column displays the highest score associated with the Match Result Name parameter. Valid range: 1 through 100%
SI/Dot Product	Specifies the search index method used to search the NIST library.
RSI/Rev Product	(Reverse search index) Specifies the method used to search the NIST library. A reverse search compares a library entry to an unknown compound (whereas a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
Library Probability Percent	Specifies the probability ranking from the NIST library. When you use a reverse search, this value is "N/A".
Fragments	Specifies the number of fragments matched in the calculated spectra relative to the total number of expected fragments.

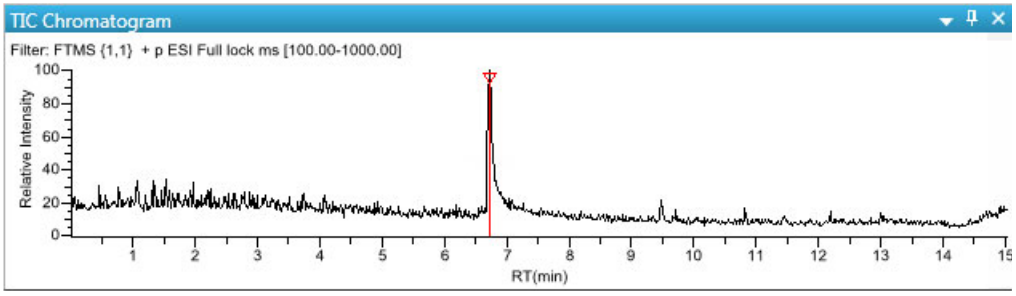
TIC Chromatogram pane

Use the TIC Chromatogram pane to display the relative intensity of a trace along the length of the sample data retention window.

v **To focus on a specific peak**

In the TIC Chromatogram pane, click any displayed peak.

The application indicates the selected peak with a red, vertical marker and updates the focus in the other Data Review panes with data for that peak.



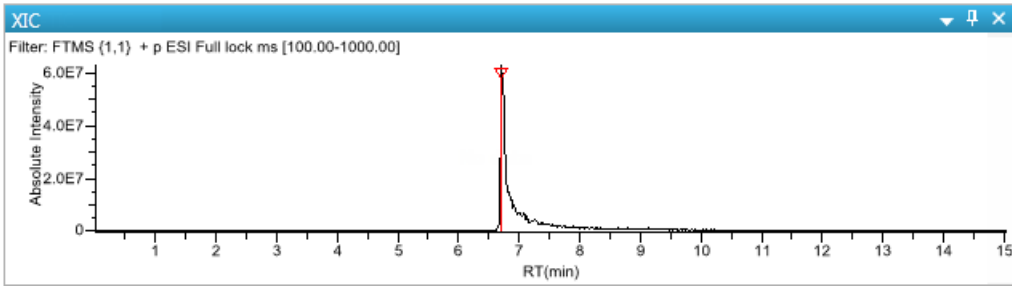
XIC pane

Use the XIC pane to display the absolute intensity of an extracted trace along the length of the sample data retention window.

v **To focus on a specific peak**

In the XIC pane, click any displayed peak.

The application indicates the selected peak with a red, vertical marker and updates the focus in the other Data Review panes with data for that peak.



XIC Overlay pane

Use the XIC Overlay pane to view specific groups of peaks. You can choose to view all peaks, selected peaks only, or the top 20 most intense peaks (by area). The XIC Overlay plot is a collection of overlaid, extracted *m/z* ion plots that use a different color for each peak.

Follow these procedures:

- To display all peaks in a sample
- To display only selected peaks in a sample
- To display the top 20 peaks in a sample
- To focus on a specific peak

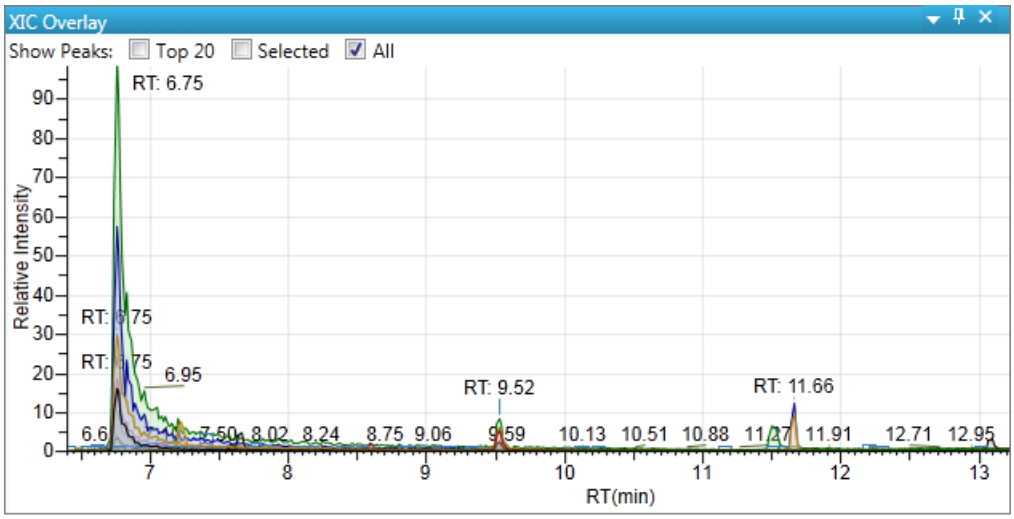
v **To display all peaks in a sample**

1. In the Sample List pane, select the sample whose peaks you want to view.
2. In the XIC Overlay pane, select the **All** check box.

   The application displays all the peaks in the selected sample. See XIC Overlay plot showing all peaks.

Note If there are more than 1000 peaks in the sample, performance might be slow.

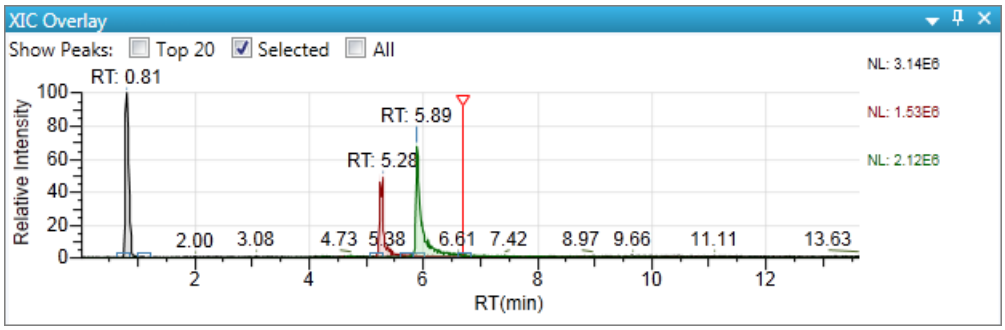
Figure 131. XIC Overlay plot showing all peaks



v **To display only selected peaks in a sample**

1. In the Sample List pane, select the sample whose peaks you want to view.
2. In the Peak List pane, select the **Selected** check box for each peak that you want to view.
3. In the XIC Overlay pane, select the **Selected** option.

   The application displays all selected peaks.

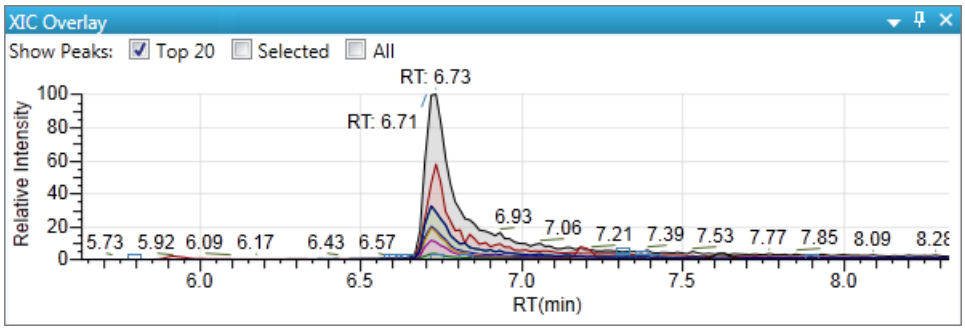


v To display the top 20 peaks in a sample

1. In the Sample List pane, select the sample whose peaks you want to view.
2. In the XIC Overlay pane, select the **Top 20** check box.

   The application displays the top 20 peaks in the selected sample.

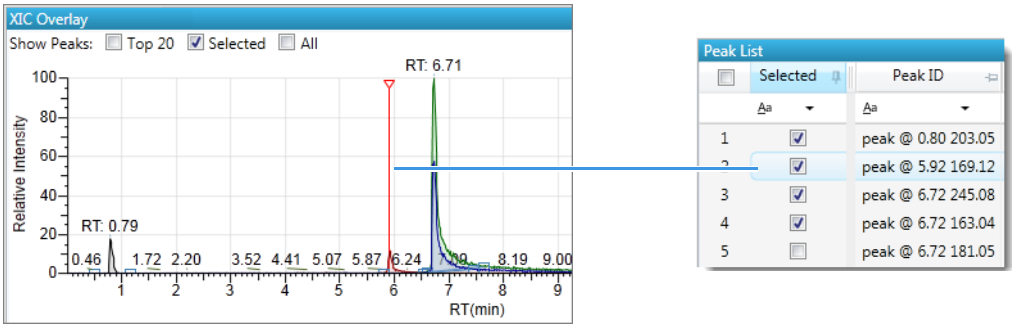
   Figure 132. XIC Overlay plot showing the top 20 peaks



v To focus on a specific peak

- In the XIC Overlay pane, click any displayed peak.

  The application indicates the selected peak with a red, vertical marker and updates the focus in the other Data Review panes with data for that peak.



Group Averages pane

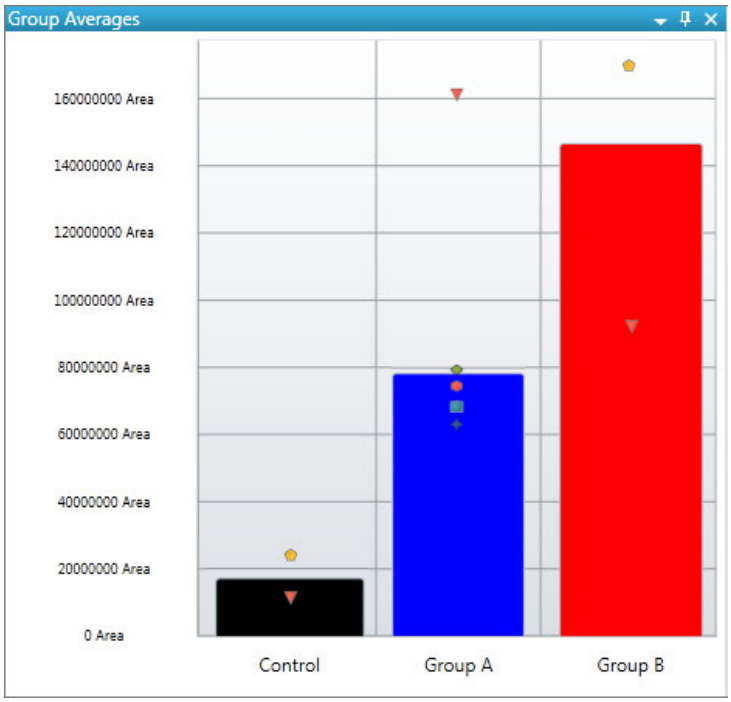
Use the Group Averages pane to compare the peak areas of different samples to a control group of samples.

The Group Averages pane is available only when you select the Alignment and Gap Filling option in the method (refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*) or select the RT Alignment option when you submit the batch (see Submitting a batch).

The control group is displayed to the left, and other samples and groups are listed in the order in which they appear in the Batch View. To specify a group as the control group, see Groups.

Each group displays a colored bar that indicates the average response of the group, as displayed in the Average Area column in the Cross Sample Peak List pane. The color of the bar matches the colors assigned to the samples and peaks in the Cross Sample Peak Overlay pane.

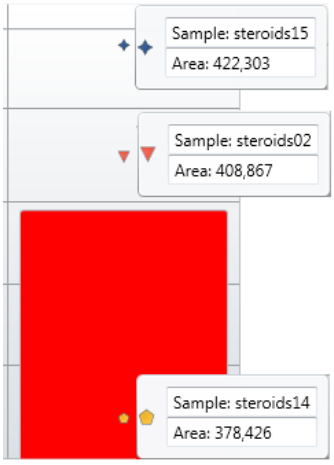
Figure 133. Group Averages pane



Display areas for each sample in the batch

- Point to an indicator icon (,).

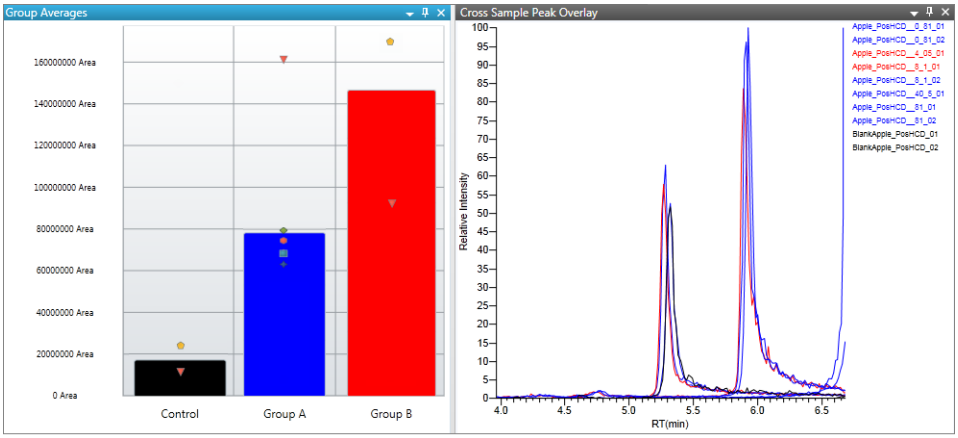
  The application displays the area for the selected compound in each represented sample.



Use the Group Averages pane with the Cross Sample Peak Overlay pane

- Display both the Group Averages pane and the Cross Sample Peak Overlay pane.

  The color of the bars in the Group Averages pane matches the colors assigned to the group samples and peaks in the Cross Sample Peak Overlay pane.



Peak Chromatogram pane

Use the Peak Chromatogram pane to display the selected chromatogram peak. The pane initially displays only the apex scan for the detected peak. You can manually integrate the peak and use the updated peak to generate reports.

Follow these procedures:

- To zoom in on a peak
- To remove a peak
- To customize the labels in the display
- To display surrounding apex times
- To manually integrate a peak
- To switch between method, manual, and user integration modes

v 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**.

v To remove a peak

Right-click the Peak Chromatogram pane, and choose **Delete Peak**.

The application removes the peak displayed in the Peak Chromatogram pane. All data for this peak are removed from the Unknown Screening View panes.

v To customize the labels in the display

1. Right-click the Peak Chromatogram pane, and choose **Peak Display Settings**.

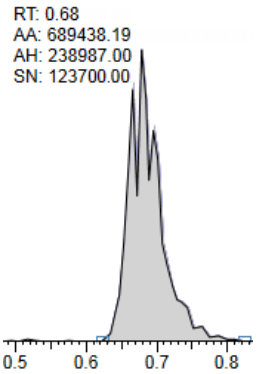
   The Peak Display Settings dialog box opens.

2. To display labels for the peak retention time (RT), mass height (MH), mass area (MA), or signal-to-noise (SN), select the appropriate check box.

3. Click **OK** in the Peak Settings dialog box.

   The chromatogram plot displays the selected labels.

   Figure 134. Example of displayed labels



v To display surrounding apex times

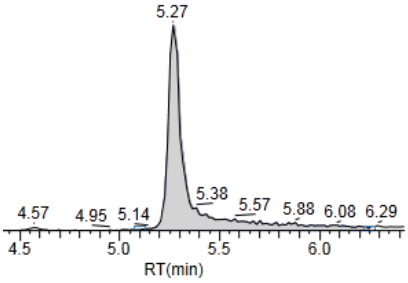
1. Right-click the Peak Chromatogram pane, and choose **Peak Display Settings**.

   The Peak Display Settings dialog box opens.

2. Select the **Show All Apex Times** check box.

3. Click **OK** in the Peak Settings dialog box.

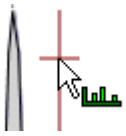
   Figure 135. Example of displayed apex times



v To manually integrate a peak

1. Right-click the Peak Chromatogram pane and then choose **Swipe Manual Integration**, or click the **Swipe Manual Integration** icon, .

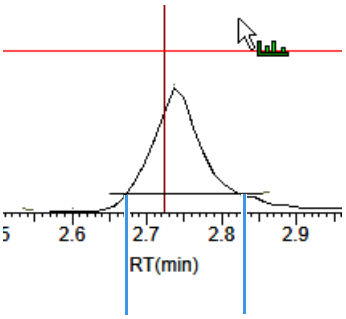
   The cursor changes to indicate the manual integration mode.



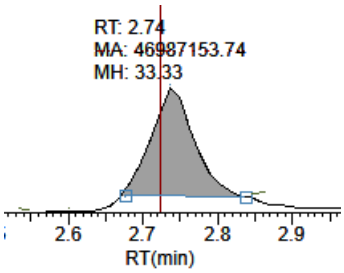
2. Drag the cursor to define the beginning and ending base points for the new peak.

   Note You must drag the cursor inside the *x* axis and *y* axis.

   Figure 136. Manually integrated peak



Drag the cursor across the peak at the base points for the



The application identifies the peak and indicates the manual integration in the

   The application updates the area of the peak to the baseline that you just added. When you regenerate the reports, they display the manually modified data.

3. To return to the original peak as defined by the method, right-click and choose **Toggle Integration Mode > Method**.

v To switch between method, manual, and user integration modes

Right-click the Peak Chromatogram pane and choose **Toggle Integration Mode > Method/Manual/User**.

Initially, the method integration and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the Peak Chromatogram plots update and the result set updates as you switch between modes.

As you switch between modes, each pane reflects the changes. The generated reports for these data identify any manual modifications.

Peak Chromatogram pane

Use the Peak Chromatogram pane to display the selected chromatogram peak.

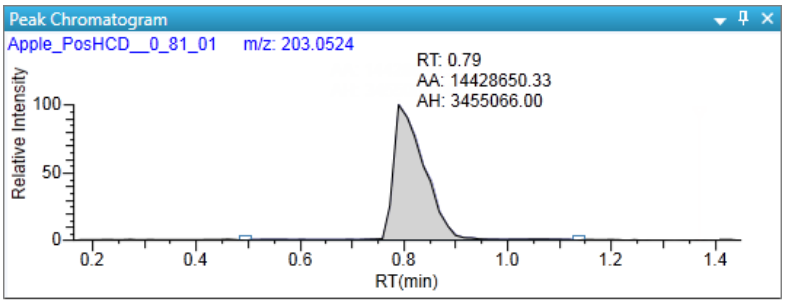


Table 70. Peak Chromatogram pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Swipe Manual Integration	Switches to manual integration mode, where you can manually define the peak. Also available from the icon in the upper right corner, .
Toggle Integration Mode (Manual or Method)	Switches the display between manual and method integration modes. You can edit the local method peak detection settings from the Peak Detection Settings menu. You can manually edit a peak with the Swipe Manual Integration command.
Delete Peak	Removes the peak and all data for this peak from the Unknown Screening View panes. Also available from the icon in the upper right corner, .
Peak Display Settings	Opens the Peak Display Settings dialog box.
Peak Detection Settings	Edit User 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. The changes that you make on the Signal page in the Peak Detection Settings dialog box can affect all quantification and ion ratio calculations and are not auto-reversible. These changes can also create a mismatch with calibration files that are not fully defined in the batch.

Peak Display Settings dialog box

Use the Peak Display Settings dialog box to customize the display settings.

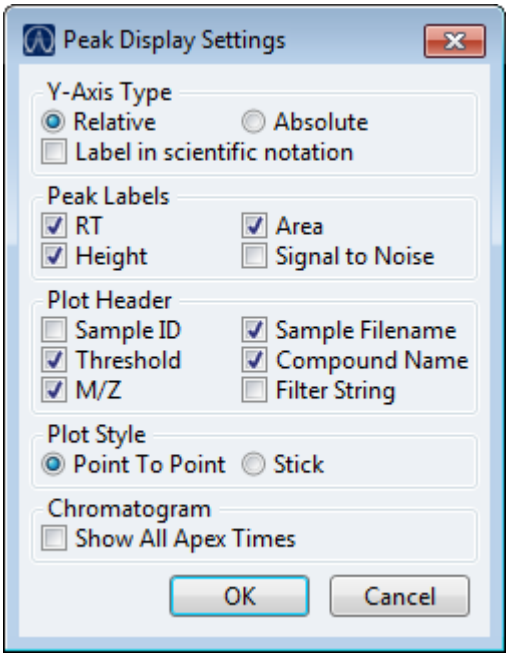
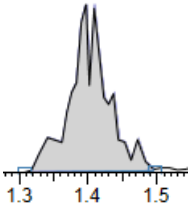
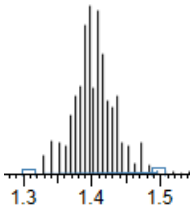


Table 71. Peak Display Settings dialog box parameters (Sheet 1 of 2)

Command	Description
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.
Peak Labels	
RT	Displays the retention time (RT) label in the peak chromatogram pane.
Height	Displays the peak height (AH) label in the peak chromatogram pane.
Area	Displays the peak area (AA) label in the peak chromatogram pane.
Signal to Noise	Displays the signal-to-noise (SN) label in the peak chromatogram pane.
Plot Header	
Sample ID	Displays a user-defined, alphanumeric string that identifies a sample.
Threshold	Displays the peak threshold.

Table 71. Peak Display Settings dialog box parameters (Sheet 2 of 2)

Command	Description
m/z	Displays the mass-to-charge ratio found in the spectra for the peak. Assumes the charge is 1.
Sample Filename	Displays the name of the current, selected sample where the peak was found.
Compound Name	Displays the compound name match in the library or compound database.
Filter String	Displays the filter used to identify the peak. Specified in the raw data file or the master method.
Plot Style	
Point To Point	Displays chromatograms in the following format: 
Stick	Displays chromatograms in the following format: 
Chromatogram	
Show All Apex Times	Displays all surrounding apex times in the plot.

Cross Sample Peak Overlay pane

Use the Cross Sample Peak Overlay pane to compare instances of a selected peak across all samples in the batch. The application overlays all occurrences of the peak in the batch.

The application displays the names of all samples in the batch where the selected peak is found. Samples that are assigned to groups are color coded, and the peaks found in those samples are color coded in the plot. To assign samples to groups, see Groups.

The retention time window displayed in the Cross Sample Peak Overlay pane is the RT window that you specified in the method.

Follow these procedures:

- To select the peak to display in the Cross Sample Peak Overlay pane
- To zoom in on a peak
- To use the Cross Sample Peak Overlay pane with the Group Averages pane

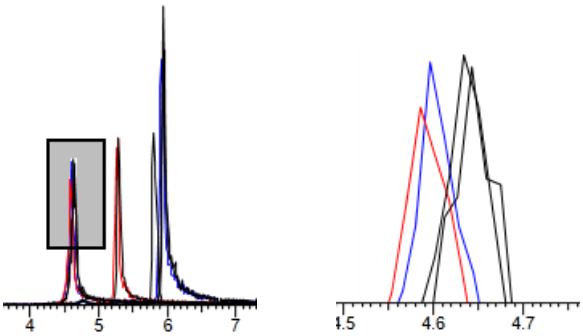
v **To select the peak to display in the Cross Sample Peak Overlay pane**

Select a peak in either the Peak List pane or the Cross Sample Peak List pane.

v **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.

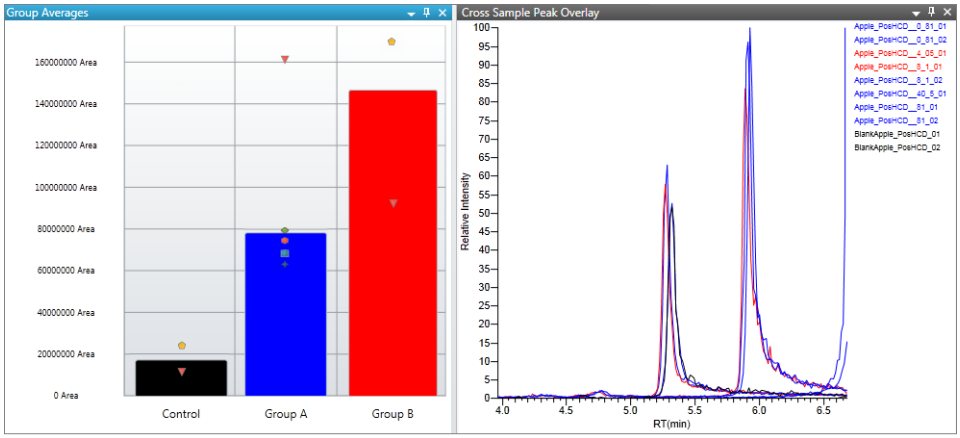


2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling**.

v **To use the Cross Sample Peak Overlay pane with the Group Averages pane**

Display both the Cross Sample Peak Overlay pane and the Group Averages pane.

The color of the bars in the Group Averages pane matches the colors assigned to the group samples and peaks in the Cross Sample Peak Overlay pane.



Cross Sample Peak Overlay pane

Use the Cross Sample Peak Overlay pane to compare instances of a selected peak across all samples in the batch.

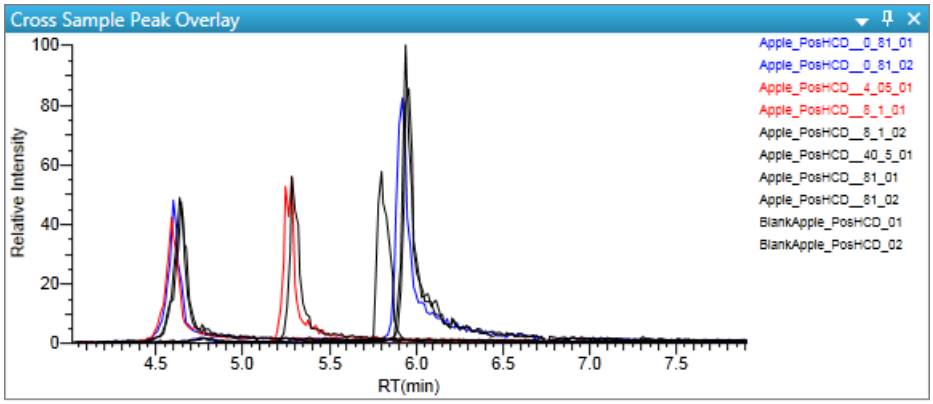


Table 72. Cross Sample Peak Overlay pane shortcut menu commands

Column	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Library Search pane

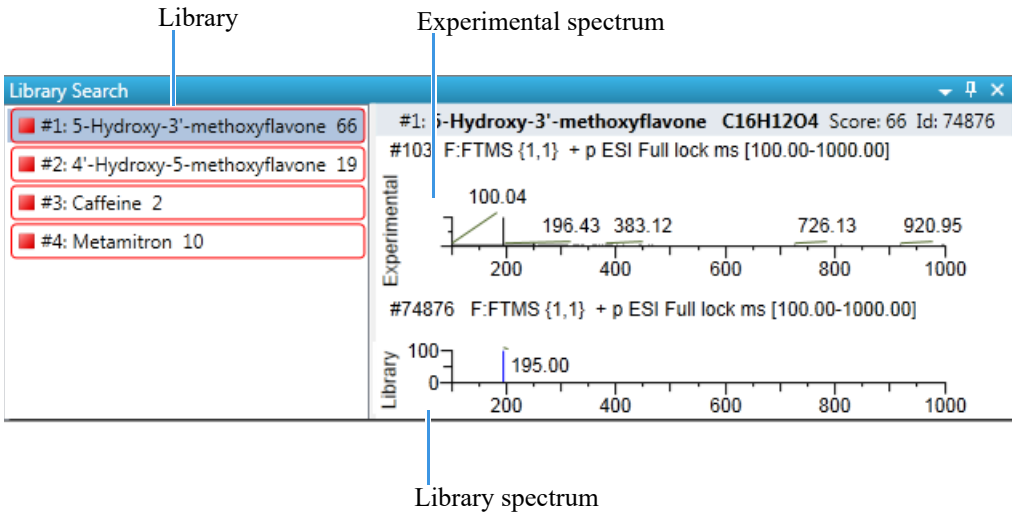
The Library Search pane displays the best library matches for the selected peak, with the highest score listed first.

Follow these procedures:

- To view the spectrum for a library match
- To display the difference between experimental and library spectra

v **To view the spectrum for a library match**

- In the Library Search pane, select a library entry.

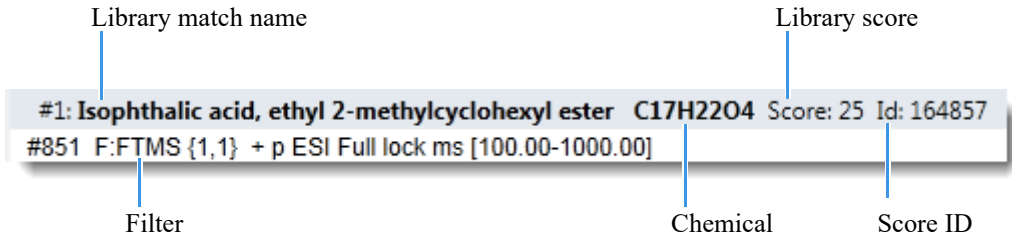


The Experimental plot displays the measured spectra for the selected compound. Library matches are colored red.

The Library plot displays the expected spectra in the library. Library matches are colored blue.

The spectra header displays the following:

- The library match name
- The chemical formula for the peak
- The score from the library fit when the library type is mzVault or NIST
- SI and RSI when the library type is NIST
- Dot Prod or Rev Dot Prod when the library is HRAM
- Molecular weight when the library type is NIST
- The ID record from the library when the library type is mzVault or NIST
- The scan number and scan filter when either is present in the library

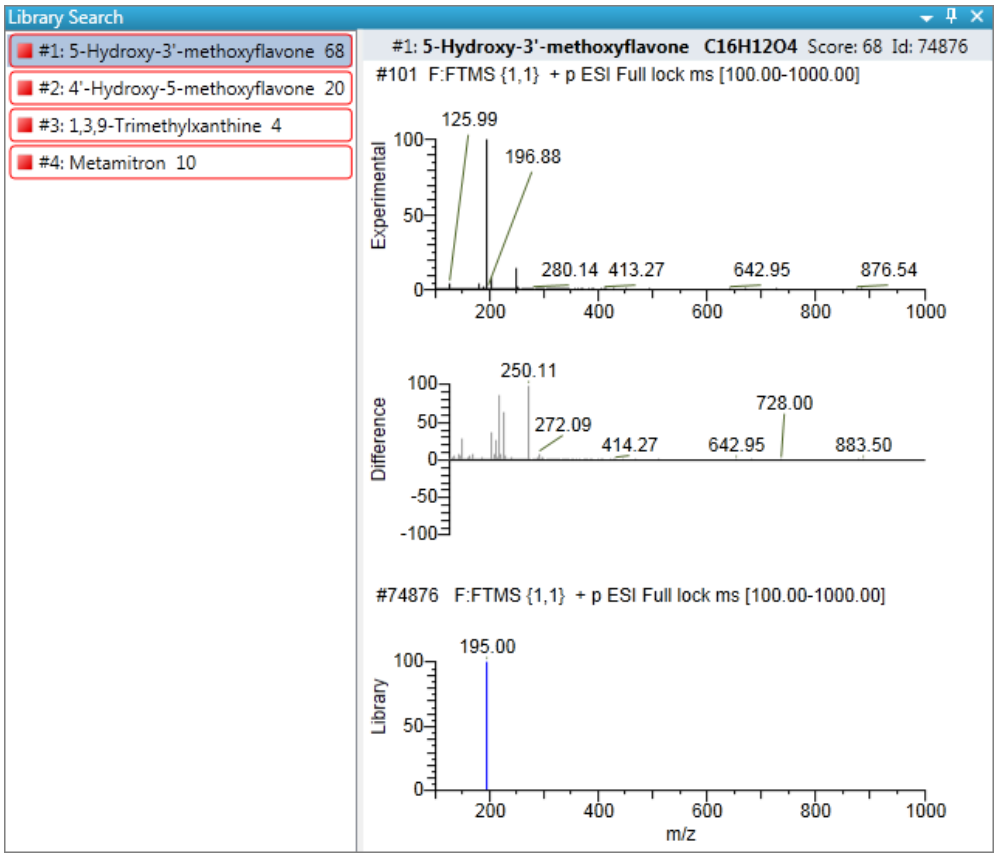


v To display the difference between experimental and library spectra

1. Right-click the spectrum plot and choose **Show Difference Plot**.

   The application displays the Experimental and Library plots and a Difference plot that shows the difference between the experimental and library spectra. When you read a difference plot, the match between the experimental and library spectra is better when fewer peaks appear.

   Figure 137. Library Search pane showing a Difference plot



2. To specify how the difference plot displays the mass tolerance, do the following:
   a. Right-click the spectrum plot and choose **Set Difference Plot Mass Tolerance.**
   b. In the dialog box that opens, select either **MMU** or **PPM** as the unit of measure.

      The default value is the tolerance set in the NIST library or mzVault library.
   c. Type a mass tolerance value.
   d. Click **OK**.

Note This command is available only when you display the difference plot.

Library Search pane

Use the Library Search pane to display the best library matches for the selected peak.

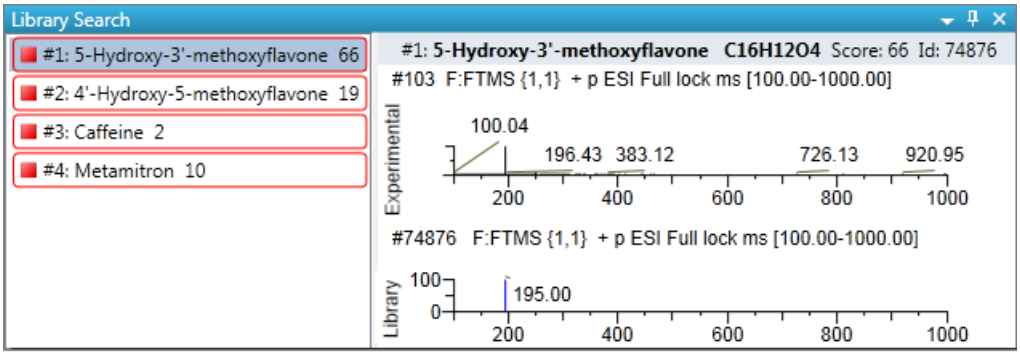
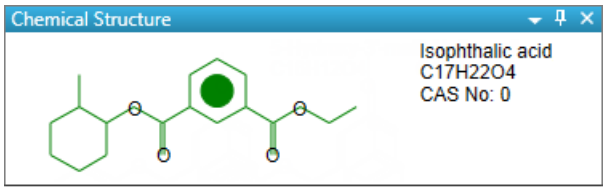


Table 73. Library Search pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra Display Stack Spectra	Overlays the two spectrum displays, or stacks the Experimental and Library spectra. When you display the Difference plot, this spectrum also displays the Difference spectrum.
Show/Hide Difference Plot	Displays or hides the Difference spectrum plot.
Set Difference Plot Mass Tolerance	Opens a dialog box where you specify the mass tolerance in either MMU or PPM units. Available only when you display the Difference Plot.

Chemical Structure pane

Use the Chemical Structure pane to view the chemical formula and structure for the peak that is currently selected in the Peak List pane.



The application displays the chemical formula (and CAS number when available) that was found in the search database that you specified in the method. Refer to Chapter 6, “Using the Method Development Mode for Unknown Screening Methods,” in the *TraceFinder Lab Director User Guide*.

Fragments pane

The Fragments pane displays the maximum number of fragments as specified in the unknown screening method. Refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*.

When a compound database search returns a match for a peak that has fragments, the Fragments pane displays the theoretical fragments.

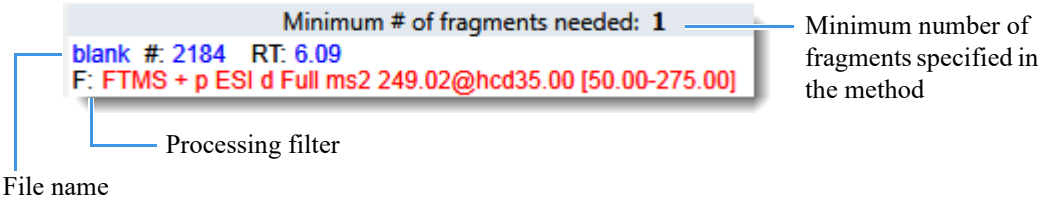
When the data has an MS/MS element that is identified as belonging to the chromatographic peak, the Fragments pane displays the fragments found in the MS/MS scan.

The Fragments pane displays the fragments in one of two ways:

- All Fragments
- Individual fragments

All Fragments

The All Fragments view displays a composite of all fragments found in the peak. The application displays the following headers, red indicating the measured peak and blue indicating the expected peak.



You can display the fragments as either stacked spectra or overlaid spectra.

Figure 138. Fragments pane with stacked spectra for all fragments

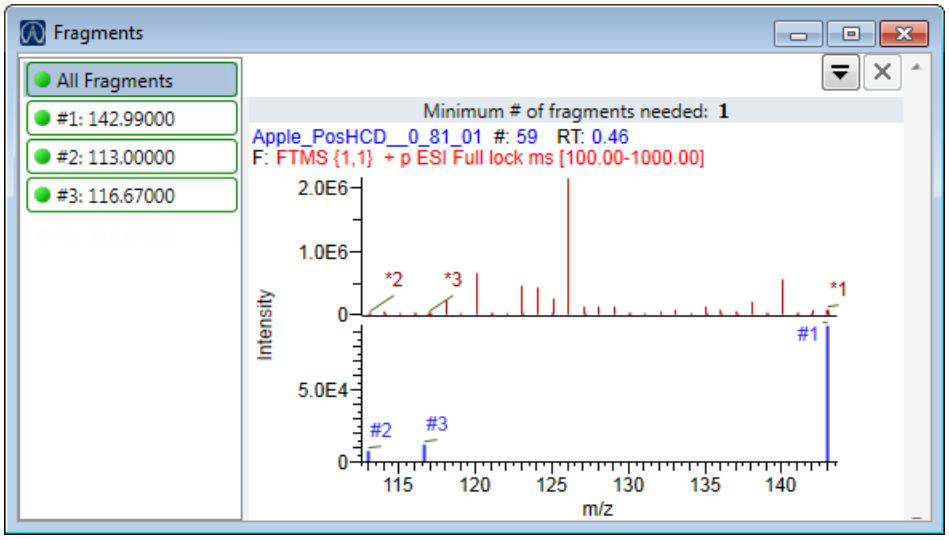
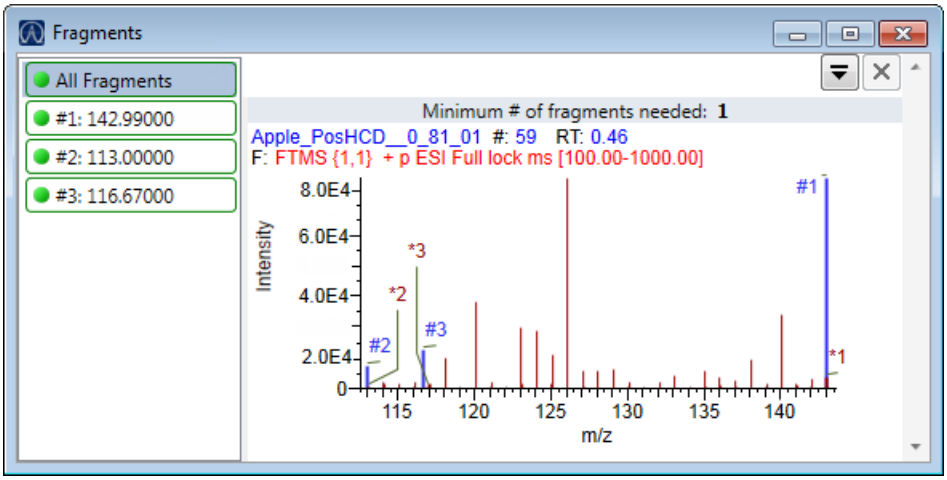
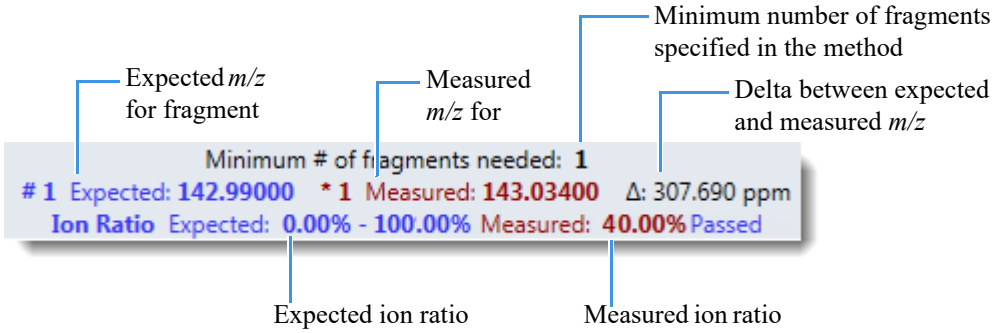


Figure 139. Fragments pane with overlaid spectra for all fragments



Individual fragments

The individual fragments view displays the expected and measured peaks for a single fragment. These are the headers for the individual fragments view.



You can display each fragment as either stacked spectra or overlaid spectra.

Figure 140. Fragments pane with stacked spectra for a single fragment

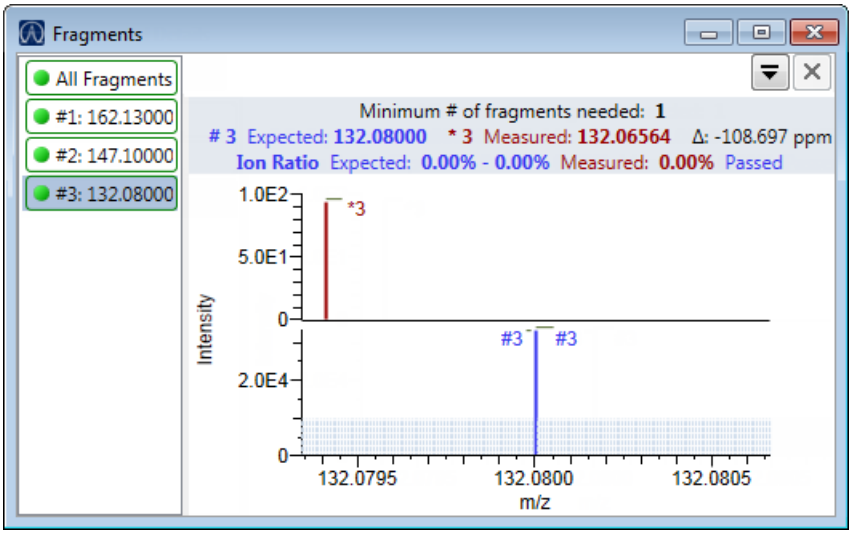
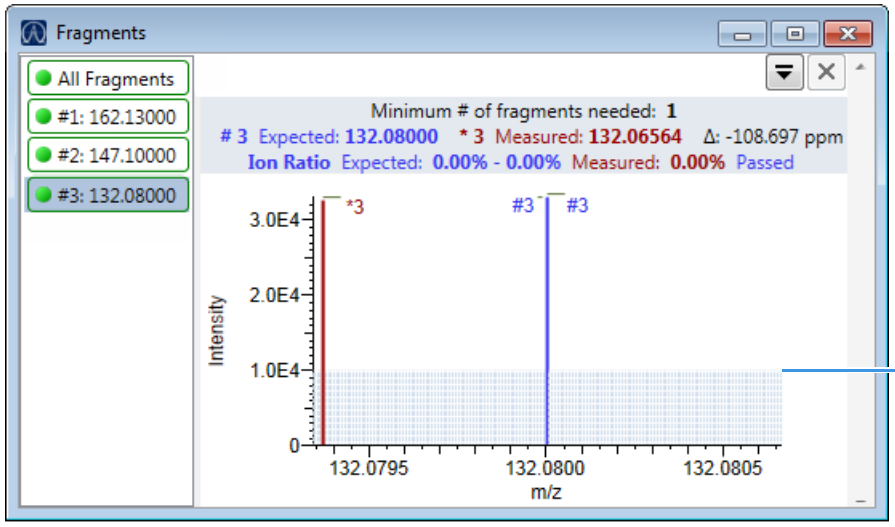


Figure 141. Fragments pane with overlaid spectra for a single fragment



Isotopes pane

The Isotopes pane displays isotopic pattern results for all adducts of a compound according to the threshold and deviation parameters defined in the unknown method.

To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

- An isotope peak is not found if its intensity, relative to the monoisotopic ion's intensity, is more than the specified intensity deviation percentage away from the theoretical relative intensity of the isotope ion.
- An isotope peak is found if its measured *m/z* is less than the specified mass deviation amount away from its expected *m/z*.

To specify the peak threshold and deviation parameters, refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*.

The Isotopes pane displays the isotopes in one of three ways:

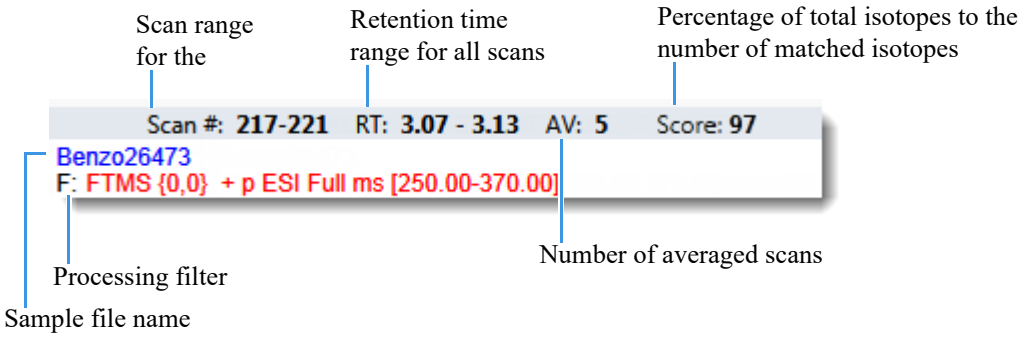
- All Isotopes
- Multi-Isotopes
- Individual isotopes

All isotopes panes use a shortcut menu so that you can specify how to display the data. See Isotopes pane shortcut menu commands.

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; it displays the expected peak as a dashed blue line.

The application displays these headers for the All Isotopes view:



You can display the isotopes as either stacked spectra or overlaid spectra.

Figure 142. Isotopes pane with stacked spectra for all isotopes

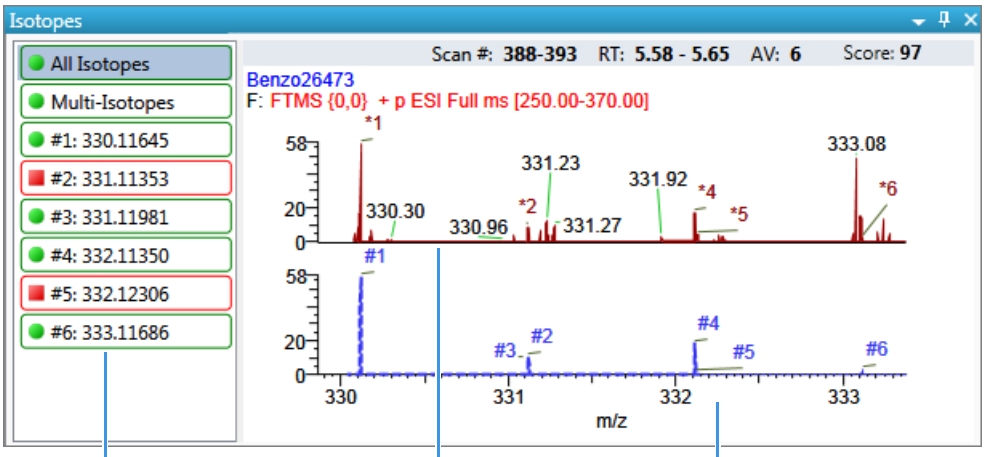
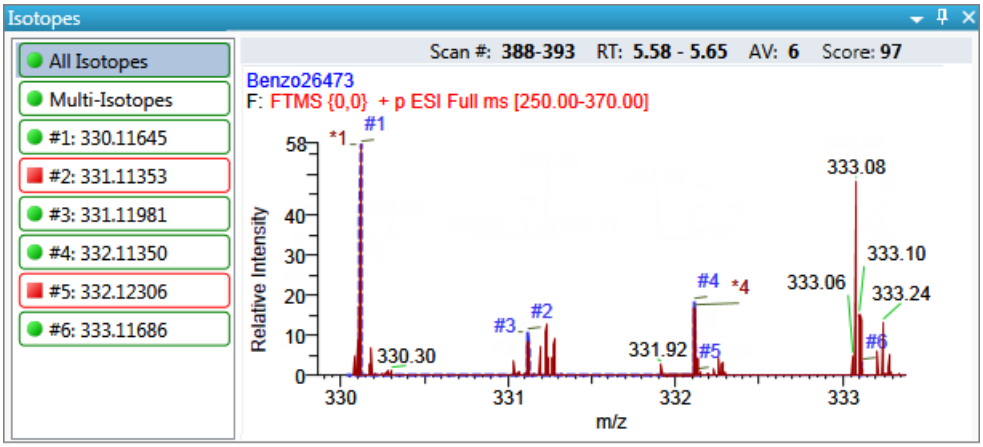


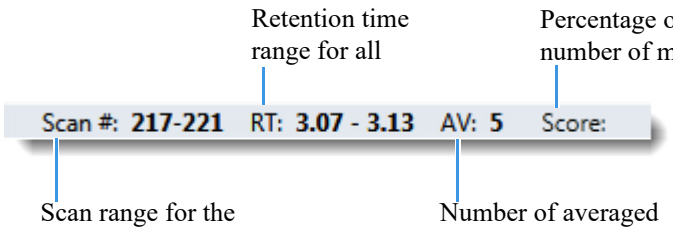
Figure 143. Isotopes pane with overlaid spectra for all isotopes



Multi-Isotopes

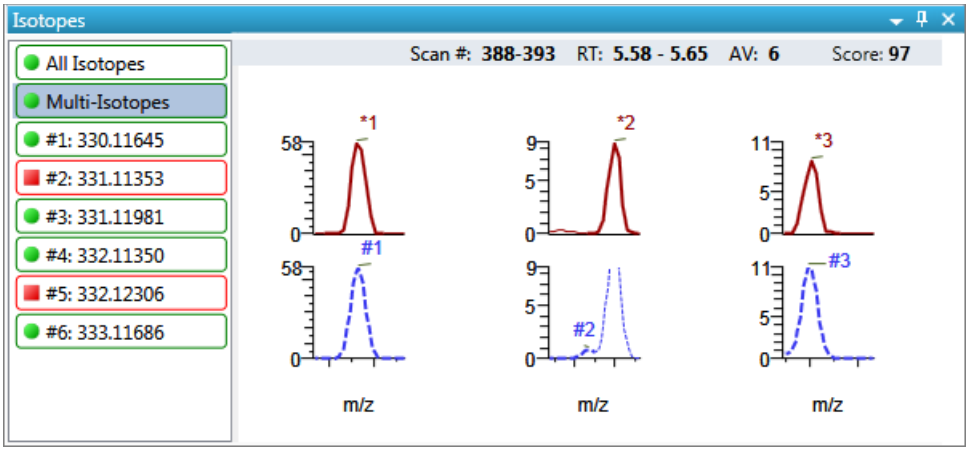
The Multi-Isotopes view displays individual plots for each isotope.

The application displays these headers for the Multi-Isotopes view:



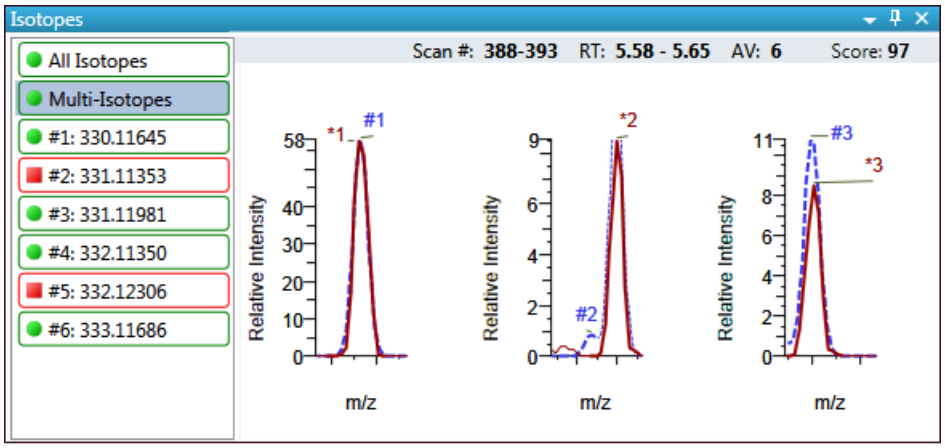
You can display the isotopes as stacked spectra, overlaid spectra, or both stacked and overlaid spectra.

Figure 144. Isotopes pane with stacked spectra for multi-isotopes



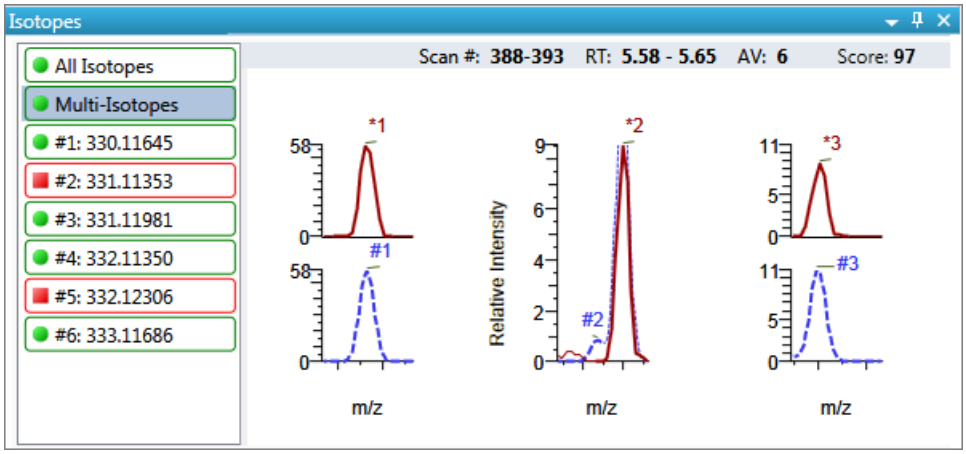
Expected spectrum in blue Measured spectrum in red

Figure 145. Isotopes pane with overlaid spectra for multi-isotopes



Expected spectrum in blue Measured spectrum in red

Figure 146. Isotopes pane with stacked and overlaid spectra for multi-isotopes

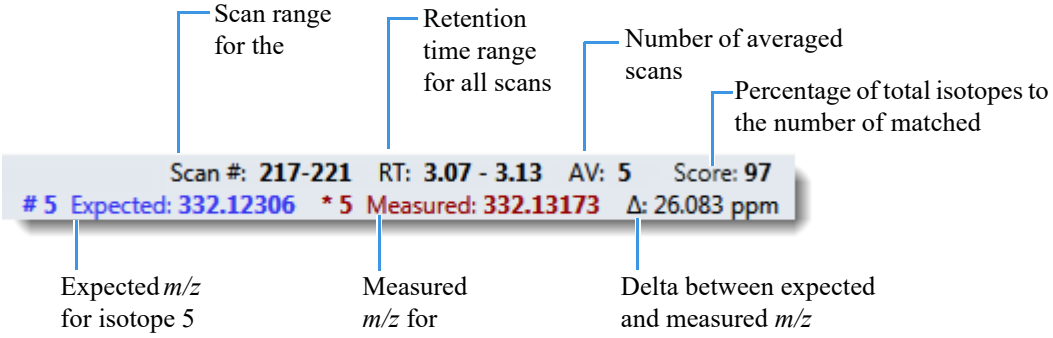


Expected spectrum in blue Measured spectrum in red

Individual isotopes

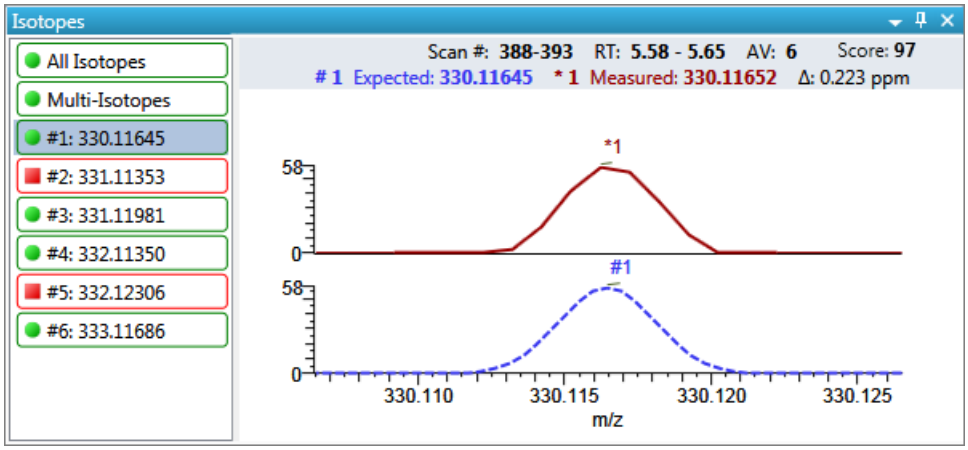
The individual isotopes view displays the expected and measured peaks for a single isotope.

The application displays these headers for the individual isotopes view:



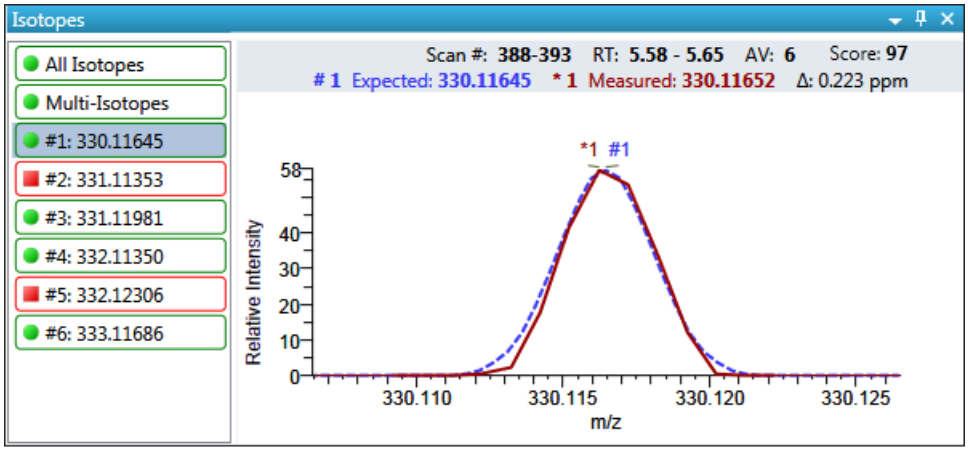
You can display the isotopes as either stacked spectra or overlaid spectra.

Figure 147. Isotopes pane with stacked spectra for a single isotope



Expected spectrum in blue Measured spectrum in red

Figure 148. Isotopes pane with overlaid spectra for a single isotope



Expected spectrum in blue Measured spectrum in red

Table 74. Isotopes pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Show/Hide Noise Label	Adds a noise label to each peak. Expected isotope peaks (displayed in blue) do not display a noise label.
Show/Hide Resolution Label	Adds a resolution label to each peak. Expected isotope peaks (displayed in blue) do not display a resolution label.

Spectrum pane

When data is available, the spectrum plot width is the full mass range in the raw data file. Otherwise, the application scales the width to the scan range.

Figure 149. Spectrum pane

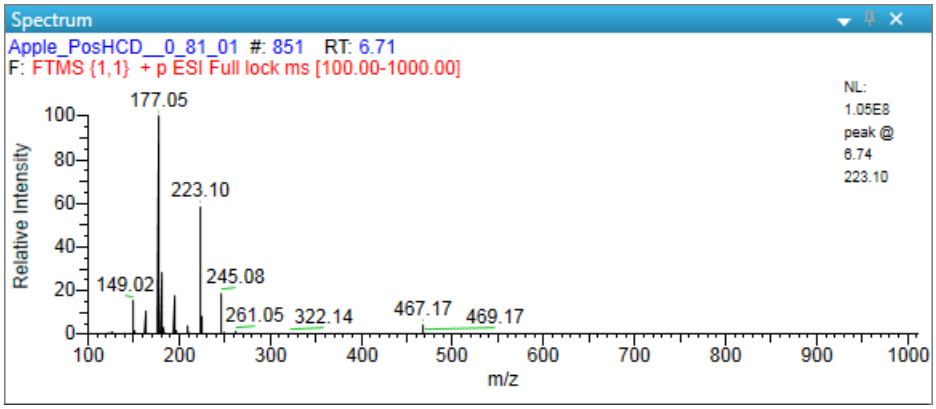


Table 75. Spectrum pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Working in the Report View for unknown screening batches

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 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

v To open the Report View

- Click **Report View** in the navigation pane.

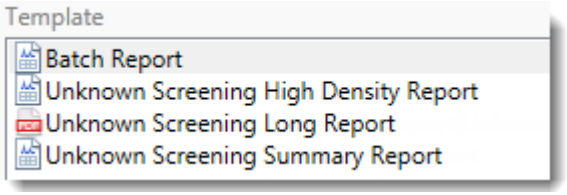
The application opens the Report View.

v 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. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

   Figure 150. Example template list for unknown screening batches



2. Click Preview.

   The application opens the Report Designer, showing the report information for the current batch in the selected report template format.

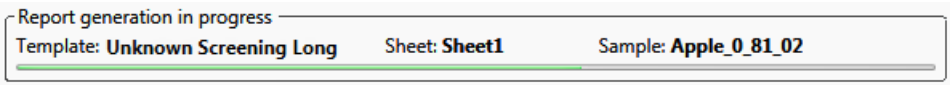
   For details about using the Report Designer, see Chapter 7, "Using the Report Designer."

v To generate a report as a PDF, an Excel, or a CSV file

1. In the Template pane, select a report template.
2. Select the check box for each of the file types that you want to create: **PDF**, **Excel**, or **CSV**.
3. Click Generate.

   The application does the following:

   - Displays a green progress bar as it generates the reports.

   - Creates a report for the current batch as a PDF, an Excel, or a CSV file, using the selected report template format.
   - Adds information about the generated report to the Generated Reports pane.

     For details about the Generated Reports pane, see Report View.
   - Saves the report files to the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

v To print a report

1. In the Template pane, select a report template.
2. Select the check box for the **Print** file format.
3. Click Generate.

   The application does the following:

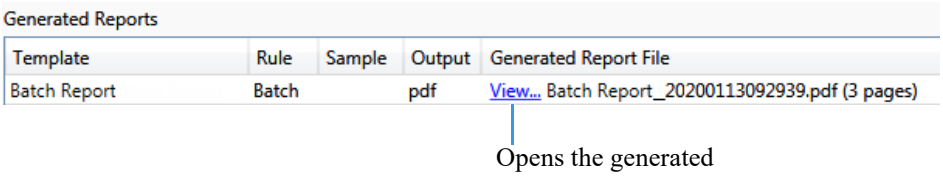
   - Creates a report for the current batch using the selected report template format.
   - Prints the report to your default printer.
   - Adds information about the generated report to the Generated Reports pane.

     For details about the Generated Reports pane, see Report View.
   - Saves the report files to the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

v To display a generated report

- In the Generated Reports pane, click **View** for the report that you want to see.

  Figure 151. Generated Reports pane showing a PDF report

  The application opens the output file.

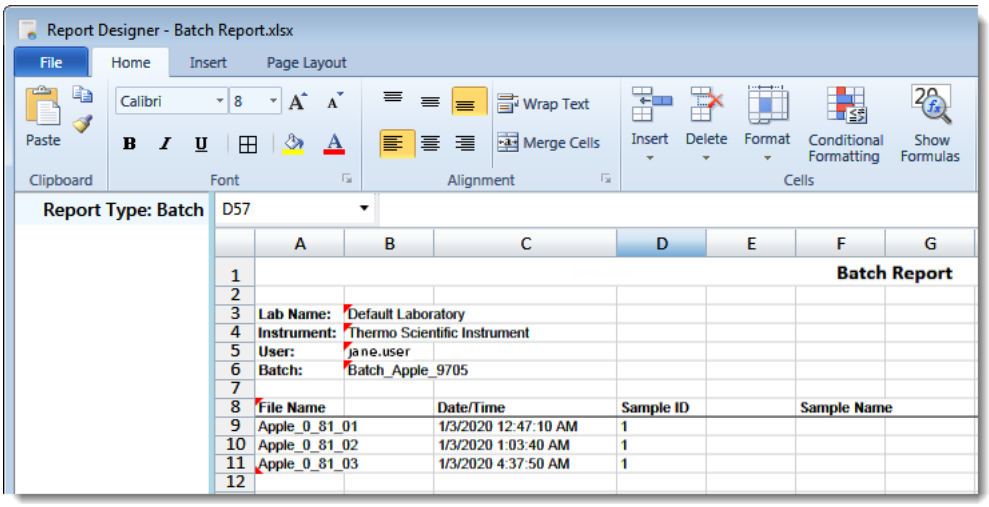
v To edit a report template

You cannot edit report templates that were provided with the TraceFinder application; however, you can open a TraceFinder template, make changes, and save it to a new template name.

1. In the Template pane, select a report template.
2. Click Open.

   The application opens the Report Designer showing the template in an Excel spreadsheet.

   Figure 152. Report Designer showing the template for the selected report



3. Use the features in the Report Designer to edit the template.

   See Chapter 7, "Using the Report Designer."

4. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

v To create a new report template

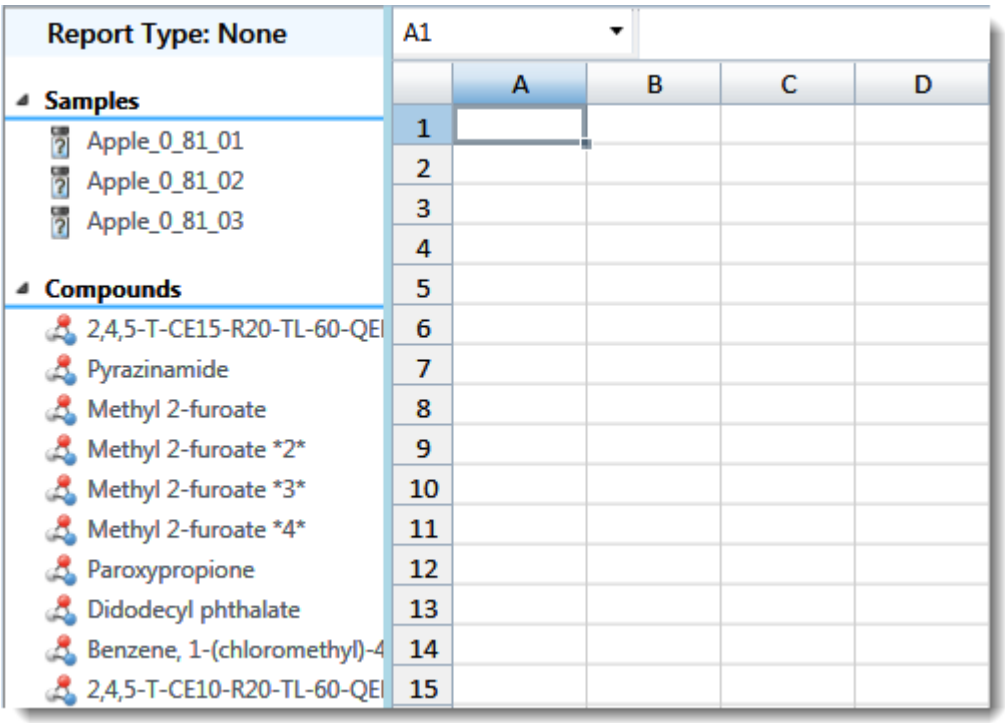
1. Click New.

   The application opens the Report Designer showing an empty template in an Excel spreadsheet. See Report Designer showing a new, empty template.

   The Report Type is None.

   In the left pane, the spreadsheet lists all samples in the current batch and all compounds in the method used for the batch.

Figure 153. Report Designer showing a new, empty template



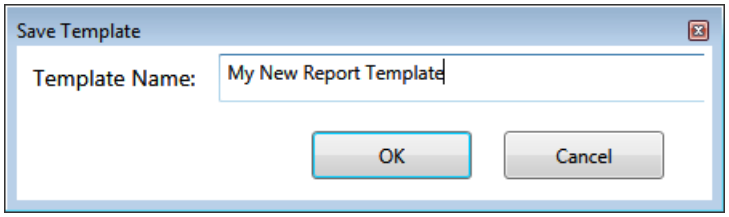
2. Use the features in the Report Designer to create the report template.

   See Chapter 7, "Using the Report Designer."

3. When you finish your changes, choose **File > Save** from the Report Designer menu bar.

   The Save Template dialog box opens.

   Figure 154. 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 155. Report View

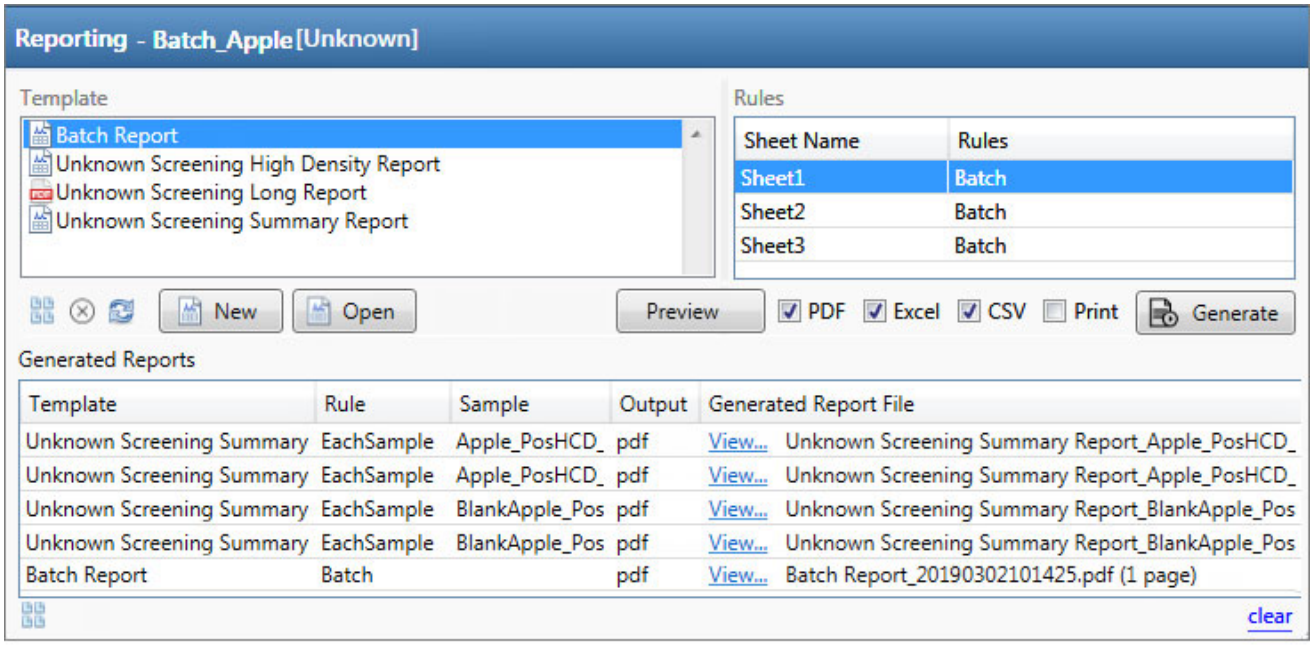


Table 76. Report View parameters (Sheet 1 of 2)

Parameter	Description
Template	
	Displays all available unknown screening report templates.
Rules	
Sheet Name	Specifies each sheet in the report.
Rules	Specifies the type of data used in each sheet in the selected report. • Batch • EachSample • SampleType: *SampleType* • CompoundType: *CompoundType* • SampleCustomFormula:
Buttons	
View Report Templates	Displays the …\TraceFinderData\Templates\ReportTemplates folder that contains all report templates.
Open	Opens the selected report template in the Report Designer.
New	Opens a blank report template in the Report Designer.

Table 76. Report View parameters (Sheet 2 of 2)

Parameter	Description
Preview	Opens the Report Designer showing the report information for the current batch in the selected report template format.
PDF	Writes the generated report to a PDF file in the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.
Excel	Writes the generated report to a PDF file in the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.
CSV	Saves the generated report as a PDF file in the …\TraceFinderData\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 for unknown screening batches.
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\Projects\…*batch*\ReportOutput folder.
View	Displays the generated output file.
View Generated Reports	Displays the …\TraceFinderData\Projects\…*batch*\ReportOutput folder that contains all report outputs.
Clear	Removes all reports from the Generated Reports display. This does not delete the reports from the …\TraceFinderData\Projects\…*batch*\ReportOutput folder.

Working in the Local Method View for unknown screening batches

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*.

v **To open the Local Method View**

1. Click **Analysis** in the navigation pane.
2. Click **Local Method**.

The Local Method View for the currently selected batch opens.

You can edit many of the method parameters in a local method. Editing the local method does not affect parameters in the master method.

For detailed descriptions of method parameters, refer to Chapter 6, "Using the Method Development Mode for Unknown Screening Methods," in the *TraceFinder Lab Director User Guide*.

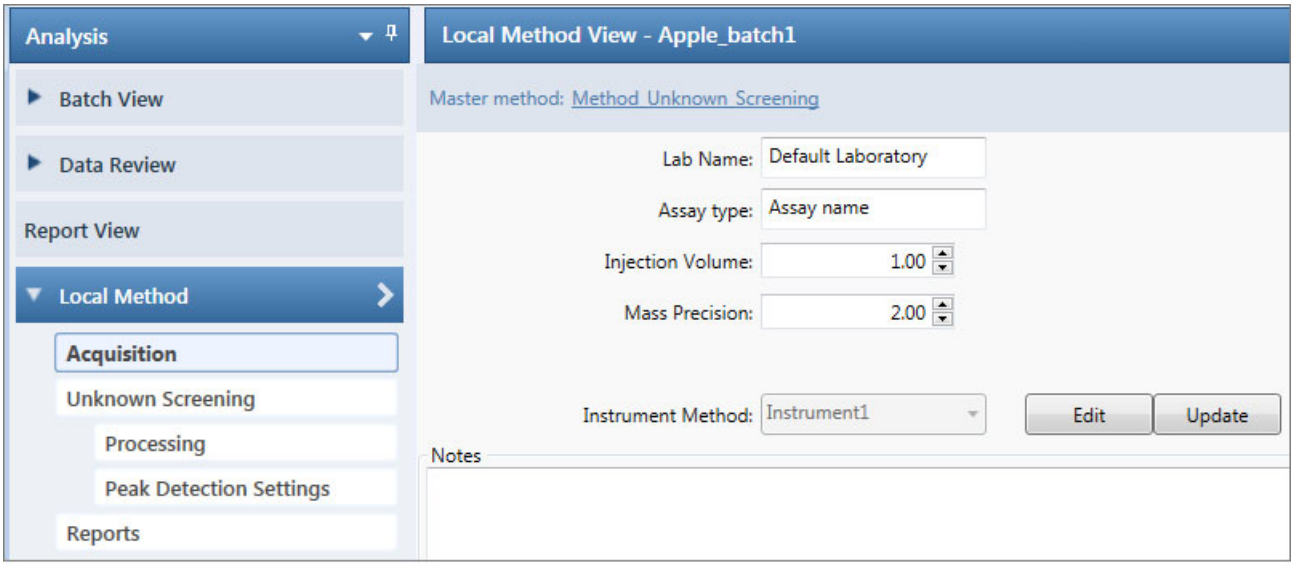
3. Enter any local changes to the method.
4. When you have finished editing the local method, choose **File > Save**.
5. To process the batch or create new reports with the edited local method, return to the Batch View and submit the batch.

v **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



7

Using the Report Designer

Use the features in the Report Designer to create or edit report templates.

You can create new report templates or edit your laboratory's report templates. You cannot edit report templates that were provided with the TraceFinder application; however, you can open a TraceFinder template, make changes, and save it with a new template name.

Contents

- Editing a template
- Toolbar reference
- Plot display properties
- Quick Tips

You can also create templates for Batch (Calibration Group) and Compound (Calibration Group). You can select these templates from the Batch and Compound Report types.

To create or edit a report template, use the Report Designer to do any of the following:

- Make changes to the template as you would in an Excel application.
- Add or remove graphics.
- Add repeated areas of many types.
- Format fonts and colors.
- Add or edit formulas.
- Edit template text and headers.

Note To edit or create a template, you must have an open batch.

Editing a template

Use the Report Designer to add or remove graphics, add tables, add repeated areas, and format headings, data, or cells.

Follow these procedures:

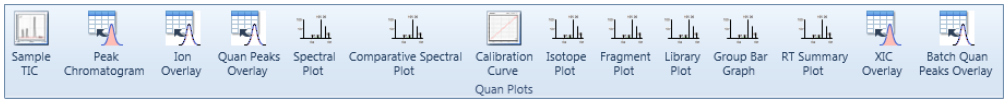
- To insert graphics into a report template
- To resize an inserted graphic
- To move an inserted graphic
- To insert a table
- To remove an inserted table
- To make changes to a table
- To format header text in the spreadsheet
- To format data in the report grid
- To format cells in the report grid
- To add repeated areas
- To insert a new sheet in a report

v To insert graphics into a report template

1. Click the **Insert** tab.

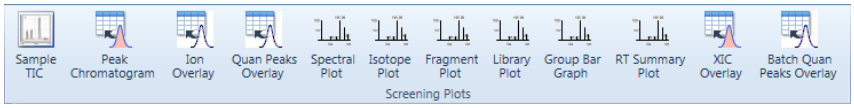
   The Insert page displays the available objects that you can insert in a quantitation, a target screening, or an unknown screening report template.

   Figure 157. Quan Plots features for quantitation batch report templates

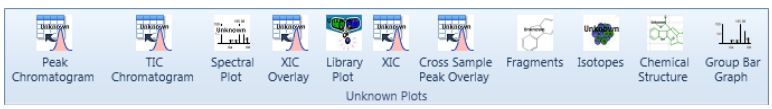
   For a description of each graphic element, see Insert toolbar – general features.

   Figure 158. Screening Plots features for target screening batch report templates

   For a description of each graphic element, see Insert toolbar – target screening reports.

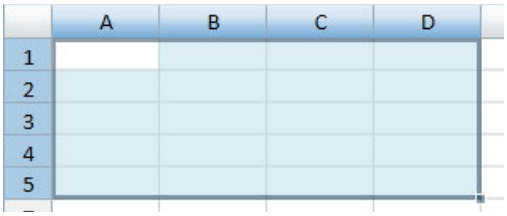
   Figure 159. Unknown Plots features for unknown screening batch report templates

For a description of each graphic element, see Insert toolbar – unknown screening reports.

Note When the method for a quantitation or target screening batch includes unknown screening, the Insert features for the report templates include Unknown Plots.

2. In the template grid, drag to select cells where you want to place the item.



Note You can also select a single row, and the application inserts the upper left corner of the graphic at the first cell, using a minimum default size.

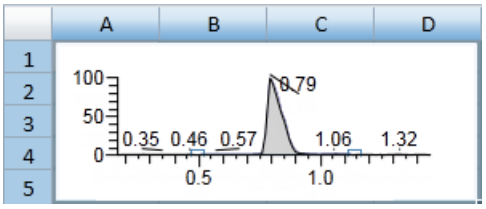
3. Select a sample from the list of samples in the left pane.

   The application uses graphical data from the selected sample when you insert a graphical plot.

4. Click a graphical plot in the toolbar to insert into the selected cells.

   The application inserts the selected plot in the template grid.

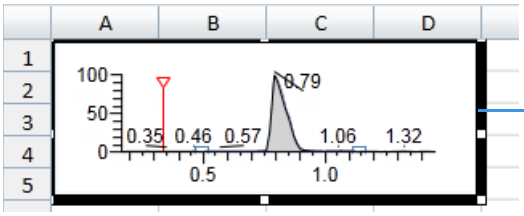
Figure 160. Inserted peak chromatogram



v **To resize an inserted graphic**

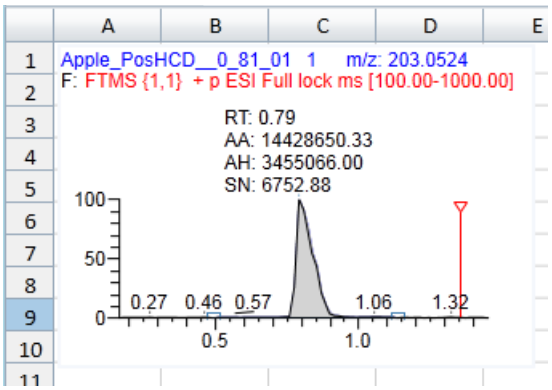
1. Right-click the graphic to make it editable.

Figure 161. Editable graphic



2. Grab a corner of the graphic and stretch it to the new size.

Figure 162. Resized graphic

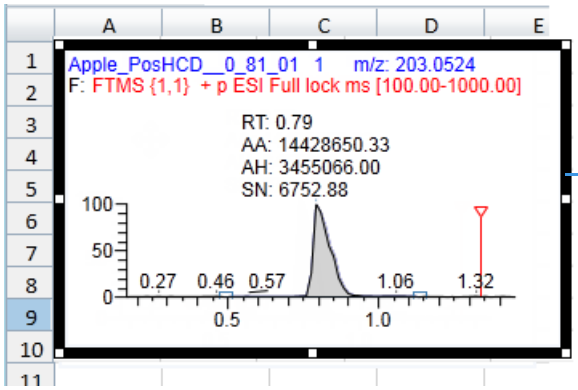


Note In this example, the original graphic was too small to display all the chromatogram data. Stretching the graphic reveals the sample name, mass, filter, and labeling.

v To move an inserted graphic

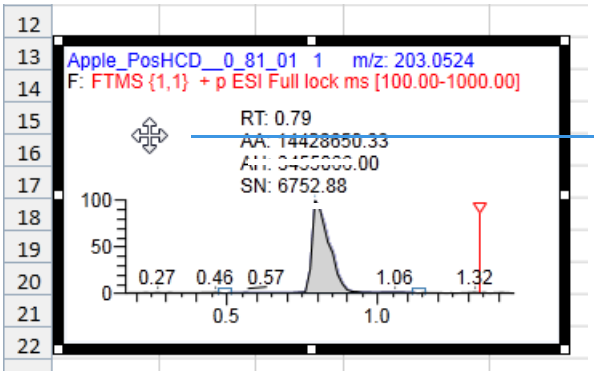
1. Right-click the graphic to make it editable.

Figure 163. Editable graphic

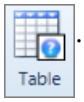


2. Click the graphic (notice the cursor change), and drag it to a new location.

Figure 164. Moved graphic

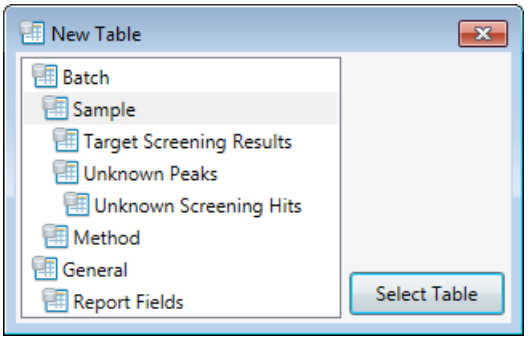


v To insert a table

1. Select a row in the report grid where you want to insert the table.
2. Click the **Insert** tab, and then click the **Table** icon, 

.

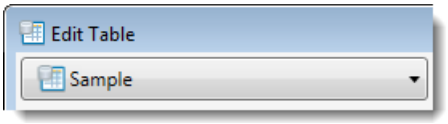
   The New Table dialog box opens.



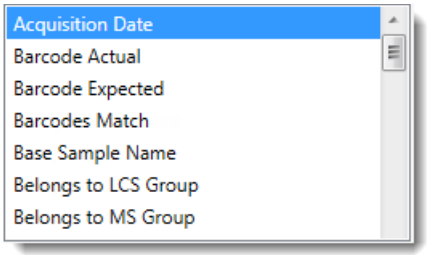
3. Select the type of table that you want to insert and click **Select Table**.

   The Edit Table dialog box opens.

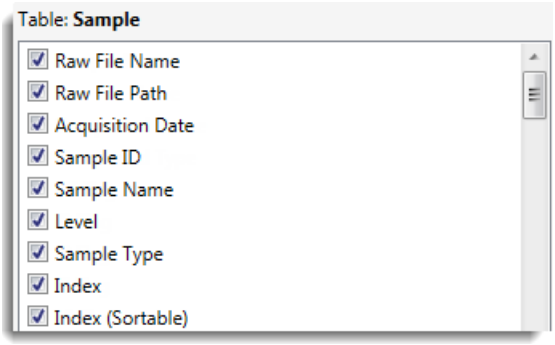
   The dropdown list in the upper left corner displays the data type for the table you selected.



   The left pane displays an alphabetical list of all available fields for the selected data type that you can include in the table. To display fields for a different data type, see step 4.

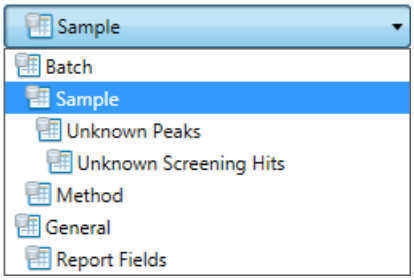


   The right pane lists the fields that are included in the new table.



You can select as many additional fields as you want. The table you create displays each selected field as a table column. By default, all available fields for the original data type are included in the table. The first field in the list is the leftmost column in the table. The last field in the list is the rightmost column in the table. To change the order of the columns, see step 6.

4. To add fields to the table from a different data type, do the following:
   a. Click the dropdown list and select a different data type.



   The left pane displays an alphabetical list of all available fields for the new data type.

   b. Select a field in the left pane and then click ›.

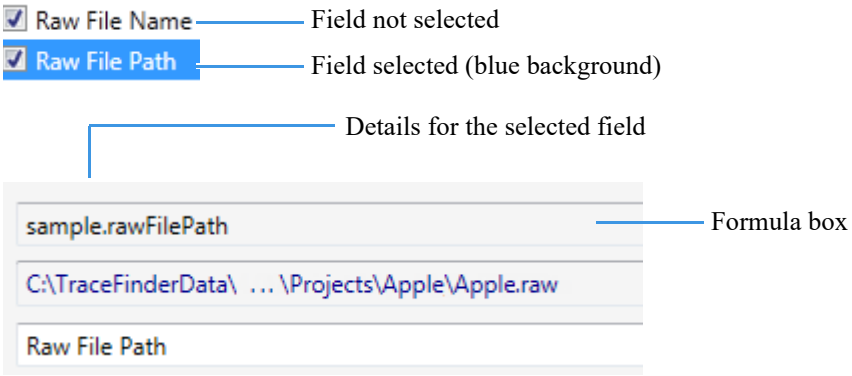
   The application moves the selected field to the rightmost pane to indicate that it is included in the inserted table.

5. To select a field that you do not want in the table, in the rightmost pane, clear the check box next to the field name.
6. To move a column up or down in the table, select the field name in the rightmost pane and click the **Up** arrow, ↑, or **Down** arrow, ↓.
7. To edit the header for a table column, select the field in the list on the right, and then type new header text in the Header box in the Field Details area.

   The default header name is the same as the field name.

8. To find the formula for a field, select the field.

   The application displays the formula in the Formula box.



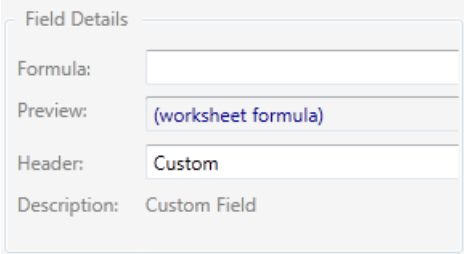
This video demonstrates how to use the Report Designer to create your own formula: Working with Formulas.

9. To create a custom column, do the following:
   a. Click **Custom,** Custom.

      The application adds a Custom field to the fields list.

   b. Select the Custom field in the list.

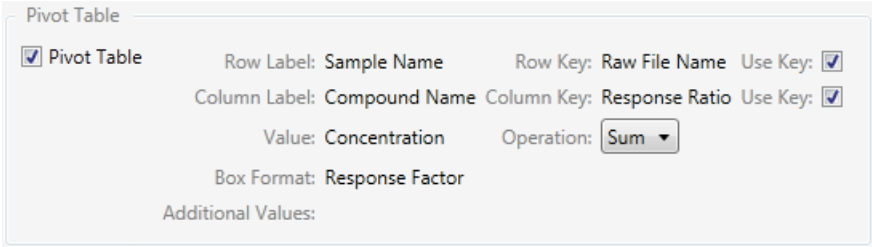
      The application display the details for the new, custom column.



   c. Enter values for the Formula and Header.

10. To create a pivot table, do the following:
    a. Select the **Pivot Table** check box.

       The Pivot Table area expands to display the pivot table options.



    b. Select the **Use Key** check box for the row label.
    c. Select the **Use Key** check box for the column label.
    d. Select the operation that you want to use to calculate the aggregate value: **Sum**, **Count**, **Average**, **First**, or **Last**.

11. When you have made all your table selections, click **OK**.

    The application inserts the table into the report template.

v To remove an inserted table

1. Select all rows and cells in the table.
2. Right-click and choose **Delete – Delete Cells and Shift Cells Left**.

   The application removes the entire table from the report template.

v **To make changes to a table**

1. In the table that you want to edit, right-click and choose **Data Table**.

   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 dialog box that you used to create a table.

2. Edit the fields for the table and click **OK**.

v **To format header text in the spreadsheet**

1. In the Report Designer window, select the header in the spreadsheet table.

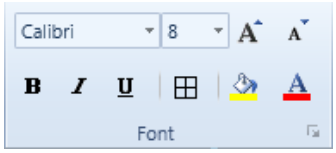
   To change all headers, select the entire header row.

   To change a single header, select the specific header cell.

   Tip You can also use the SHIFT key to select sequential cells or the CTRL key to select nonsequential cells anywhere in the grid.

2. Click the **Home** tab.

3. Use the Font icons to change the font format.



v **To format data in the report grid**

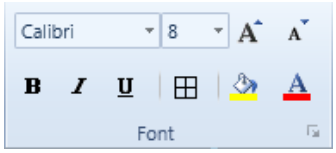
1. Select the data that you want to format.

   To format all rows in a column, select the header row.

   To format a single cell of data, select only that cell.

   Tip You can also use the SHIFT key to select sequential cells or the CTRL key to select nonsequential cells anywhere in the grid.

2. Click the **Home** tab and use the toolbar icons to edit the font or cells as appropriate:



   - Change the font or font size.
   - Make the selected text bold.
   - Make the selected text italics.

- Underline the selected text.
- Apply borders to the currently selected cells.
- Increase or decrease font size.
- Apply color to the background for selected cells.
- Change the font color.

v **To format cells in the report grid**

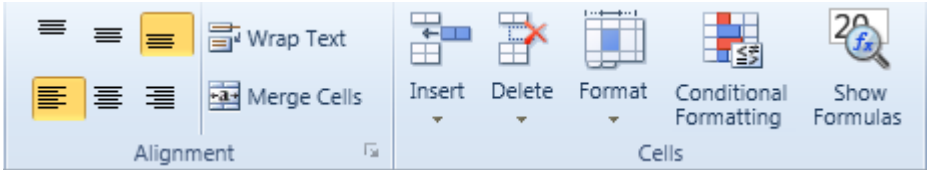
1. Select the cells that you want to modify:

   To change all cells in a row, select the entire row.

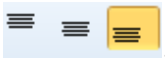
   To change a single cell, select only that cell.

   Tip You can also use the SHIFT key to select sequential cells or the CTRL key to select nonsequential cells.

2. Click the **Home** tab and use the Alignment or Cells toolbar icons to edit the cells.



3. To align the cell text to the top, center, or bottom of the cell, click one of these icons:



4. To align the cell text to the left, center, or right of the cell, click one of these icons:

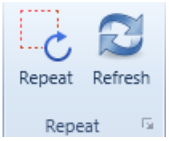
5. To make all contents visible within a cell, click **Wrap Text**.
6. To join selected cells into one cell, click **Merge Cells**.
7. To insert cells, rows, or columns into the template, click **Insert**.
8. To delete rows or columns from the template, click **Delete**.
9. To change the row height or column width, organize sheets, or protect or hide cells, click **Format**.
10. To highlight or emphasize useful cells based on specific criteria, click **Conditional Formatting** to use data bars, color scales, or icon sets.
11. To show formulas for selected cells instead of the resulting value, click **Show Formulas**.

v To add repeated areas

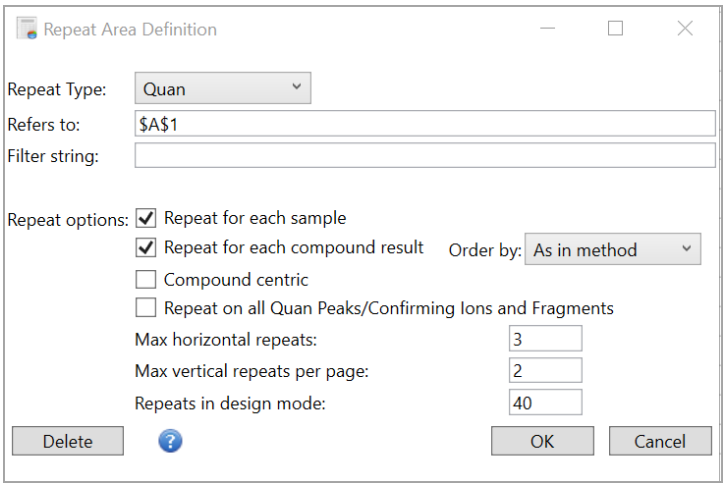
1. To define a repeat area, select the cells that you want to repeat.

   You can repeat only one area per worksheet, but you can repeat it many times. You cannot insert data tables beneath a repeated area. See Example of repeated areas.

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.

   Note For the Batch (Calibration) and Compound (Calibration) report types, when a repeat area is in the template and the "Repeat for each sample" and "Repeat for each compound result" options are enabled, then it will loop through the calibration groups instead of every sample. Calibration fields and plots inside that repeat area are based on the calibration group it is in.

   For the sample template type, the calibration fields and plots are based on the calibration group each sample belongs to.

4. Select to repeat for each sample, for each compound, or for both.

5. Define whether the repeat area repeats first for samples or first for compounds:

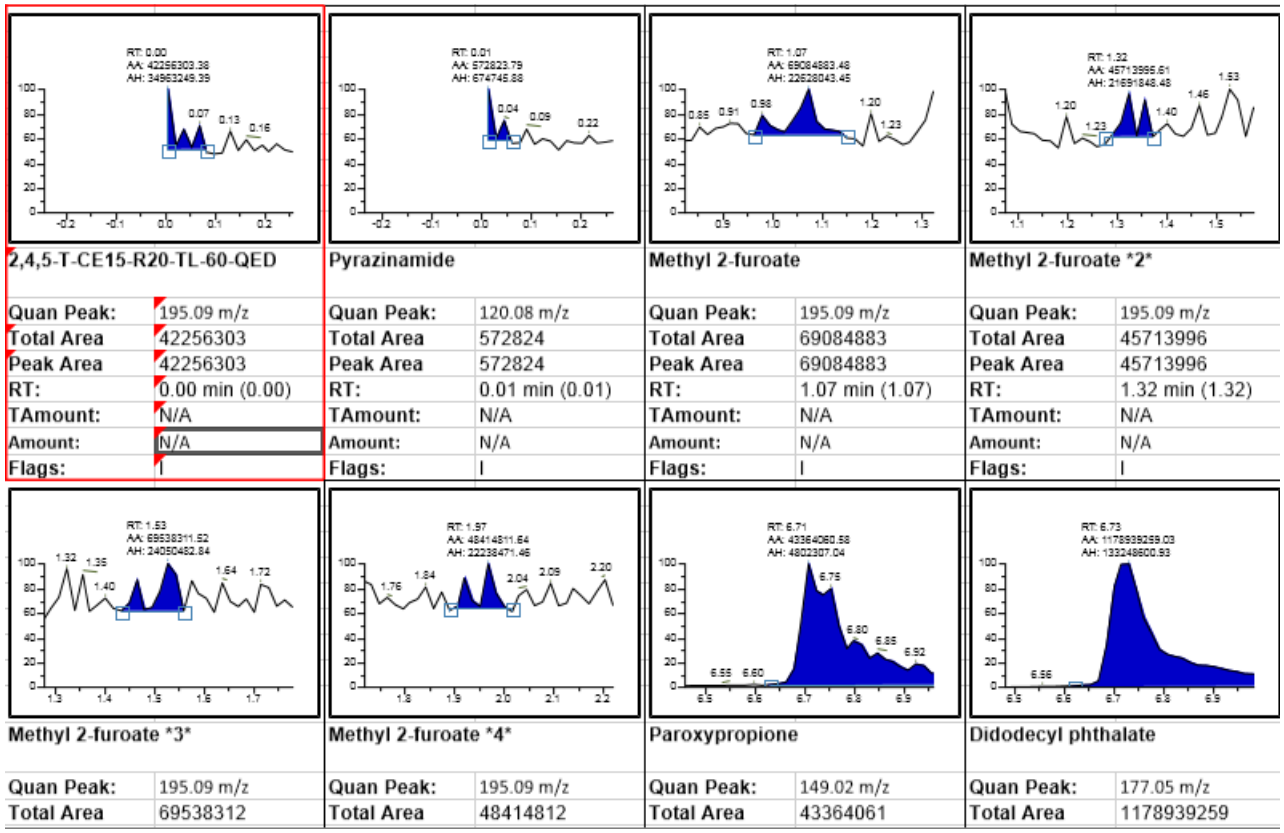
   - To have the repeat area repeat first for samples and then for compounds, clear the **Compound Centric** check box.
   - To have the repeat area repeat first for compounds and then for samples, select the **Compound Centric** check box.

6. To define the number of times to repeat horizontally before wrapping to the next row, type a number in the Max Horizontal Repeats box.
7. To define the number of times to repeat vertically before inserting an auto-page break, type a number in the Max Vertical Repeats Per Page box.
8. To define the maximum suggested number of repeats, type a number in the Repeats in Design Mode box.

   This maximum number of repeats is intended to limit the size of the report while you are editing the report in the Report Designer. When generating an actual report, the application does not enforce this limit.

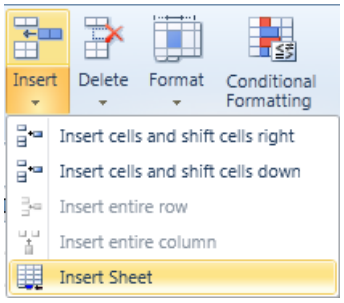
In this example, the repeated area (outlined in red) displays the peak chromatogram, target peak, total area, peak area, retention time, theoretical amount, actual amount, and reported flags, if any, for each compound.

Figure 165. Example of repeated areas



v **To insert a new sheet in a report**

1. Click the **Home** tab.
2. In the Cells area, choose **Insert Sheet** from the Insert menu.



The application adds a new sheet to the report.

Edit Table dialog box

Use the options in the Edit Table dialog box to edit the fields in a table.

For the Batch and Compound calibration report types, when there is a data table in the template, the application displays a row for each group instead of a row for every sample. Calibration Fields inside that table are based on its calibration group.

Figure 166. Edit Table dialog box

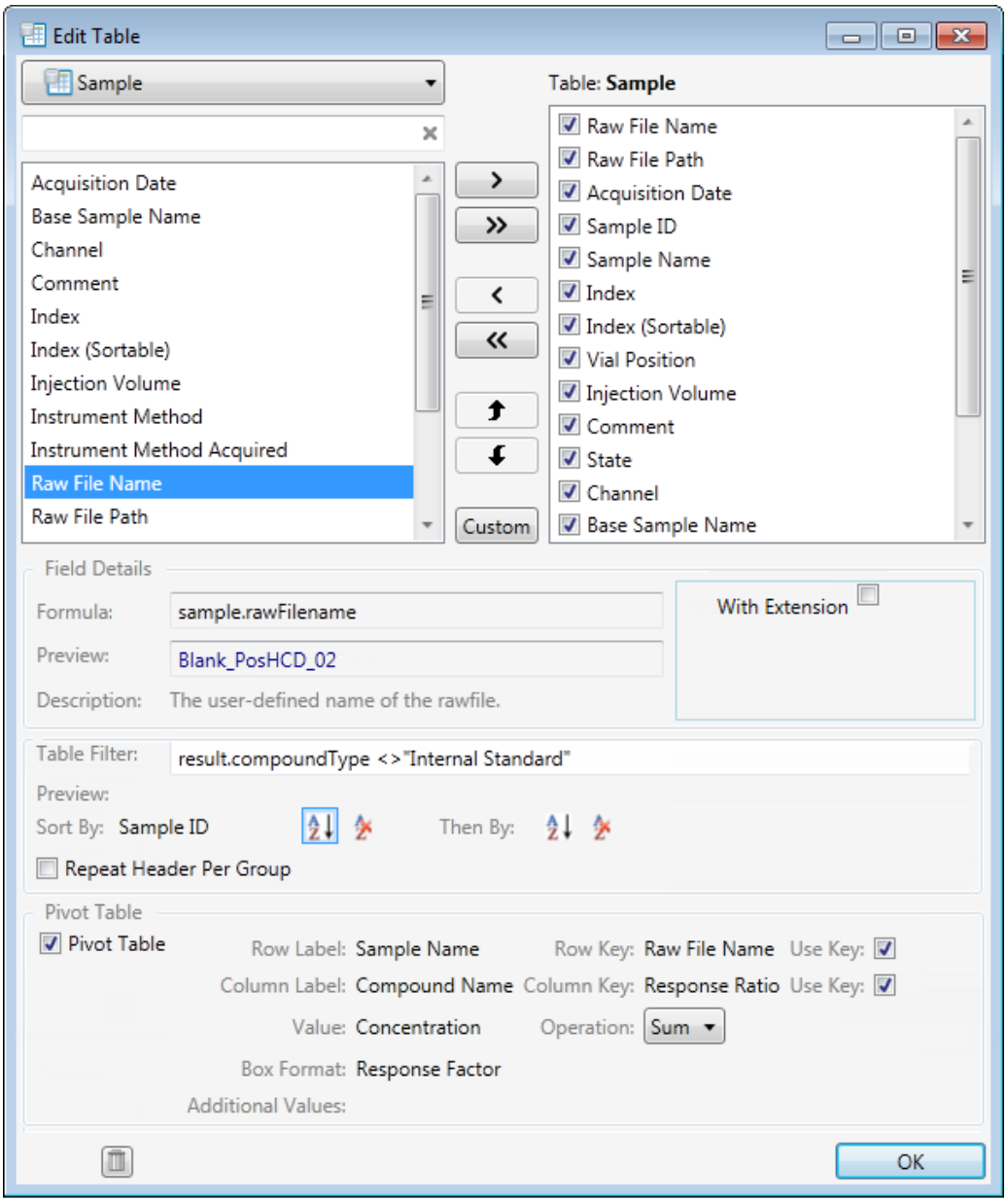


Table 77. Edit Table dialog box parameters (Sheet 1 of 2)

Parameter	Description
Dropdown List	Specifies the type of table you are editing.
Field List	Lists all available table fields.
Table	Displays the selected table type and the fields included in the table.
Field Details	
Formula	Specifies the functions and arguments used to define the field.
Preview	Specifies the name of the raw data file used for the report.
Header	Specifies the header name for the column in the spreadsheet.

Table 77. Edit Table dialog box parameters (Sheet 2 of 2)

Parameter	Description
Description	Specifies the type of field.
Table Filter	
Table Filter	Specifies the filter used for the sample compounds.
Preview	–
Sort By	Sorts the data by ascending or descending values.
Pivot Table	
Pivot Table	Enables the Pivot Table features.
Row Label	–
Row Key	–
Column Label	–
Column Key	–
Value	–
Operation	Specifies the operation used to calculate the aggregate value. Valid values: Sum, Count, Average, First, Last
Box Format	–
Additional Values	–
Delete	Deletes the selected table from the template.

Toolbar reference

The Report Designer includes the following toolbars.

- Home toolbar
- Insert toolbar – general features
- Insert toolbar – quantitation reports
- Insert toolbar – target screening reports
- Insert toolbar – unknown screening reports
- Page Layout toolbar

Home toolbar

Use the options in the Home toolbar to modify fonts, align cell data, and format cells.

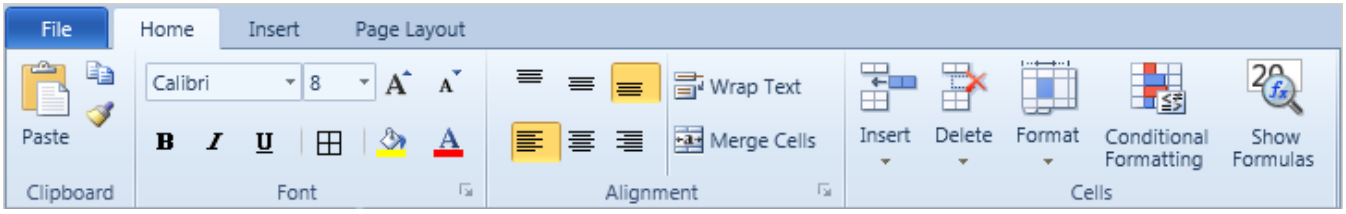


Table 78. Home toolbar options (Sheet 1 of 2)

Option	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 lists	Use the dropdown lists to change the font or font size.
Bold	Make the selected text bold.
Italic	Make the selected text italics.
Underline	Underline the selected text.
Border	Apply borders to the currently selected cells.
Font size	Increase or decrease the font size.
Fill color	Apply color to the background for selected cells.
Font color	Change the font color.
Alignment	
	Align the cell text to the top, center, or bottom of the cell.
	Align the cell text to the left, center, or right of the cell.

Table 78. Home toolbar options (Sheet 2 of 2)

Option	Description
Wrap text	Make all contents visible within a cell.
Merge cells	Join selected cells into one cell.
Cells	
Insert	Insert cells, rows, columns, or sheets into a template.
Delete	Delete rows or columns from a template.
Format	Change the row height or column width, organize sheets, or protect or hide cells.
Conditional Formatting	Based on specific criteria, highlight or emphasize useful cells using data bars, color scales, and icon sets.
Show Formulas	Show formulas for selected cells instead of the resulting value.

Insert toolbar – general features

Use the features on the Insert page to create and edit tables, formulas, graphic plots, charts, and illustrations.

Graphic plots can represent data from quantitative, target screening, or unknown screening data. The Insert page displays the available data plots for the type of batch: quantitation, quantitation plus unknown screening, target screening, target screening plus unknown screening, or unknown screening only.

The following graphic outlines all three plot types for illustrative purposes only.

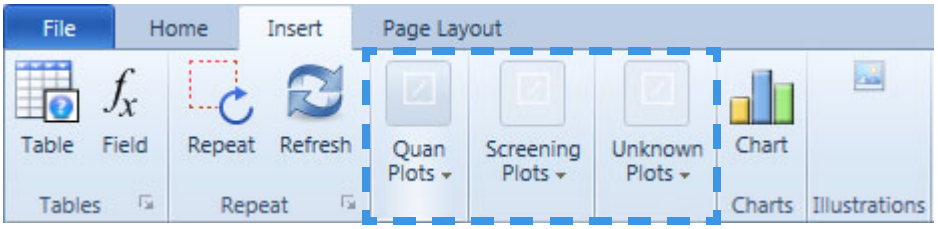
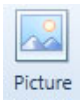


Table 79. Insert toolbar options (Sheet 1 of 2)

Option	Description
Tables	
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.

Table 79. Insert toolbar options (Sheet 2 of 2)

Option	Description
Quan Plots	Can be stand-alone or used with Unknown plots. For descriptions of quantitation plots, see Insert toolbar – quantitation reports.
Screening Plots	Can be stand-alone or used with Unknown plots. For descriptions of target screening plots, see Insert toolbar – target screening reports.
Unknown Plots	Can be stand-alone or used with either Quan plots or Screening plots. For descriptions of unknown screening plots, see Insert toolbar – unknown screening reports.
Charts	
	Adds a custom chart. To define the chart, double-click the inserted blank chart.
Illustrations	
	Insert a picture from a file.

Insert toolbar – quantitation reports

Use the options in the Insert toolbar to add graphics, plots, and other objects to a template or report. You can also set up repeating objects and define functions.

For each inserted plot, you can customize the display properties. See Quantitation and target screening plots.

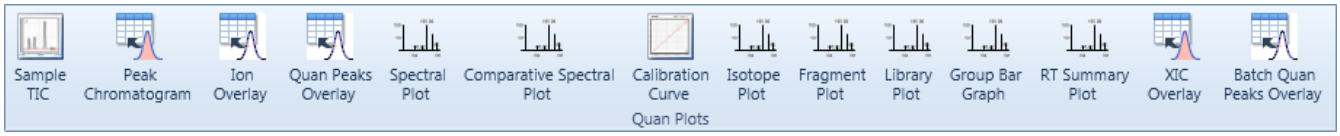


Table 80. Insert toolbar Quantitation options (Sheet 1 of 3)

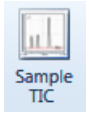
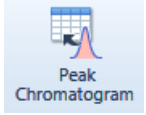
Option	Description
	Adds a sample TIC. For information about sample TIC data in the Data Review results, see Peaks pane.
	Adds a peak chromatogram. For information about peak chromatogram data in the Data Review results, see Quan Peak.

Table 80. Insert toolbar Quantitation options (Sheet 2 of 3)

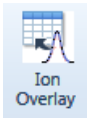
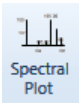
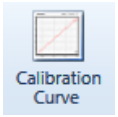
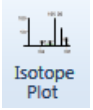
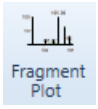
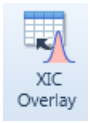
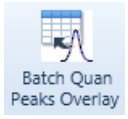
Option	Description
	Adds an ion overlay. For information about ion overlay data in the Data Review results, see Ion Overlay.
	Adds a quantitation peaks overlay plot. For information about quantitation peaks overlay data in the Data Review results, see Quan Peaks Overlay.
	Adds a spectral plot. For information about spectral data in the Data Review results, see Spectra.
	Adds a comparative spectral plot. For information about comparative spectral data in the Data Review results, see Spectra.
	Adds a calibration curve plot. For information about calibration curve data in the Data Review results, see Calibration Curve.
	Adds an isotope plot to display the number of isotopes found, the score, a pass/fail flag, and a plot of the isotopes. For information about isotope plot data in the Data Review results, see Isotope.
	Adds a fragment plot. For information about fragment plot data in the Data Review results, see Fragments.
	Adds a library plot. For information about library plot data in the Data Review results, see Library Match.
	Adds a group averages plot. For information about group averages data in the Data Review results, see Group Averages.
	Adds an RT summary plot. For information about retention time summary data in the Data Review results, see Retention Time Summary.

Table 80. Insert toolbar Quantitation options (Sheet 3 of 3)

Option	Description
	Adds an XIC summary plot. For information about XIC summary data in the Data Review results, see XIC Overlay.
	Adds a Batch Quan Peaks Overlay plot that displays all quantitative peaks in the batch.

Insert toolbar – target screening reports

Use the options in the Insert toolbar to add graphics, plots, and other objects to a template or report. You can also set up repeating objects and define functions.

For each inserted plot, you can customize the display properties. See Quantitation and target screening plots.

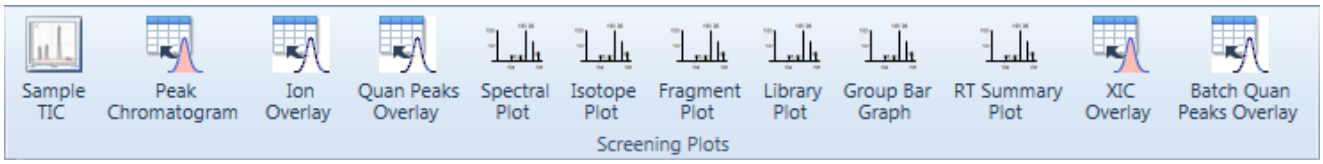


Table 81. Insert toolbar target screening options (Sheet 1 of 2)

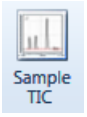
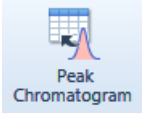
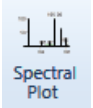
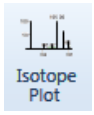
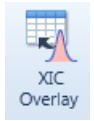
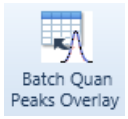
Option	Description
	Adds a sample TIC plot.
	Adds a peak chromatogram plot. For information about peak chromatogram data in the Data Review results, see Chromatogram pane.
	Adds an ion overlay plot.
	Adds a quantitation peaks overlay plot.
	Adds a spectral plot. For information about spectral plot data in the Data Review results, see Spectrum.

Table 81. Insert toolbar target screening options (Sheet 2 of 2)

Option	Description
	Adds an isotope plot to display the number of isotopes found, the score, a pass/fail flag, and a plot of the isotopes. For information about isotope plot data in the Data Review results, see Isotopes.
	Adds a fragment plot. For information about fragment plot data in the Data Review results, see Fragments.
	Adds a library plot. For information about library plot data in the Data Review results, see Library.
	Adds a group averages plot. For information about group averages data in the Data Review results, see Groups.
	Adds an RT summary plot.
	Adds an XIC summary plot.
	Adds a Batch Quan Peaks Overlay plot that displays all quantitative peaks in the batch.

Insert toolbar – unknown screening reports

Use the options in the Insert toolbar to add graphics, plots, and other objects to a template or report. You can also set up repeating objects and define functions.

For each inserted plot, you can customize the display properties. See Unknown screening plots.

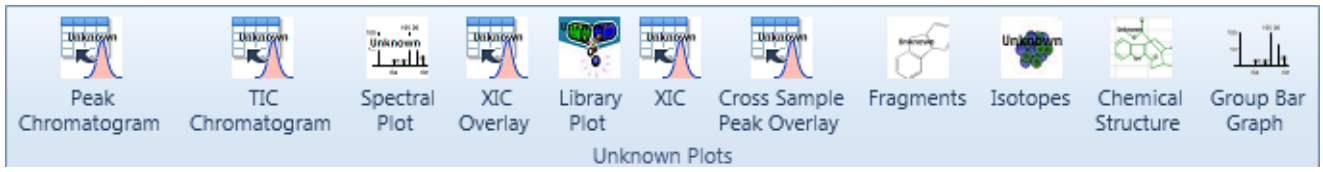
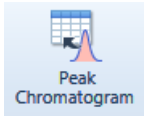
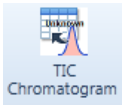
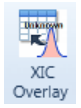
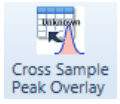
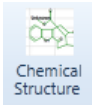


Table 82. Insert toolbar unknown screening options

Option	Description
	Adds a peak chromatogram. For information about peak chromatogram data in the Data Review results, see Peak Chromatogram pane.
	Adds a TIC chromatogram. For information about TIC chromatogram data in the Data Review results, see TIC Chromatogram pane.
	Adds a spectral plot. For information about spectral plot data in the Data Review results, see Spectrum pane.
	Adds an XIC overlay plot. For information about XIC overlay data in the Data Review results, see XIC Overlay pane.
	Adds a library plot. For information about library plot data in the Data Review results, see Library Search pane.
	Adds an XIC plot. For information about XIC plot data in the Data Review results, see XIC pane.
	Adds a cross-sample peak overlay plot. For information about cross-sample peak overlay data in the Data Review results, see Cross Sample Peak Overlay pane.
	Adds a fragments plot. For information about fragments plot data in the Data Review results, see Fragments pane.
	Adds an isotopes plot. For information about isotopes plot data in the Data Review results, see Isotopes pane.
	Adds a chemical structure plot. For information about chemical structure plot data in the Data Review results, see Chemical Structure pane.
	Adds a group averages plot. For information about group averages data in the Data Review results, see Group Averages pane.

Page Layout toolbar

Use the options in the Page Layout toolbar to adjust margins, orientation, paper size, and page breaks. To see your changes, click **Print Preview**.

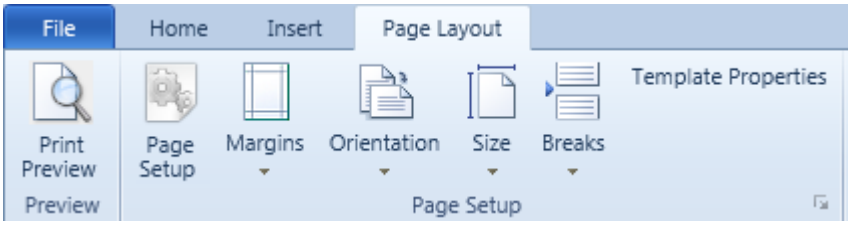
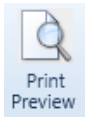
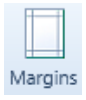
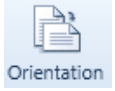


Table 83. Page Layout toolbar options

Option	Description
	View the report before printing it.
	Define page details.
	Select page margins for the current view or the entire document.
	Switch the pages from portrait to landscape view.
	Choose a page size for the current view or the entire document.
	Specify where a new page begins in the printed copy.
Template Properties	Open the Template Properties dialog box where you can specify the expected batch type for the report template. The Template Properties dialog box also displays the Used Range so that you can identify when there is empty white space in the report template. Extra white space to the right or left of the report content can cause unwanted page breaks.

Plot display properties

For plot types that you insert in the spreadsheet, you can change the display properties.

Note This topic shows examples of all plot types; however, the following plots do not have editable plot properties: Calibration Curve, Group Bar Graph, and RT Summary.

v **To change the plot display properties**

1. Insert a plot in the spreadsheet.
2. Right-click the plot to select it.
3. Right-click the plot again to display the shortcut menu.
4. Choose **Properties**.

   The Plot Properties dialog box opens, displaying the editable display properties for the selected plot type.

The following topics show the plots in the report templates and describe their properties.

- Quantitation and target screening plots
- Unknown screening plots

Quantitation and target screening plots

To customize the display in the quantitation and target screening reports, use the Plot Properties dialog box for each plot.

- Sample TIC plot
- Peak Chromatogram plot
- Ion Overlay plot
- Quan Peaks Overlay plot
- Spectral plot
- Comparative Spectral plot (quantitation reports only)
- Calibration Curve plot (quantitation reports only)
- Isotope plot, Fragment plot, or Library plot
- Group Bar Graph plot
- RT Summary plot
- XIC Overlay plot
- Batch Quan Peaks Overlay plot

Sample TIC plot

Click

to insert a sample TIC Chromatogram plot.

Figure 167. TIC Chromatogram plot

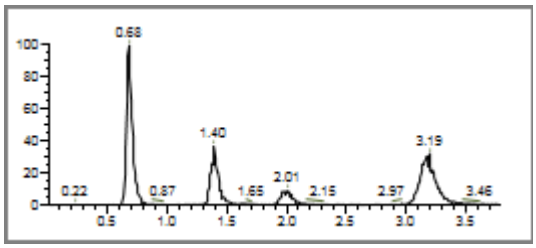


Figure 168. Plot Properties dialog box for a TIC Chromatogram plot

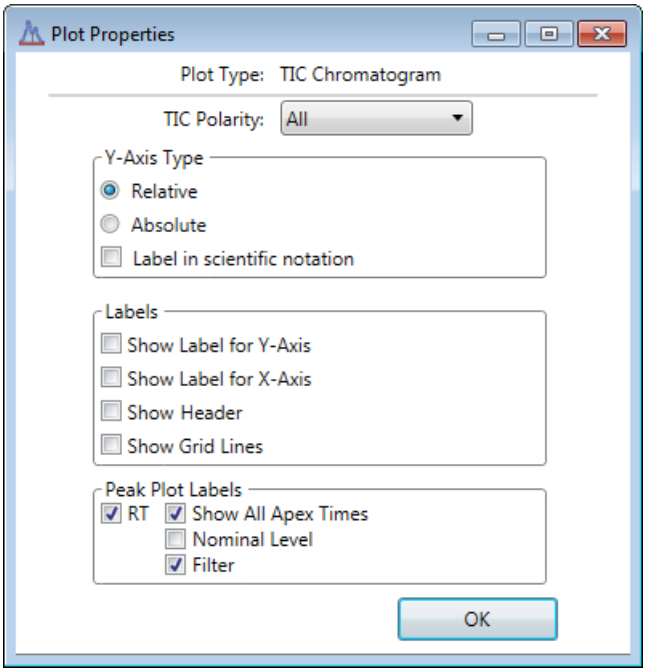


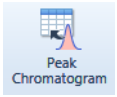
Table 84. Plot Properties parameters for a TIC Chromatogram (Sheet 1 of 2)

Command	Description
TIC Polarity	Specifies the polarity of adducts displayed in the plot. All: Displays positive, negative, and analog adducts. Positive: Displays only positive adducts. Negative: Displays only negative adducts. Analog: Displays only analog adducts.
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
Absolute	Displays the *y*-axis scale from 0 to the actual value of the most intense peak in the group.

Table 84. Plot Properties parameters for a TIC Chromatogram (Sheet 2 of 2)

Command	Description
Label in Scientific Notation	Displays the *y*-axis scale in scientific notation.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Header	Displays the raw data file path at the top of the plot.
Show Grid Lines	Displays the grid lines in the plot background.
Peak Plot Labels	
RT	Displays the retention time (RT) for each peak in the plot.
Show All Apex Times	Displays all surrounding apex times in the plot.
Nominal Level	Displays the nominal level (NL) values for each peak in the plot.

Peak Chromatogram plot

Click 

to insert a Peak Chromatogram plot.

Figure 169. Peak Chromatogram plot

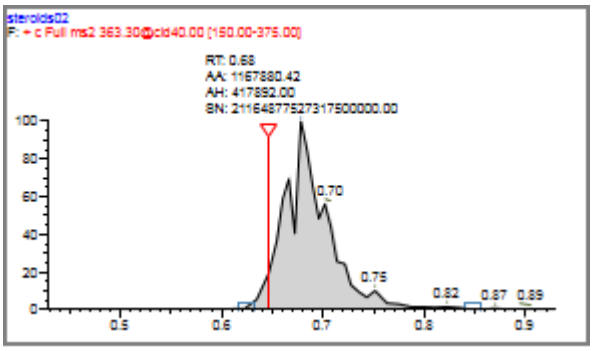


Figure 170. Plot Properties dialog box for Peak Chromatogram plot

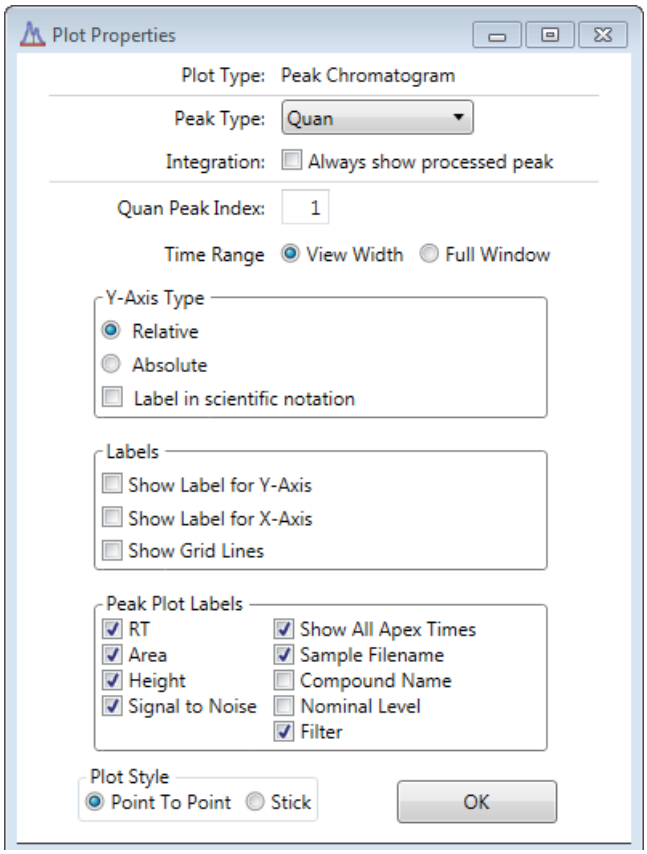
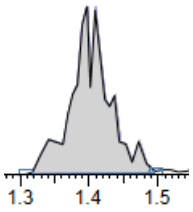
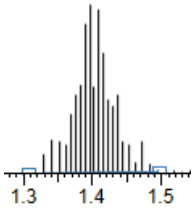


Table 85. Plot Properties parameters for a Peak Chromatogram plot (Sheet 1 of 2)

Command	Description
Peak Type	Specifies the type of peak to display in the plot: • Quan • Confirming • InternalStandard • InternalStandardConfirming
Integration: Always Show Processed Peak	Specifies that the plot always displays the processed peak.
Quan Peak Index	Valid values: 1 through 9
Time Range	Specifies that the plot display one of the following: • View Width: Zooms the display on the peak of interest. • Full Window: Displays the full width of the scan.
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
Absolute	Displays the *y*-axis scale from 0 to the actual value of the most intense peak in the group.

Table 85. Plot Properties parameters for a Peak Chromatogram plot (Sheet 2 of 2)

Command	Description
Label in Scientific Notation	Displays the *y*-axis scale in scientific notation.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Grid Lines	Displays the grid lines in the plot background.
Peak Plot Labels	
RT	Displays the retention time (RT) label in the peak chromatogram plot.
Area	Displays the peak area (AA) label in the peak chromatogram plot.
Height	Displays the peak height (AH) label in the peak chromatogram plot.
Signal to Noise	Displays the signal-to-noise (SN) label in the peak chromatogram plot.
Show All Apex Times	Displays all surrounding apex times in the plot.
Sample Filename	Displays the name of the sample file.
Compound Name	Displays the compound name.
Nominal Level	Displays the nominal level (NL) values for each peak in the plot.
Filter	Displays the filter used for the scan. The plot displays the filter name below the raw data file name.
Plot Style	
Point To Point	Displays chromatograms in the following format: 
Stick	Displays chromatograms in the following format: 

Ion Overlay plot

Click

to insert an Ion Overlay plot.

Figure 171. Ion Overlay plot

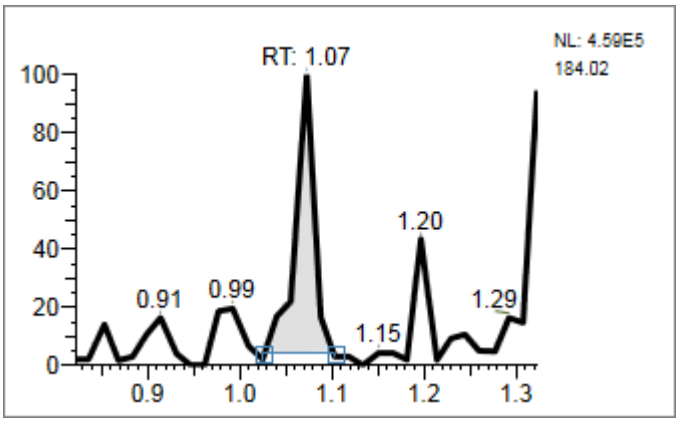


Figure 172. Plot Properties dialog box for an Ion Overlay plot

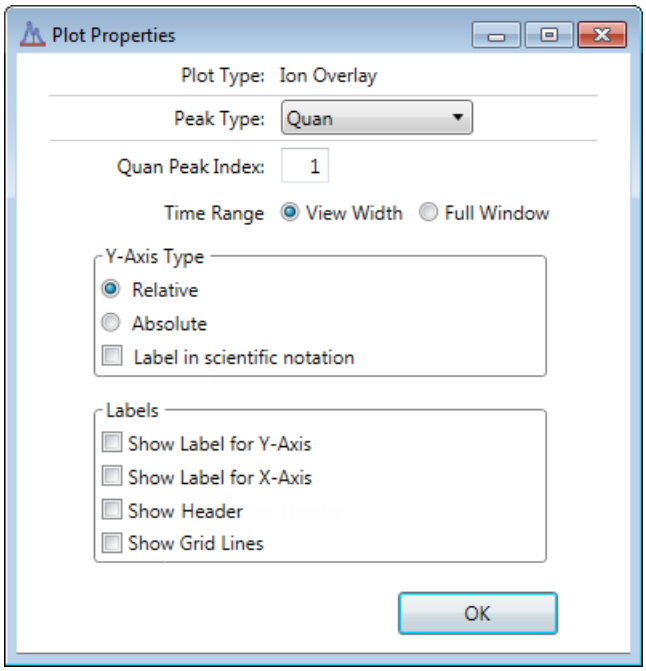


Table 86. Plot Properties parameters for an Ion Overlay plot (Sheet 1 of 2)

Command	Description
Peak Type	Specifies the type of peak to display in the plot: Quan or InternalStandard
Quan Peak Index	Valid values: 1 through 9

Table 86. Plot Properties parameters for an Ion Overlay plot (Sheet 2 of 2)

Command	Description
Time Range	Specifies that the plot display one of the following: • View Width: Zooms the display on the peak of interest. • Full Window: Displays the full width of the scan.
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Header	Displays the raw data file name and compound name.
Show Grid Lines	Displays the grid lines in the plot background.

Quan Peaks Overlay plot

Click

to insert a Quan Peaks Overlay plot.

Figure 173. Quan Peaks Overlay plot

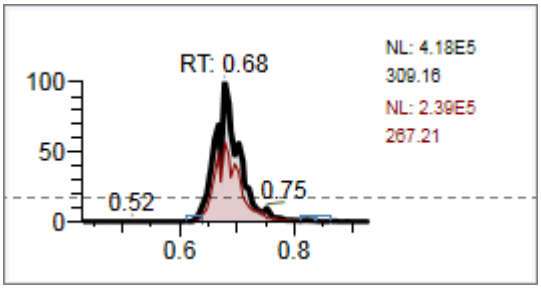


Figure 174. Plot Properties dialog box for a Quan Peaks Overlay plot

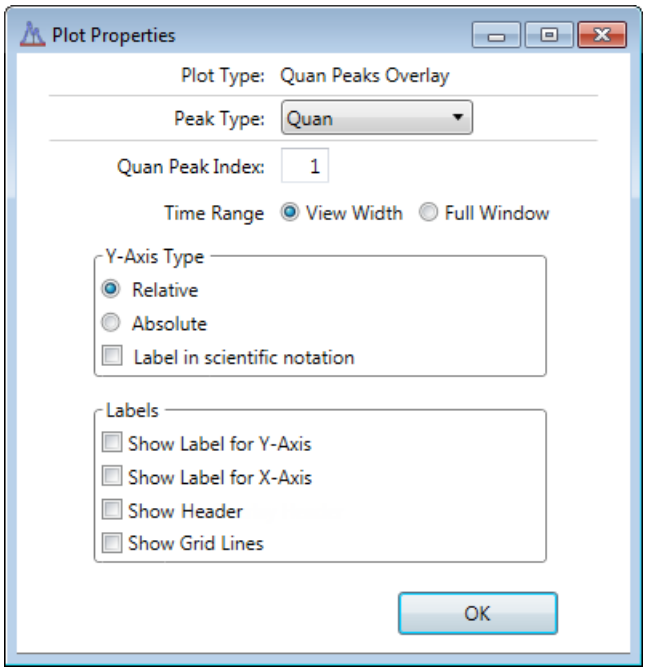


Table 87. Plot Properties parameters for a Quan Peaks Overlay plot

Command	Description
Peak Type	Specifies the type of peak to display in the plot: Quan or InternalStandard
Quan Peak Index	Valid values: 1 through 9
Time Range	Specifies that the plot display one of the following: • View Width: Zooms the display on the peak of interest. • Full Window: Displays the full width of the scan.
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Header	Displays the raw data file name and compound name.
Show Grid Lines	Displays the grid lines in the plot background.

Spectral plot

Click

to insert a Spectral plot.

Figure 175. Spectral plot

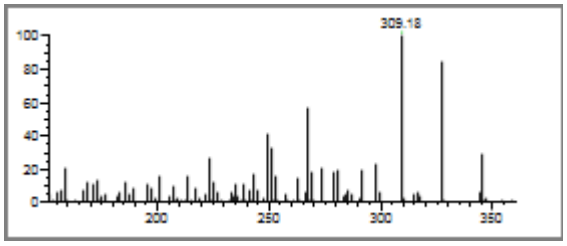


Figure 176. Plot Properties dialog box for a Spectral plot

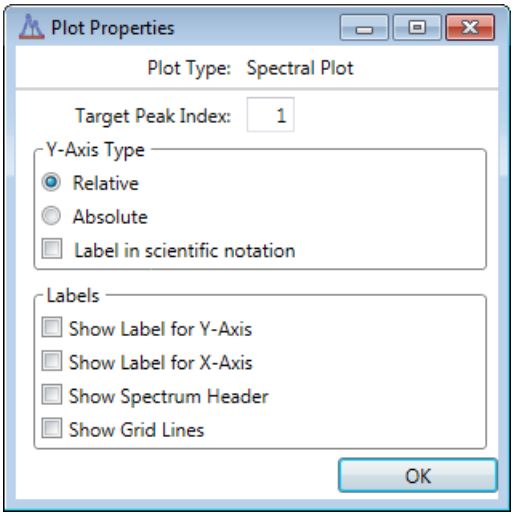


Table 88. Plot Properties parameters for a Spectral plot

Command	Description
Target Peak Index	Valid values: 1 through 9
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Header	Displays the raw data file name and compound name.
Show Grid Lines	Displays the grid lines in the plot background.

Comparative Spectral plot (quantitation reports only)

Click

to insert a Comparative Spectral plot.

Figure 177. Comparative Spectral plot

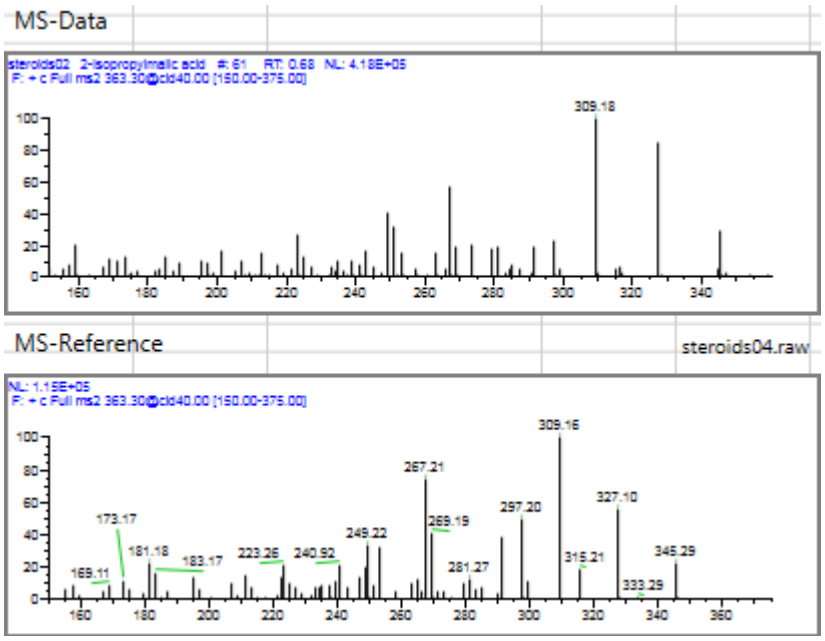


Figure 178. Plot Properties dialog box for a Comparative Spectral plot

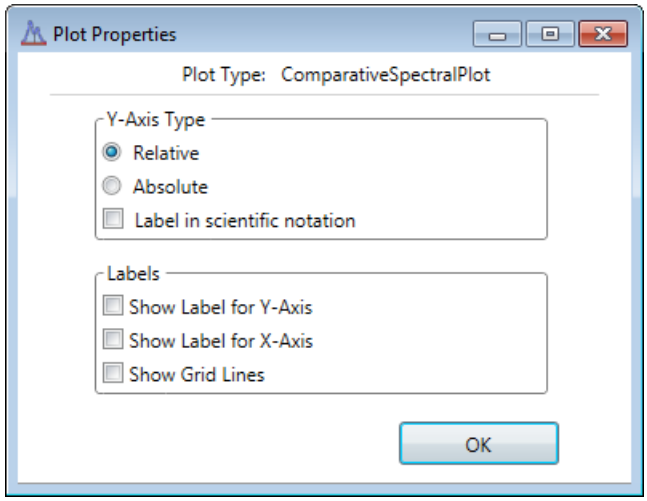


Table 89. Plot Properties parameters for a Comparative Spectral plot (Sheet 1 of 2)

Command	Description
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
Absolute	Displays the *y*-axis scale from 0 to the actual value of the most intense peak in the group.

Table 89. Plot Properties parameters for a Comparative Spectral plot (Sheet 2 of 2)

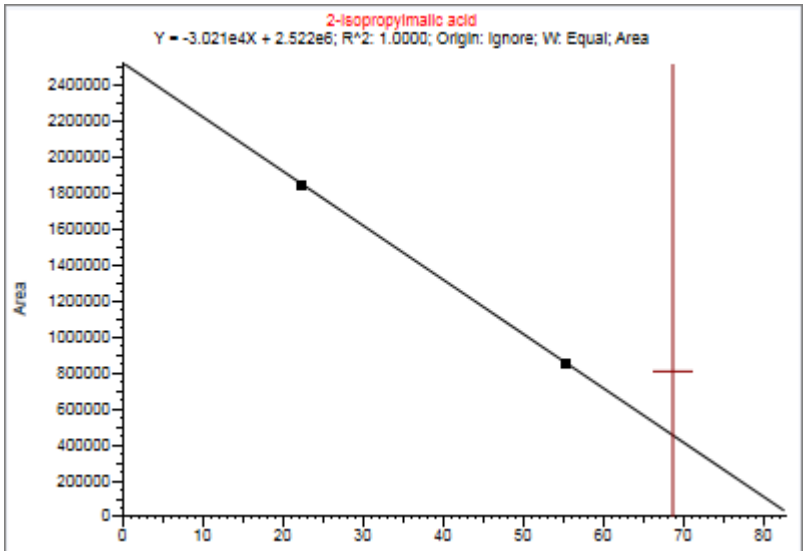
Command	Description
Label in Scientific Notation	Displays the *y*-axis scale in scientific notation.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Grid Lines	Displays the grid lines in the plot background.

Calibration Curve plot (quantitation reports only)

Click

to insert a Calibration Curve plot.

Figure 179. Calibration Curve plot



Note There are no plot properties for a calibration curve plot.

Isotope plot, Fragment plot, or Library plot

Do one of the following:

- Click

to insert an Isotope plot.
- Click

to insert a Fragment plot.
- Click

to insert a Library plot.

The Isotope, Fragment, and Library plots use identical plot properties.

Figure 180. Isotope plot

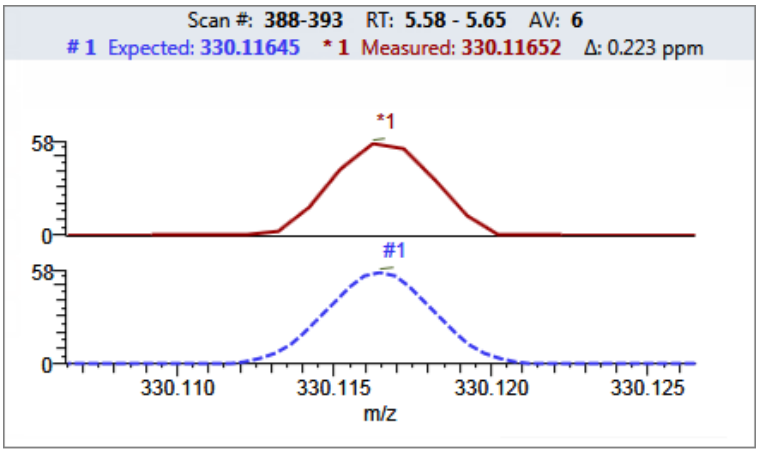


Figure 181. Fragment plot

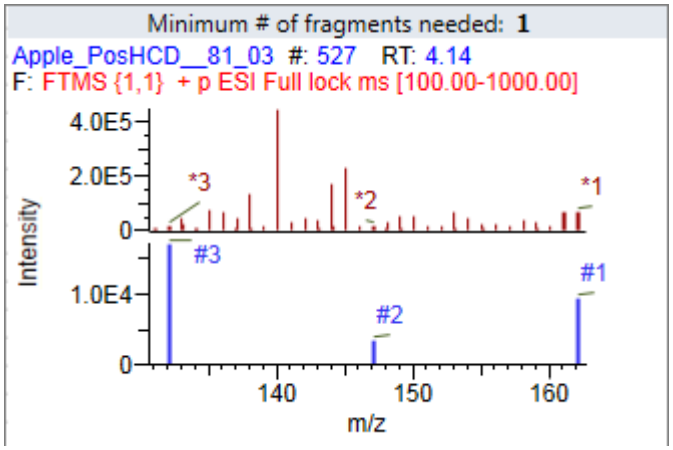


Figure 182. Library plot

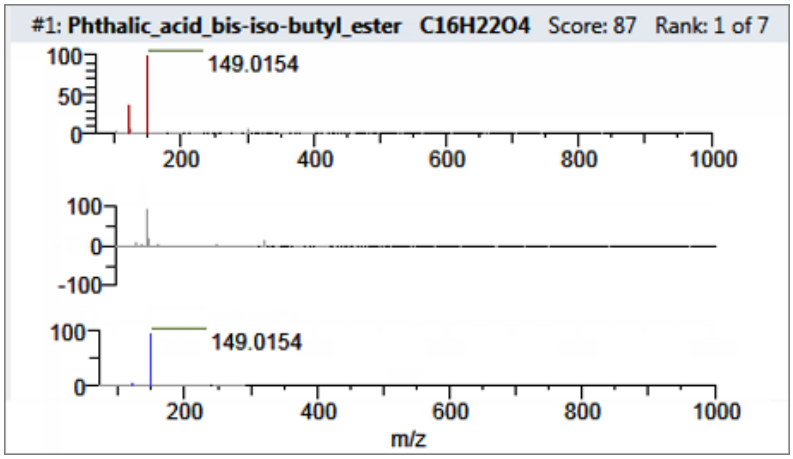


Figure 183. Plot Properties dialog box for an Isotope plot, a Fragment plot, or a Library plot

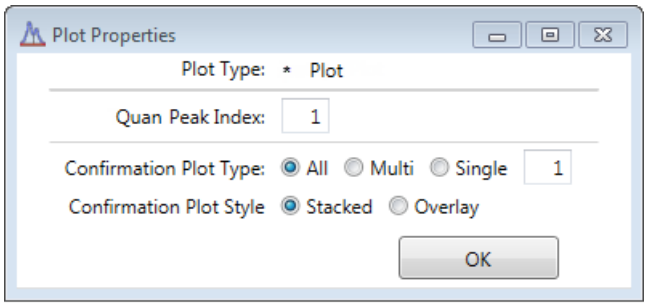


Table 90. Plot Properties parameters for an Isotope plot, a Fragment plot, or a Library plot

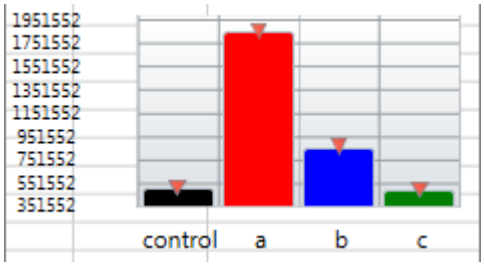
Command	Description
Target Peak Index	Specifies the number of peak plots to display. Valid values: 1 through 9
Confirmation Plot Type	Specifies that the plot display one of the following: • All: Displays isotopes, fragments, or library hits. • Multi: Displays individual plots for each isotope. You can individually stack or overlay the plots for each isotope. • Single: Displays only the selected isotope, fragment, or library hit. For examples of these display types, see Isotope, Fragments, or Library Match.
Confirmation Plot Style	Specifies that the plot display one of the following: • Stacked: Stacks the simulated spectrum and the peak apex spectrum. • Overlay: Overlays the two spectrum displays. For examples of these display types, see Isotope, Fragments, or Library Match.

Group Bar Graph plot

Click

to insert a Group Bar Graph plot.

Figure 184. Group Bar Graph plot



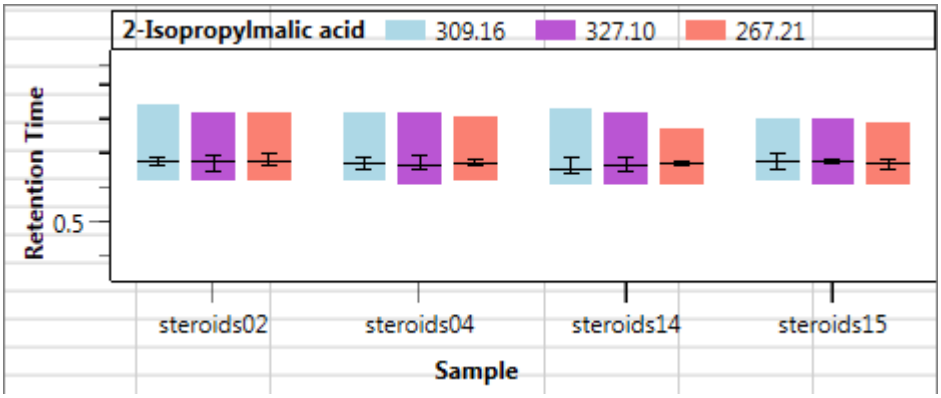
Note There are no plot properties for a group bar graph plot.

RT Summary plot

Click

to insert an RT Summary plot.

Figure 185. RT Summary plot



Note There are no plot properties for an RT summary plot.

XIC Overlay plot

Click

to insert an XIC Overlay plot.

Figure 186. XIC Overlay plot

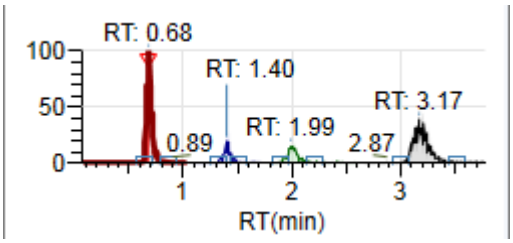


Figure 187. Plot Properties dialog box for an XIC Overlay plot

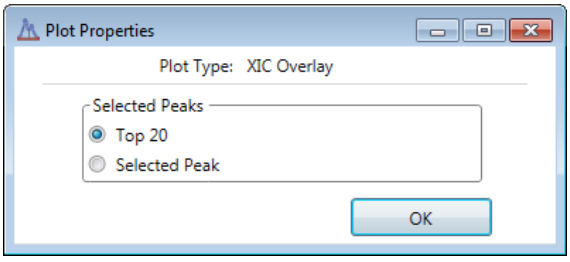
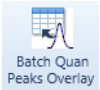


Table 91. Plot Properties parameters for an XIC Overlay plot

Command	Description
Selected Peaks	
Top 20	Displays the top 20 peaks.
Selected Peak	Displays only the selected peak.

Batch Quan Peaks Overlay plot

Click 

to insert a Batch Quan Peaks Overlay plot.

Figure 188. Batch Quan Peaks Overlay plot

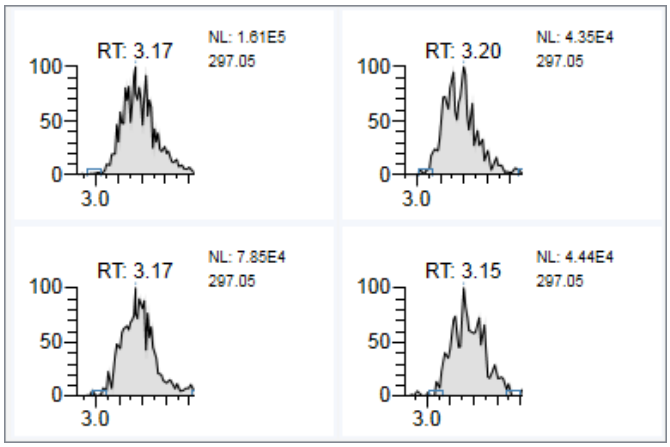


Figure 189. Plot Properties dialog box for a Batch Quan Peaks Overlay plot

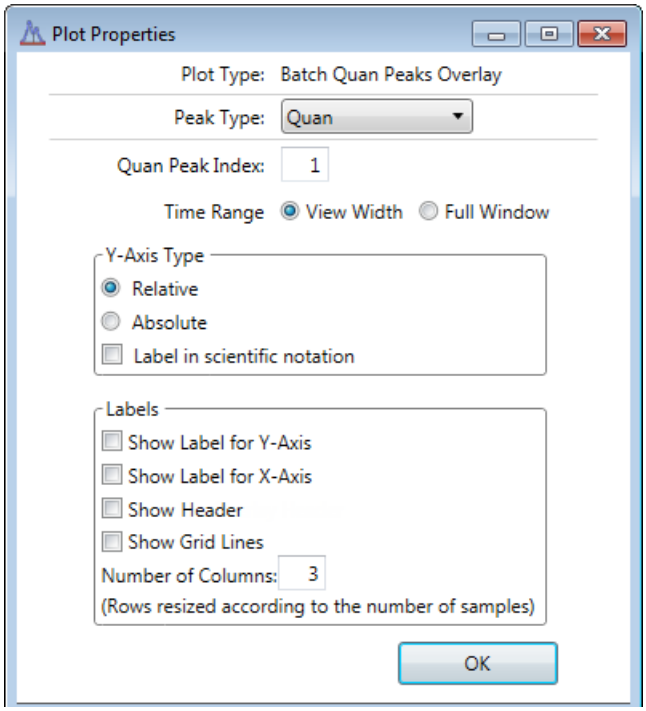


Table 92. Plot Properties parameters for a Batch Quan Peaks Overlay plot

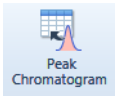
Command	Description
Quan Peak Index	Valid values: 1 through 9
Time Range	Specifies that the plot display one of the following: • View Width: Zooms the display on the peak of interest. • Full Window: Displays the full width of the scan.
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Header	Displays the raw data file name and compound name.
Show Grid Lines	Displays the grid lines in the plot background.
Number of Columns	Specifies the number of columns that you want to display in the inserted graphic. The application resizes the images to fit the specified number of columns.

Unknown screening plots

To customize the display in the unknown screening report, use the Plot Properties dialog box for each plot.

- Peak Chromatogram plot
- TIC Chromatogram plot
- Spectral plot
- XIC Overlay plot
- Library plot, Fragments plot, or Isotopes plot
- XIC plot
- Cross Sample Peak Overlay plot
- Chemical Structure plot
- Group Bar Graph plot

Peak Chromatogram plot

Click 

to insert a Peak Chromatogram plot.

Figure 190. Peak Chromatogram plot

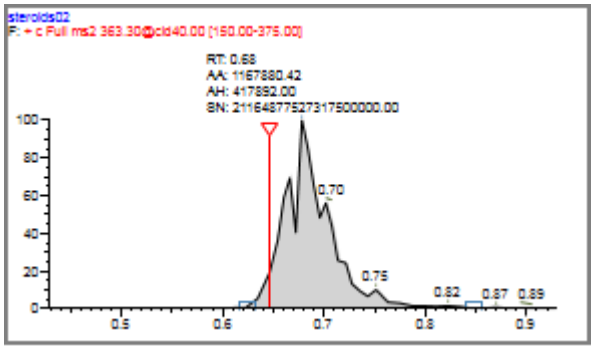


Figure 191. Plot Properties dialog box for Peak Chromatogram plot

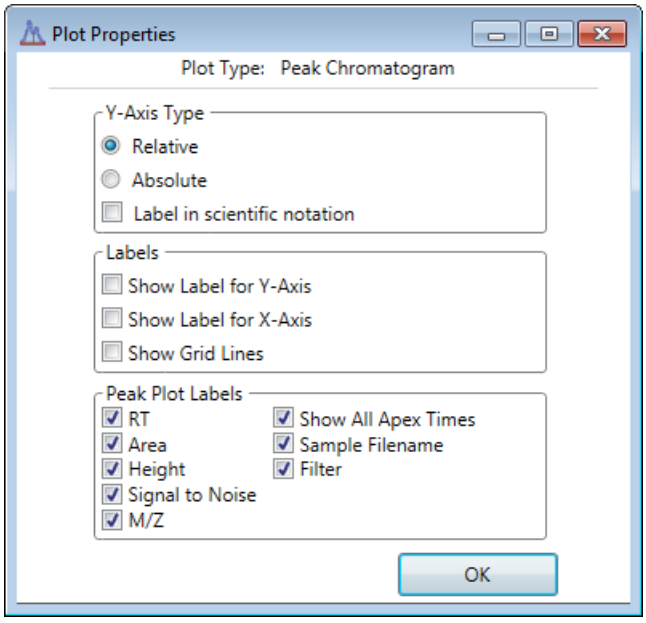


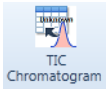
Table 93. Plot Properties parameters for a Peak Chromatogram plot (Sheet 1 of 2)

Command	Description
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.

Table 93. Plot Properties parameters for a Peak Chromatogram plot (Sheet 2 of 2)

Command	Description
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Grid Lines	Displays the grid lines in the plot background.
Peak Plot Labels	
RT	Displays the retention time (RT) label in the peak chromatogram plot.
Area	Displays the peak area (AA) label in the peak chromatogram plot.
Height	Displays the peak height (AH) label in the peak chromatogram plot.
Signal to Noise	Displays the signal-to-noise (SN) label in the peak chromatogram plot.
M/Z	Displays the peak mass.
Show All Apex Times	Displays all surrounding apex times in the plot.
Sample Filename	Displays the name of the sample file.
Filter	Displays the filter used for the scan. The plot displays the filter name below the raw data file name.

TIC Chromatogram plot

Click 

to insert a TIC Chromatogram plot.

Figure 192. TIC Chromatogram plot

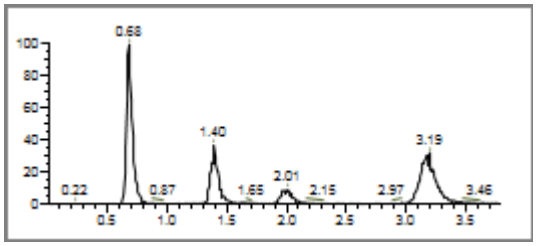


Figure 193. Plot Properties dialog box for a TIC Chromatogram plot

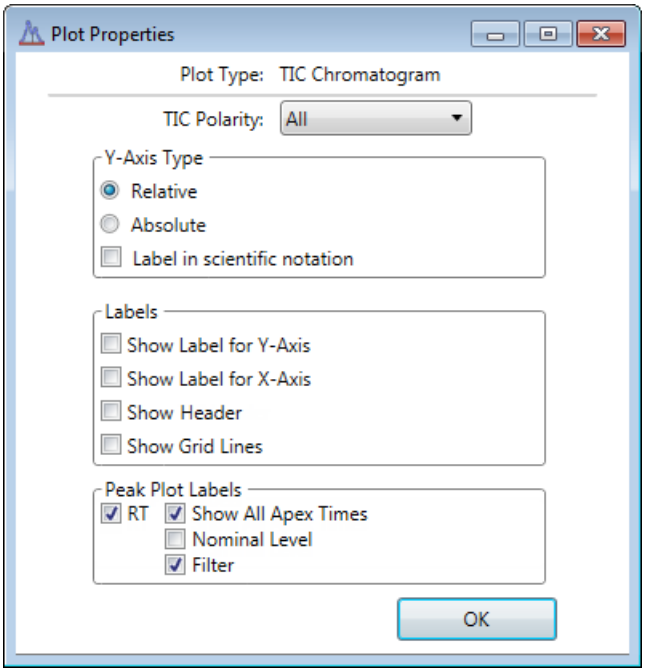


Table 94. Plot Properties parameters for a TIC Chromatogram plot (Sheet 1 of 2)

Command	Description
TIC Polarity	Specifies the polarity of adducts displayed in the plot. All: Displays positive, negative, and analog adducts. Positive: Displays only positive adducts. Negative: Displays only negative adducts. Analog: Displays only analog adducts.
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Header	Displays the raw data file name.
Show Grid Lines	Displays the grid lines in the plot background.
Peak Plot Labels	
RT	Displays the retention time (RT) label in the TIC chromatogram plot.
Show All Apex Times	Displays all surrounding apex times in the plot.

Table 94. Plot Properties parameters for a TIC Chromatogram plot (Sheet 2 of 2)

Command	Description
Nominal Level	Displays the nominal level (NL) values for each peak in the plot.
Filter	Displays the filter used for the scan. The plot displays the filter name below the raw data file name.

Spectral plot

Click

to insert a Spectral plot.

Figure 194. Spectral plot

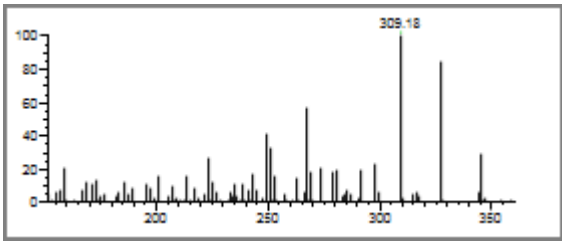


Figure 195. Plot Properties dialog box for a Spectral plot

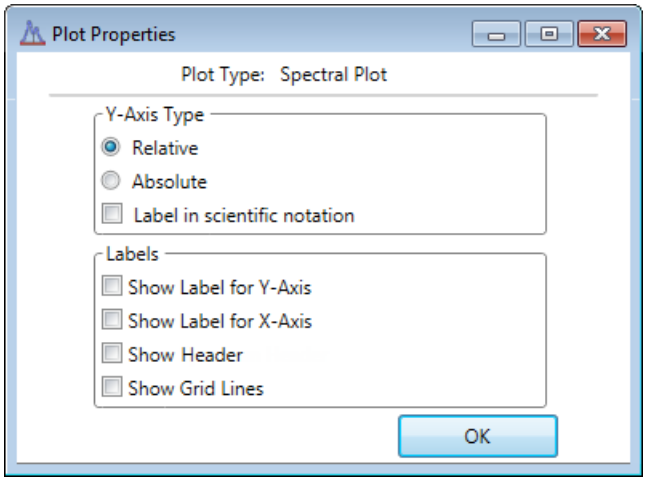


Table 95. Plot Properties parameters for a Spectral plot (Sheet 1 of 2)

Command	Description
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.
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.

Table 95. Plot Properties parameters for a Spectral plot (Sheet 2 of 2)

Command	Description
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Header	Displays the name of the sample file, the name of the compound, the retention time, the nominal level, and the filter used for the scan.
Show Grid Lines	Displays the grid lines in the plot background.

XIC Overlay plot

Click

to insert an XIC Overlay plot.

Figure 196. XIC Overlay plot

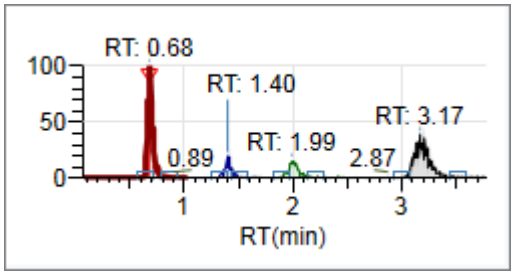


Figure 197. Plot Properties dialog box for an XIC Overlay plot

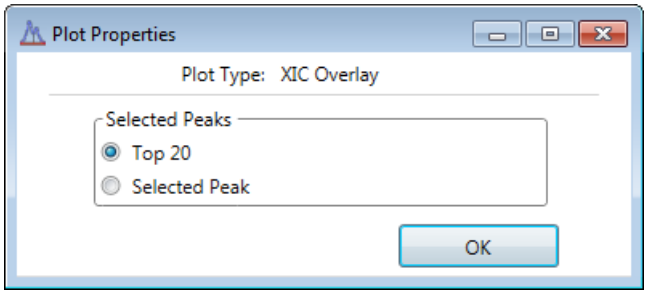


Table 96. Plot Properties parameters for an XIC Overlay plot

Command	Description
Selected Peaks	
Top 20	Displays the top 20 peaks.
Selected Peak	Displays only the selected peak.

Library plot, Fragments plot, or Isotopes plot

Do one of the following:

- Click

to insert a Library plot.
- Click

to insert a Fragments plot.
- Click

to insert an Isotopes plot.

The Library, Fragments, and Isotopes plots use identical plot properties.

Figure 198. Library plot

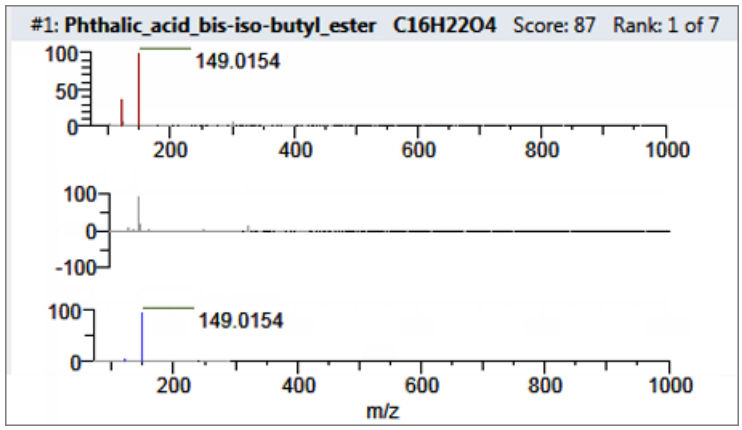


Figure 199. Fragments plot

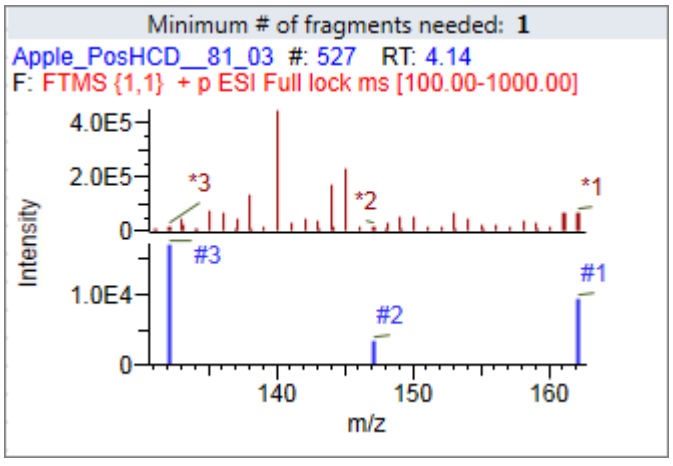


Figure 200. Isotopes plot

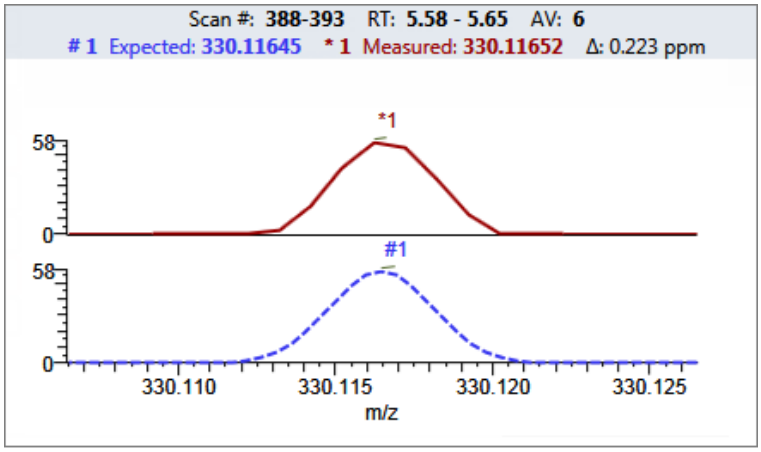


Figure 201. Plot Properties dialog box for a Library plot, a Fragments plot, or an Isotopes plot

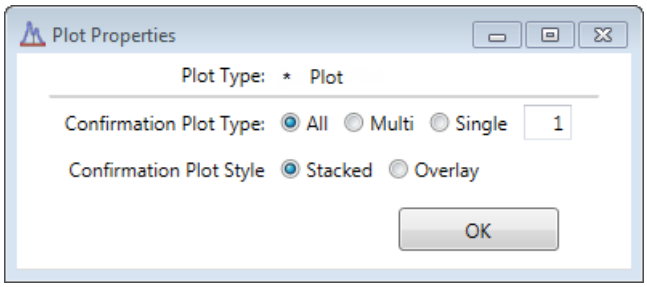


Table 97. Plot Properties parameters for a Library plot, a Fragments plot, or an Isotopes plot

Command	Description
Confirmation Plot Type	Specifies that the plot display one of the following: • All: Displays isotopes, fragments, or library hits. • Multi: Displays individual plots for each isotope. You can individually stack or overlay the plots for each isotope. • Single: Displays only the selected isotope, fragment, or library hit. For examples of these display types in the Data Review, see Library Search pane, Fragments pane, or Isotopes pane.
Confirmation Plot Style	Specifies that the plot display one of the following: • Stacked: Stacks the simulated spectrum and the peak apex spectrum. • Overlay: Overlays the two spectrum displays. For examples of these display types in the Data Review, see Library Search pane, Fragments pane, or Isotopes pane.

XIC plot

Click to insert an XIC plot.

Figure 202. XIC plot

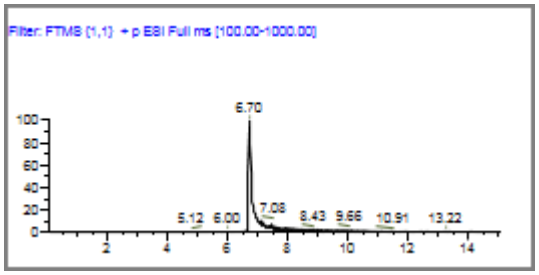


Figure 203. Plot Properties dialog box for an XIC plot

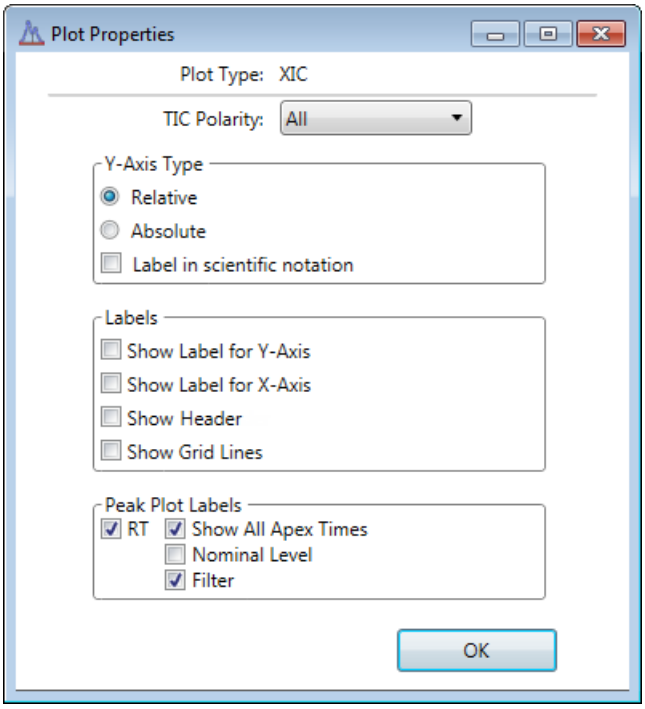


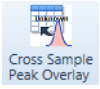
Table 98. Plot Properties parameters for an XIC plot (Sheet 1 of 2)

Command	Description
TIC Polarity	Specifies the polarity of adducts displayed in the plot. All: Displays positive, negative, and analog adducts. Positive: Displays only positive adducts. Negative: Displays only negative adducts. Analog: Displays only analog adducts.
Y-Axis Type	
Relative	Displays the *y*-axis scale from 0 through 100.

Table 98. Plot Properties parameters for an XIC plot (Sheet 2 of 2)

Command	Description
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.
Labels	
Show Label for Y-Axis	Displays the relative intensity value on the *y* axis.
Show Label for X-Axis	Displays the retention time (RT) value on the *x* axis.
Show Header	
Show Grid Lines	Displays the grid lines in the plot background.
Peak Plot Labels	
RT	Displays the retention time (RT) values for each peak in the plot.
Show All Apex Times	Displays all surrounding apex times in the plot.
Nominal Level	Displays the nominal level (NL) values for each peak in the plot.
Filter	Displays the filter used for the scan. The plot displays the filter name below the raw data file name.

Cross Sample Peak Overlay plot

Click 

to insert a Cross Sample Peak Overlay plot.

Figure 204. Cross Sample Peak Overlay plot

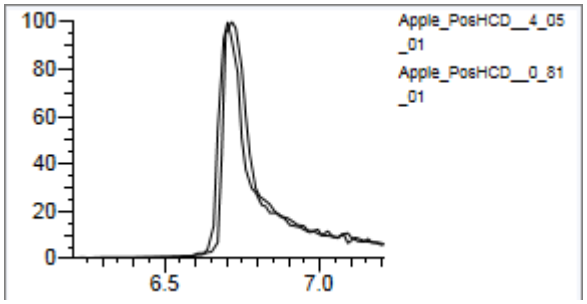


Figure 205. Plot Properties dialog box for a Cross Sample Peak Overlay plot

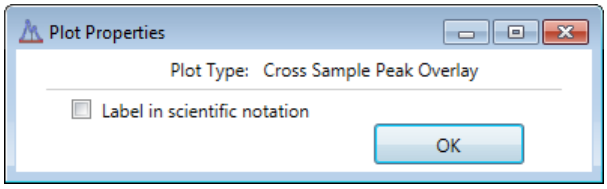


Table 99. Plot Properties parameter for a Cross Sample Peak Overlay plot

Command	Description
Label in Scientific Notation	Displays the *y*-axis scale in scientific notation.

Chemical Structure plot

Click

to insert a Chemical Structure plot.

Figure 206. Chemical Structure plot

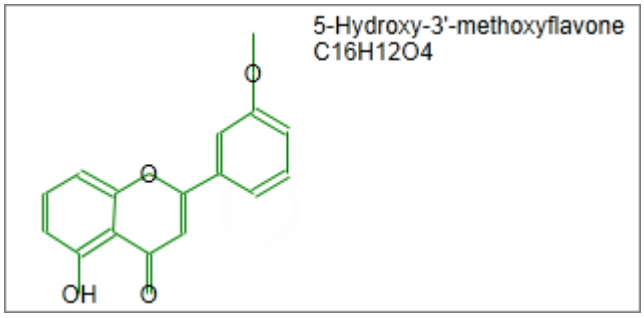


Figure 207. Plot Properties dialog box for a Chemical Structure plot

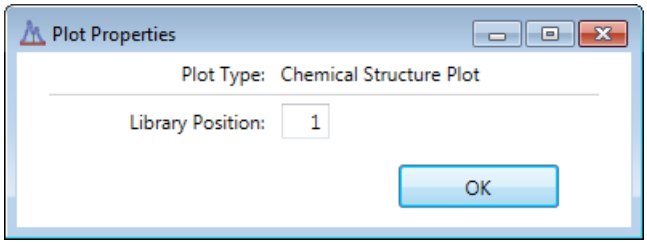


Table 100. Plot Properties parameter for a chemical structure plot

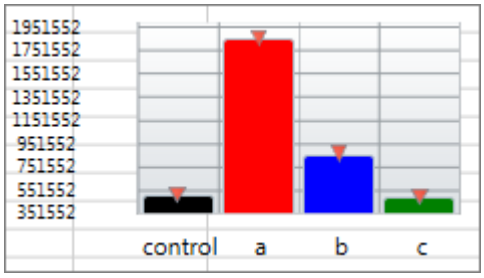
Command	Description
Library Position	Specifies the hierarchical position in the library when there are multiple chemical structures.

Group Bar Graph plot

Click

to insert a Group Bar Graph plot.

Figure 208. Group Bar Graph plot



Note There are no plot properties for a group bar graph plot.

Quick Tips

Follow these tips to make the most of the Report Designer features.

v **To move a report to the Archive folder**

1. With a report open for editing, choose **File > Archive** from the Report Designer main menu.
2. At the confirmation prompt, click **Yes**.

   The application deletes the report from the …*batch*\ReportOutput folder.

v **To insert items in the Report Designer**

- Insert a data table when the selected cell is above or below any other table, but not in the same row as a field. You cannot insert tables in repeat areas.
- Insert a data field when the selected cell is not in the same row as a table.
- Use these shortcut keys:

CTRL+T	Insert a table.
CTRL+T	Edit a table when the selected cell is inside a table.
CTRL+SHIFT+T	Insert or edit a field.
CTRL+R	Insert or edit a repeating area.

v **To format cells and group headers**

1. 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.
2. To sort fields, select a field, and then click **A-Z** to sort the data in ascending or descending order.

8

Confirming audited changes and using the Audit Viewer

In the Administrator 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, whether a user can submit a custom reason, and if a password is required. To use the auditing administration tools, refer to the instructions in the *TraceFinder Administrator Console User Guide*.

When auditing is enabled in the Administrator Console, the TraceFinder application records the following in a log file: all user access, including logging in, logging out, data creation and editing (batches, methods, and templates), and manual integration.

As specified in the Administrator Console, a user who performs an audited event can be required to give a reason. When security is enabled in the Administrator Console, a user who performs an audited event can be required to enter a password.

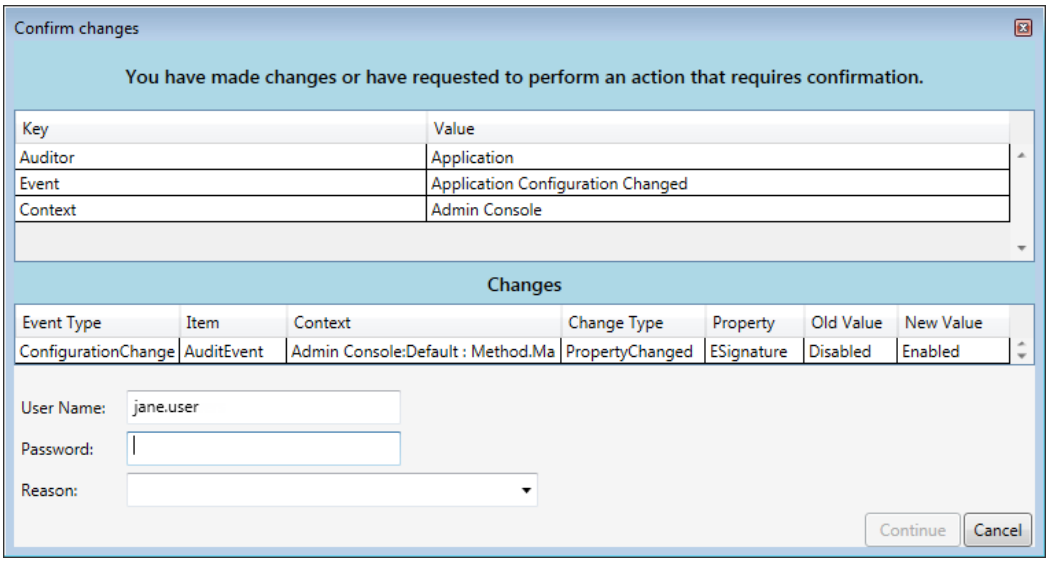
You can use the Audit Viewer to view the resulting log files to track modifications to the data. When an event requires confirmation (as specified in the Administrator Console), the audit log records who confirmed each change to a batch, method, or template. When no confirmation is required, then the audit log records the user who was logged in when the change occurred.

Contents

- Confirming audited changes
- Audit trail log files
- Audit log file functions
- Audit Viewer

Confirming audited changes

When you perform any audited action that requires a reason or password, the application displays the Confirm Changes dialog box.



- When the audited event requires a challenge, select a reason from the list of default reasons or type a custom reason in the Reason box.
- When the audited event requires an electronic signature, enter a password in the Password box.

> **IMPORTANT** Deactivating Security in the Administrator Console also deactivates the password feature in the Confirm Changes dialog box.

To view or edit the required confirmation for an audited event, refer to the Chapter 3, "Using the Audit View," in the *TraceFinder Administrator Console User Guide*.

Audit trail log files

The application creates the following audit trail log files:

- Application: Records all user access, such as starting and stopping the application, logging in, logging out, and accessing or saving data in batches and methods. The log file with this data is saved in …\TraceFinderData\Admin\AuditLog.adb.
- Master Method: Records all user interactions with master methods, such as creating, opening, or editing a master method. The log file with this data is saved in …\TraceFinderData\Methods*MasterMethodName*\5.2\AuditLog.adb.
- Batch: Records all user interactions with batches, such as creating, opening, editing, acquiring, processing, or generating reports for a batch. The log file with this data is saved in …\TraceFinderData\Projects*SubFolder**BatchName*\Batch\5.2\AuditLog.adb.

Audit log file functions

The Audit Viewer displays all saved audit log files, and you can filter and sort the audit data.

Note The Audit Viewer is available only when you have enabled auditing from the Administrator Console. Refer to the *TraceFinder Administrator Console User Guide*.

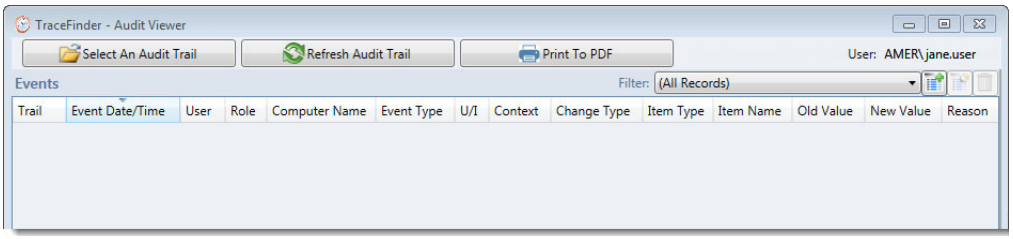
Follow these procedures:

- To access the Audit Viewer
- To select an audit trail
- To create a filter for audit log events
- To create a filter for an audit log

v To access the Audit Viewer

Choose **Tools > Audit Viewer** from the TraceFinder main menu, or click the **Audit Viewer** icon, .

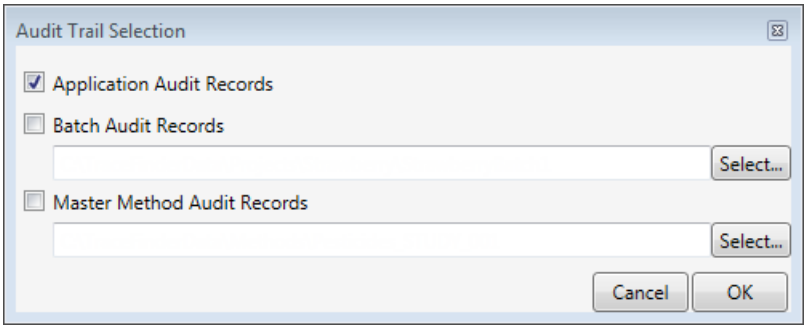
The Audit Viewer opens.



v To select an audit trail

1. Click Select An Audit Trail.

   The application opens the Audit Trail Selection dialog box.



2. Select the check box for each type of record that you want to display in the Audit Viewer.
   - **Application Audit Records** display all events: application, batch, batch template, method, security, or instrument.
   - **Batch Audit Records** display only batch events.
   - **Master Method Audit Records** display only method events.

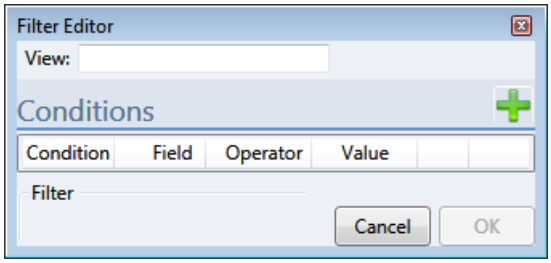
3. When you select batch or master method records, click **Select** and locate the batch or method whose records you want to display.
4. Click **OK**.

   The Audit Viewer displays the contents of the selected audit log files.

v **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.

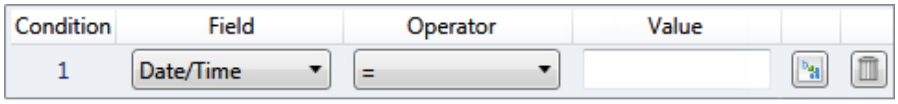
   

2. In the View box, type a name for the new filter.

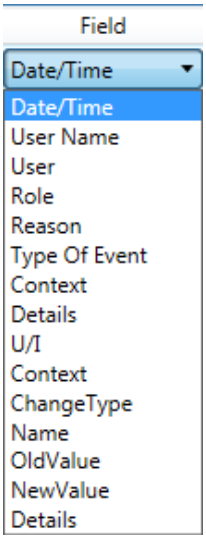
   You can also leave the View box empty when you enter your filter criteria. When you finish adding conditions and click OK (step 8), the application filters the current events list based on the filter criteria you specify, but the filter is not saved. The Filter list in the viewer identifies this filter as (Custom).

3. Click the **Add** icon, .

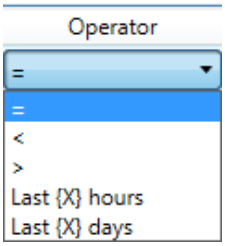
   The application adds a new, undefined condition to the Condition list.

4. In the Field list, select one of the following field types.



5. In the Operator list, select one of the available operators.



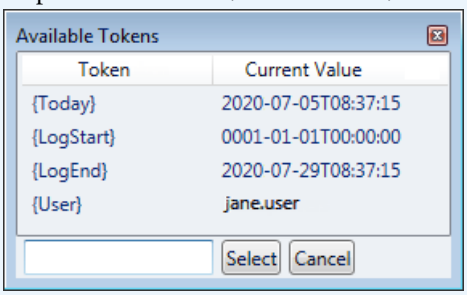
The available operators depend on the field type that you selected.

This example shows the

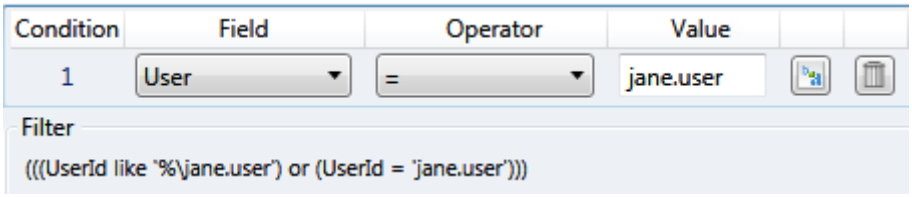
6. In the Value box, type a value or select a value from the list.

   - For the Date/Time field, type a numerical value in the Value box.
   - For fields that require a text entry, type the appropriate text in the Value box. This value is case sensitive.
   - For fields that have a list of values, such as the Type of Event field, select a value from the list.

Tip You can also click the Tokens icon, , and select a token for the Value. Tokens are predefined values, such as dates, user names, and sample or compound identifiers.



The Filter area at the bottom of the Filter Editor dialog box displays the complete definition for the filter.



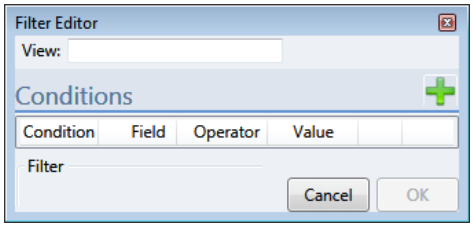
7. Repeat step 3 through step 6 for each condition that you want to include in your filter.
8. When you have added all your conditions, click **OK**.

   The application creates the new filter with the specified conditions.

v **To create a filter for an audit log**

1. Click the **Create New Filter** icon, .

   The Filter Editor dialog box opens.

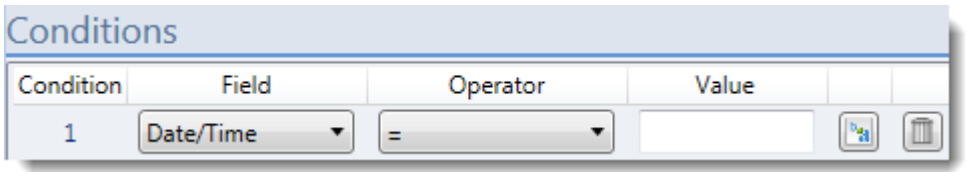
   

2. In the View box, type a name for the new filter.

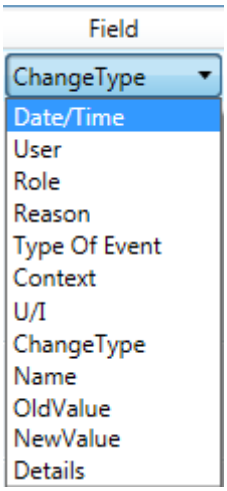
   You can also leave the View box empty when you enter your filter criteria. When you finish adding conditions and click OK (step 8), the application filters the current history list based on the criteria you specify, but the filter is not saved. The Filter list in the viewer identifies this filter as (Custom).

3. Click the **Add** icon, .

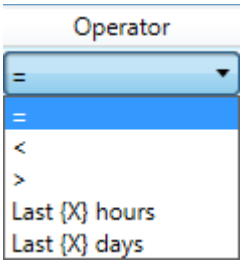
   The application adds a new, undefined condition to the Conditions list.

4. In the Field list, select one of the following field types.



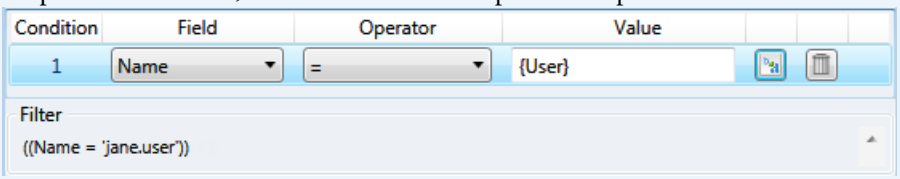
5. In the Operator list, select from the available operators.



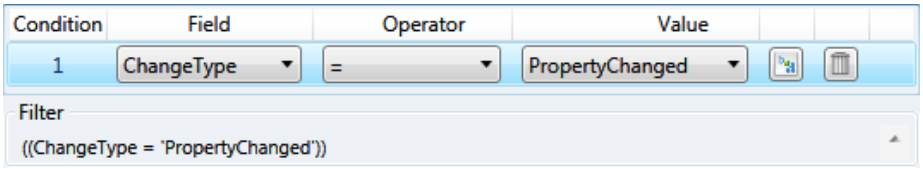
The available operators depend on the field type that you selected.

6. In the Value box, type or select a value from the list.

Tip 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.

Audit Viewer

Use the Audit Viewer to track user access and modifications to the audit log data. See Audit Viewer parameters.

Figure 209. Audit Viewer

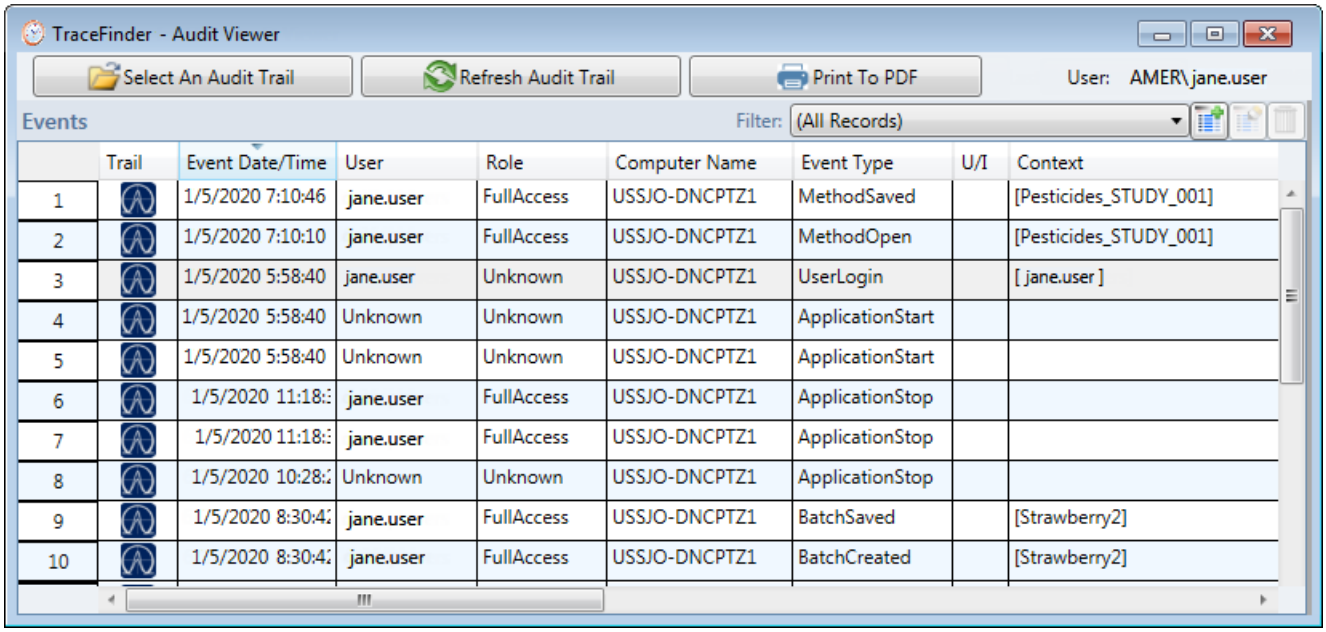


Table 101. Audit Viewer parameters (Sheet 1 of 2)

Parameter	Description
Select An Audit Trail	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.
Refresh Audit Trail	Refreshes the current audit log file in the viewer.
Print To PDF	Prints the currently filtered audit records to a PDF file.
Events	
Filter	Select a filter view to use for displaying the event log entries. Filter: (All Records) 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.

Table 101. Audit Viewer parameters (Sheet 2 of 2)

Parameter	Description
Trail	Indicates any event: application, batch, batch template, method, security, or instrument. Indicates a method event. Indicates a batch event.
Event Date/Time	Time stamp of the event.
User Name	Full name of the user (when available).
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.
Role	Security role assigned to the user in the Administrator Console.
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 Administrator Console User Guide*.
U/I	Associated user interface, such as the Administrator Console or Configuration Console.
Context	Name of the sample, batch, or method where the event occurred.
Change Type	One of the predefined ChangeType values in the filter definition.
Item Type	One of the predefined ItemType values.
Item Name	A user-defined name for the filter.
Old Value/New Value	Original parameter value and the changed value.
Reason	Default or custom reason that the user entered for the event.

A

Using quick acquisition

Use the quick acquisition feature to quickly submit samples from any mode in the application.

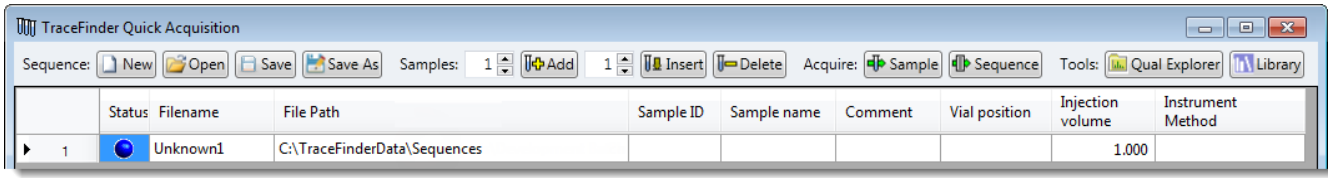
Note The Quick Acquisition feature is available only when you activate it in the Configuration console. Refer to Chapter 1, "Using the Configuration Console," in the *TraceFinder Lab Director User Guide*.

Tip (Animation) To view "Quick Acquisition," choose **Help > Animations**.

v **To run a quick acquisition**

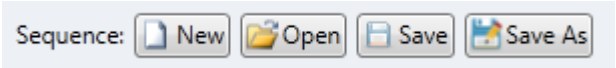
1. Choose **Tools > Quick Acquire Sample** from the main menu or click the **Quick Acquire Sample** icon, .

   The TraceFinder Quick Acquisition window opens.



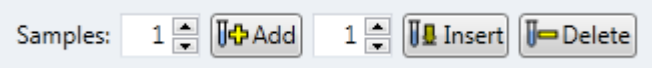
2. To create the sequence of samples that you want to acquire, do any of the following:

   - Use the Sequence buttons in the toolbar to open and save Xcalibur sequence (.sld) files.



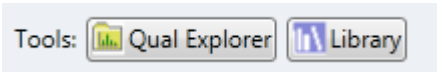
Button	Description
New	Replaces the current sequence with a new sequence that contains one Unknown sample.
Open	Opens the Open dialog box where you can open a saved SLD file.
Save	Saves the current sequence as an SLD file in the …\TraceFinderData\Sequences folder.
Save As	Opens the Save As dialog box where you can save the current sequence to a new file name or location.

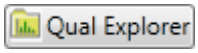
- Use the Samples buttons in the toolbar to create a sequence of samples.



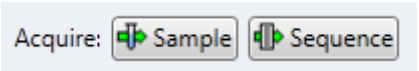
Button	Description
	Adds the specified number of new, empty samples to the end of the sample list.
	Inserts a new, empty sample or samples above the selected sample.
	Removes the selected samples from the sample list.

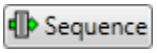
- (Optional) Use the Tools buttons in the toolbar to open a qualitative browser or the NIST library browser.



Button	Description
	Opens the qualitative explorer that you configured as your default qualitative explorer in the Configuration console. See Launching a qualitative explorer application.
	Opens the NIST library browser. See Launching the NIST Library Browser.

3. When you have completed your sequence of samples, click either of the Acquire buttons.



Button	Description
	Submits only the selected samples for acquisition, processing, or report generation.
	Submits the sequence for acquisition, processing, or report generation.

The application submits the samples for acquisition, processing, and report generation. See Real Time Status – Acquisition page.

B

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.

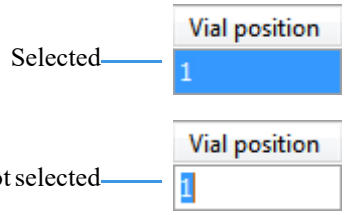
Follow these procedures:

- To automatically copy column values
- To automatically enter sequential column values
- To specify a range of values

v 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**.

   The value is copied to all rows below the selected row.

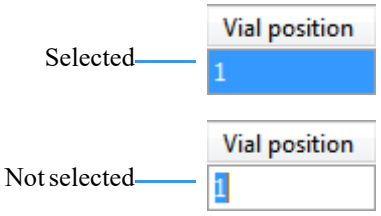
v To automatically enter sequential column values

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**.

   The application enters sequential column values starting with the value in the selected row and ending with the last row in the column.

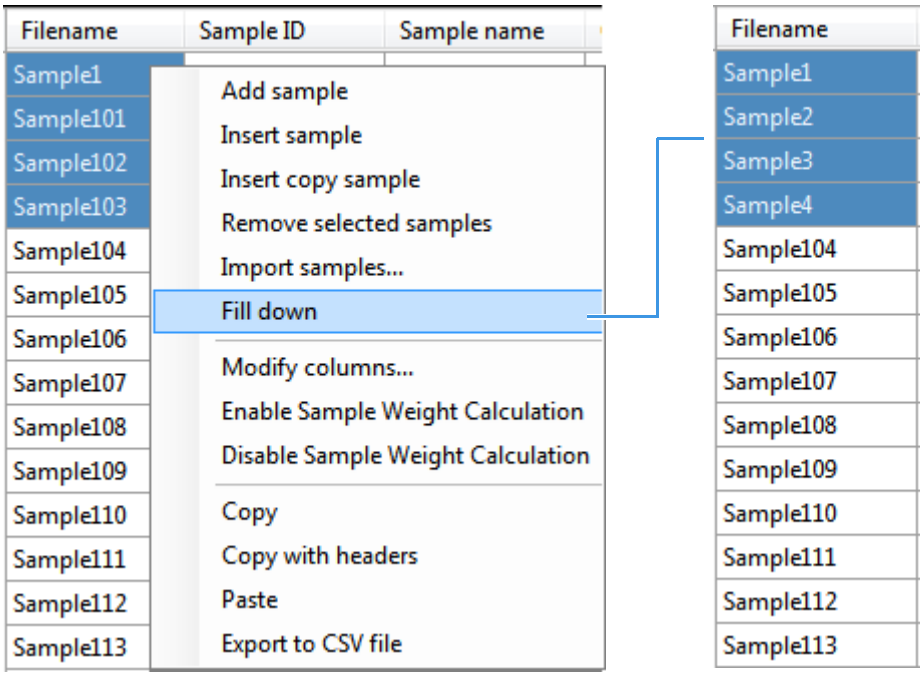
   You can repeatedly use the Fill Down command to create multiple sequences.

Vial position
A:A1
A:A2
A:A1
A:A2
A:A1
A:A2
A:A3
A:A4

   When you use the Fill Down command for the Vial Position column with an autosampler configured, the application knows the number of vial positions configured in your autosampler and numbers the positions accordingly.

Vial position
A:A1
A:A2
A:A3
A:A4
A:A5
A:A6
A:B1
A:B2
A:B3
A:B4
A:B5
A:B6

v To specify a range of values

1. Use the Copy Down or Fill Down command to specify a range of samples.To select a range of sample values, do one of the following:
   - Drag your cursor to select a contiguous group of sample values.
   - 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.