Thermo

TraceFinder

User Guide

Software Version 3.1
Optimized for Forensic Toxicology

XCALI-97540   Revision A   June 2013

DOCUMENTATION
SURVEY

Thermo
SCIENTIFIC

Contents

Contents

Preface

Thermo TraceFinder™ 3.1 is the newest application in the Thermo Scientific™ series of GC/MS and LC/MS analytical software.

Contents

- Related Documentation
- Safety and Special Notices
- System Activation
- Contacting Us

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

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

DOCUMENTATION SURVEY

Related Documentation

TraceFinder includes Help and these manuals as PDF files:

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

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

Choose **Start > All Programs > Thermo TraceFinder > Manuals**.

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

1. Open the TraceFinder application and choose **Help > TraceFinder Help.**

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

   • To create your own bookmarks, use the Favorites pane.

2. To view one of the user guides or one of the quick reference guides, choose **Help > Manuals > * User Guide** or * **Quick Reference Guide**.

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

Safety and Special Notices

Make sure you follow the precautionary statements presented in this guide. The safety and other special notices appear in boxes.

Safety and special notices include the following:

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

> **Note** Highlights information of general interest.

> **Tip** Highlights helpful information that can make a task easier.

System Activation

> **Tip** Highlights helpful information that can make a task easier.

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

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

Two types of licenses are available:

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

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

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

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

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

❖ **To request an activation key**

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

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

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

   The form of the barcode number is either *xxxx-xxxx-xxxx* or *xxxx-xxxx-xxxx-xxxx*.
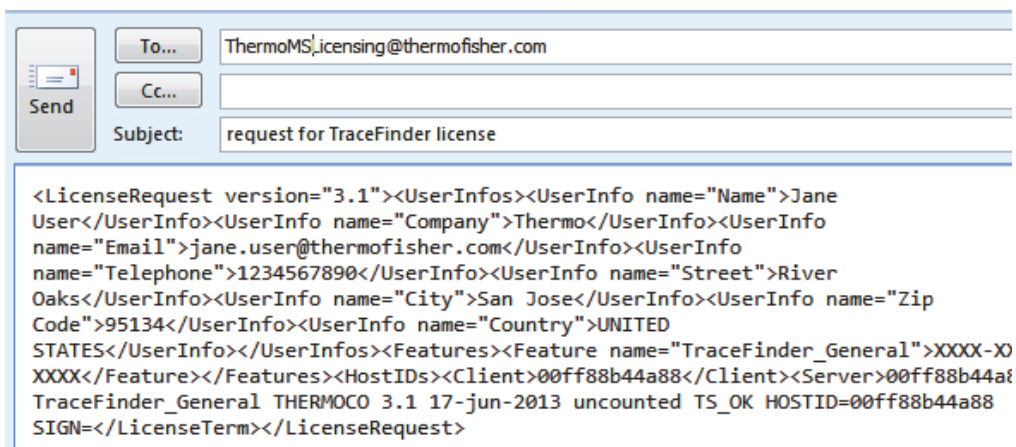
   Note The barcode might already be filled in for you.

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

   The application copies this XML text to the Clipboard.

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

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

You will receive an e-mail response containing the activation key.

❖ **To use your activation key**

1. When you receive your activation key, copy it from the e-mail.

2. Choose **Help > License Activation** from the TraceFinder menu.

   The License Activation window opens.

   > **Note** The License Activation window for power modules automatically opens when
   > you try to enable the power module features in the Configuration console.

3. Click **Paste**.

   The application pastes the contents of the Clipboard to the License Text box.

4. Click **Set.**

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

Contacting Us

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

❖ **To contact Technical Support**

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

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

❖ **To contact Customer Service for ordering information**

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

❖ **To get local contact information for sales or service**

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

Introduction

This chapter describes general features of the TraceFinder software.

Contents

About the TraceFinder Application

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

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

The TraceFinder application can import the following file types:

- Sample lists in .csv or .xml format

  See "Defining the Sample List" on page 340.

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

  For detailed information about creating processing methods, see "Working with Master Methods" on page 85.

  For detailed information about creating instrument methods, see "Working with Instrument Methods" on page 309.

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

  See "Editing Compounds in the Database" on page 285.

- Batches, methods, or templates from the following applications:
  - TraceFinder 1.0, 1.1, 2.0, 2.1, or 3.0
  - QuanLab Forms or ToxLab Forms 2.5 or 3.0

  See "Converting Legacy Data" on page 20.

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

Supported File Types

The TraceFinder application supports the following file types:

- Comma-separated values (.csv): A set of file formats used to store tabular data in which numbers and text are stored in plain textual form that can be read in a text editor. Lines in the text file represent rows of a table, and commas in a line separate fields in the tables row.

- Extensible Markup Language (.xml): A generic framework for storing any amount of text or any data whose structure can be represented as a tree. The only indispensable syntactical requirement is that the document has exactly one root element (also called the document element). This means that the text must be enclosed between a root start-tag and a corresponding end-tag.

- Instrument method (.meth): A proprietary file format for the Xcalibur software suite with specific instructions that enable scientific instruments to perform data acquisition.

- Processing method (.pmd): A proprietary file format for the Xcalibur software suite with specific instructions on processing data that was acquired through the instruments attached to the system.

- Raw data (.raw): The file type for acquired samples on the system.

- Compound database (.cdb): The file type for TraceFinder or ExactFinder compound database data.

- Library (.db): A library used for target screening.
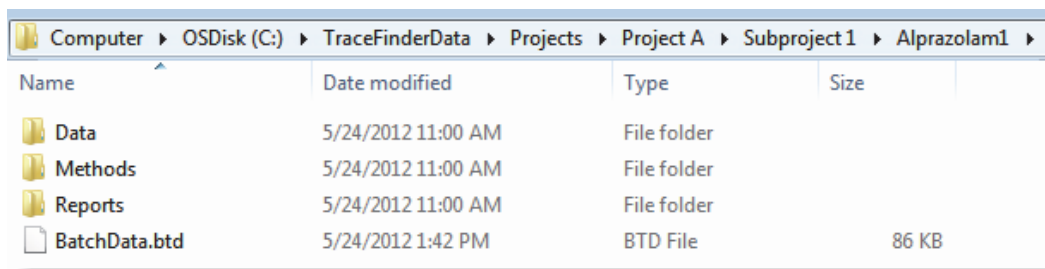
TraceFinder Directory Structure

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

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

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

Figure 1. Example batch directory structure

TraceFinder Summary of Features

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

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

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

Key features include the following:

- Role-based authorization for 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, screening library selection, and customized columns and flags

- Method Development mode for editing instrument methods, setting processing and error flag parameters, and setting report options

- Choice of acquisition wizards:

  – Acquisition batch mode that guides you in creating batches and running samples

  – Batch template wizard similar to the interface used in the ToxLab Forms application

- Analysis mode with batch views, data review, local method views, and report views

- Database-capable method development

- Quantification workflows, supporting capabilities present in the LCquan™ and ToxLab Forms applications

- Target screening workflows

- Standard and customized report formats

Features of the common workflow core include the following:

- Acquisition and processing

- Peak detection

- Quantification to include calibration

- Error analysis and flag setting

- Reporting

- Data persistence

- Raw data file handling

TraceFinder Workflow

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

When using the TraceFinder application, follow these basic steps:

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

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

   - How the raw data is acquired and processed

   - How the error checking information evaluates the results

   - How the results appear in reports

2. Create and submit a batch using one of the batch wizards.

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

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

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

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

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 currently selected batch.

Reporting Features

The report engine can generate several different types of reports designed to meet the needs of the laboratory, the laboratory's customers, and key regulatory agencies that might review the results. The following types of reports meet the requirements of various methods and worldwide regulatory agencies, helping to track the performance of LC and GC systems and methods. The reports divide into four groups: Standard, Custom, Target Screening, and ToxID.

For additional information about standard, custom, target screening, or ToxID™ reports and examples of each standard report type, see "Reports" on page 591.

Examples of standard reports (as PDF files) are also located in the following folder:

C:\Thermo\TraceFinder\3.1\Forensic\ExampleReports

Standard Report Types

- Batch Report
- Batch Summary Report
- Batch Report Rev 1
- Calibration Report
- Calibration Curve Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- High Density Calibration Report
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Intelligent Sequencing Report
- Internal Standard Summary Report
- Ion Ratio Failure Report
- Manual Integration Report
- Method Report
- Negative Report
- Qualitative Peak Report
- Qualitative Summary Report
- Quality Control Report
- Quantitation Report
- Quantitation Report - 2
- Sample Report
- Sample Report Long
- Solvent Blank Report

Custom Report Types

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

Target Screening Report Types

- Target Screening High Density Sample Report
- Target Screening Summary Report

ToxID Report Types

- Target Screening Long Report
- Target Screening Summary Report

Getting Started

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

Contents

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

Installing the TraceFinder Application

To initially install the TraceFinder 3.1 application, follow the instructions in the *TraceFinder Installation Guide*. Later, you might need to reinstall the TraceFinder application or other features on the InstallShield Wizard, such as the power modules.

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

❖ **To reinstall the TraceFinder application**

1. From the Thermo Foundation Instrument Configuration window, remove all instruments.

2. From the Windows™ Control Panel, uninstall the TraceFinder application and then uninstall all Thermo instrument drivers.

3. Insert the TraceFinder CD, and install both the TraceFinder 3.1 application and the NIST library as follows:

   a. Open the TraceFinder launcher and click **Next**.

The InstallShield Wizard opens.
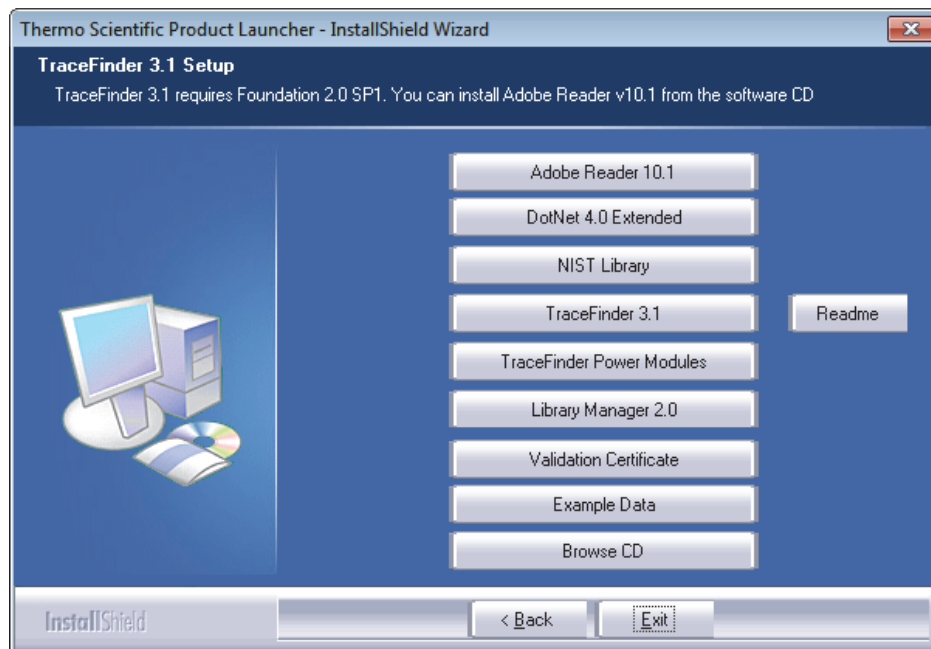
b. Click **TraceFinder 3.1**, and follow the instructions in the InstallShield Wizard.

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

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

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

e. Click **TraceFinder 3.1**, and follow the instructions in the InstallShield Wizard.

> **IMPORTANT** For the TraceFinder application to properly install, you might be prompted to uninstall Thermo Foundation™. Do the following:
>
> 1. Click **Yes**, and then when prompted to restart your computer, click **OK**.
>
>   The wizard continues the TraceFinder installation.
>
> 2. When prompted to install Thermo Foundation, click **Yes**, and then when prompted to restart your computer, click **OK**.
>
>   The wizard continues the installation.

f. When prompted, choose to install either the **GC** or **LC** version of the software.

g. When the installation completes, open the TraceFinder launcher again and click **Next**.

h. (Required for ToxID) If you have not previously installed the NIST library, click **NIST Library** and follow the instructions to install the library.

3. (Optional) Click **Example Data**, and follow the instructions to install an example project that contains example batch data.

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

Follow these instructions to start the TraceFinder application.

❖ **To start the TraceFinder application**

1. Configure your instruments.

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

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

   By default, user security is not activated and the application does not require a password. To activate user security, see "ToxID" on page 65.

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

> **Note** Before you can log in to the TraceFinder application when user security is activated, a system administrator must set up a user account for you. The administrator assigns you a user name and password and gives you permission to access specific modes.

1. Enter your assigned user name in the TraceFinder login window. See "TraceFinder login window" on page 13.

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

2. Enter your password.

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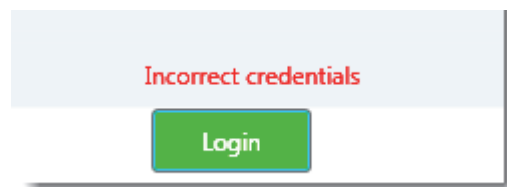
   Correct the user name or password, or contact your system administrator.

3. Click **Login**.

   The TraceFinder login window opens. See TraceFinder main window.

Figure 2. TraceFinder main window

User name and Log Off button available
only when user security is activated
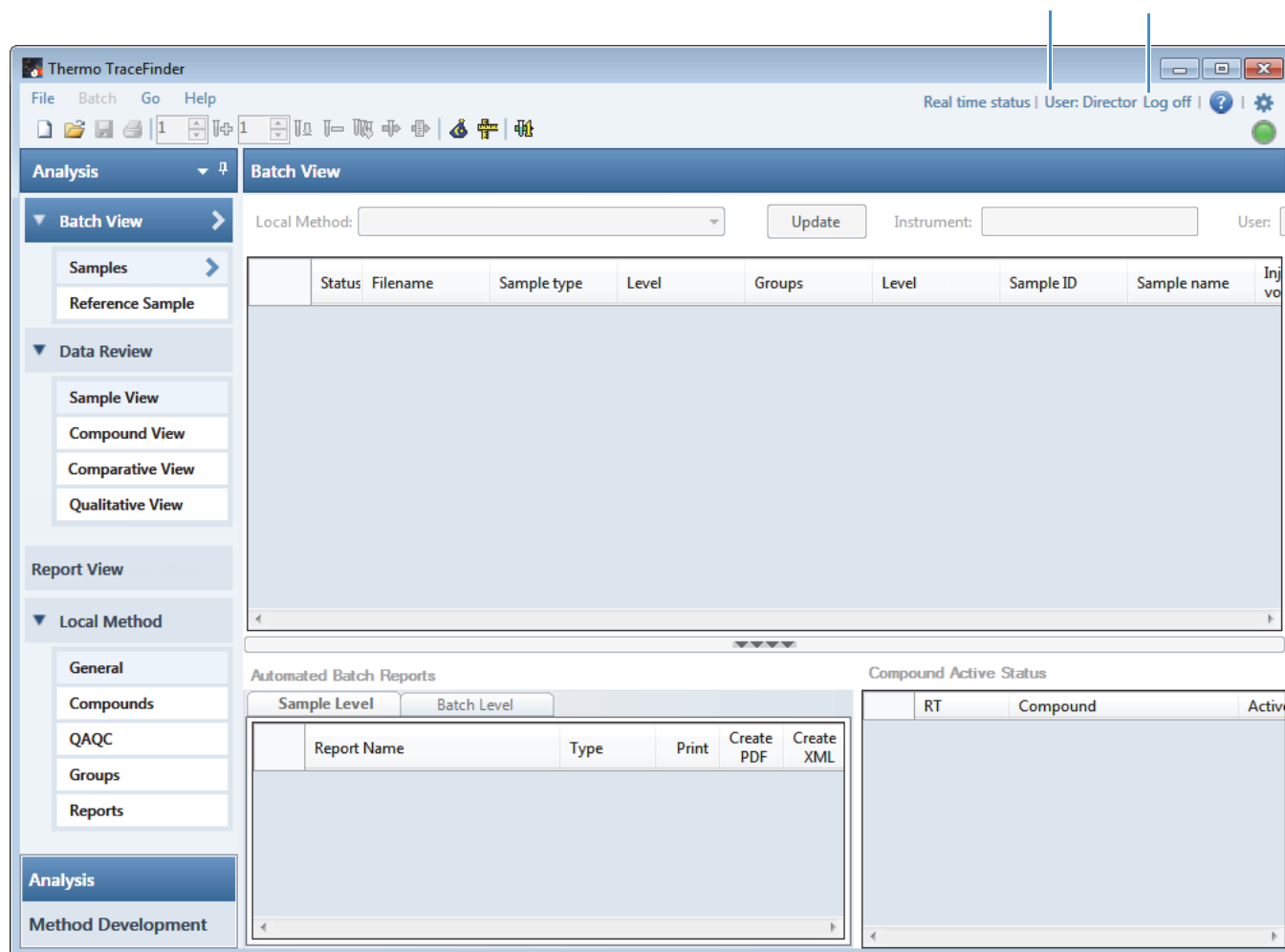
Figure 3. TraceFinder login window
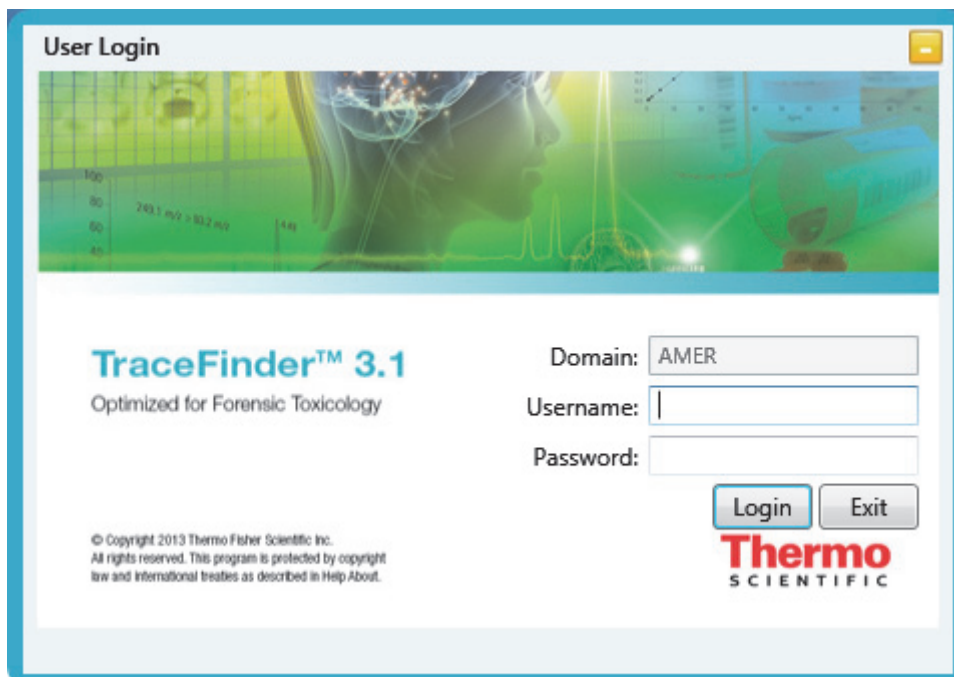
Table 1. Login window parameters

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

Installing the Power Modules

Follow these instructions to install and activate the TraceFinder power modules for multiplexing and intelligent sequencing.

❖ **To install the power modules**

1. Follow the instructions to install the TraceFinder application.

   See "Installing the TraceFinder Application" on page 9.

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

3. Click **TraceFinder Power Modules**, and follow the instructions to install the multiplexing and intelligent sequencing modules.

4. License the power modules.

   To license the power modules, follow the same procedures for licensing the TraceFinder application. See "System Activation" on page ix.

   The features associated with these power modules are mutually exclusive and are not automatically activated.

5. To activate these power modules, see "Activating Optional Features" on page 64.

Installing the NIST and QED Libraries

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

❖ **To install the NIST library**

1. Open the TraceFinder launcher, and click **Next**.

2. Click **NIST Library**.

   The NIST 08 MS Search and AMDIS Setup wizard opens.

3. Follow the instructions in the setup wizard.

4. When the wizard prompts you to select a destination folder, select **C:\Program Files\NISTMS**.

❖ **To install the QED library**

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

   The Thermo Xcalibur Roadmap opens.
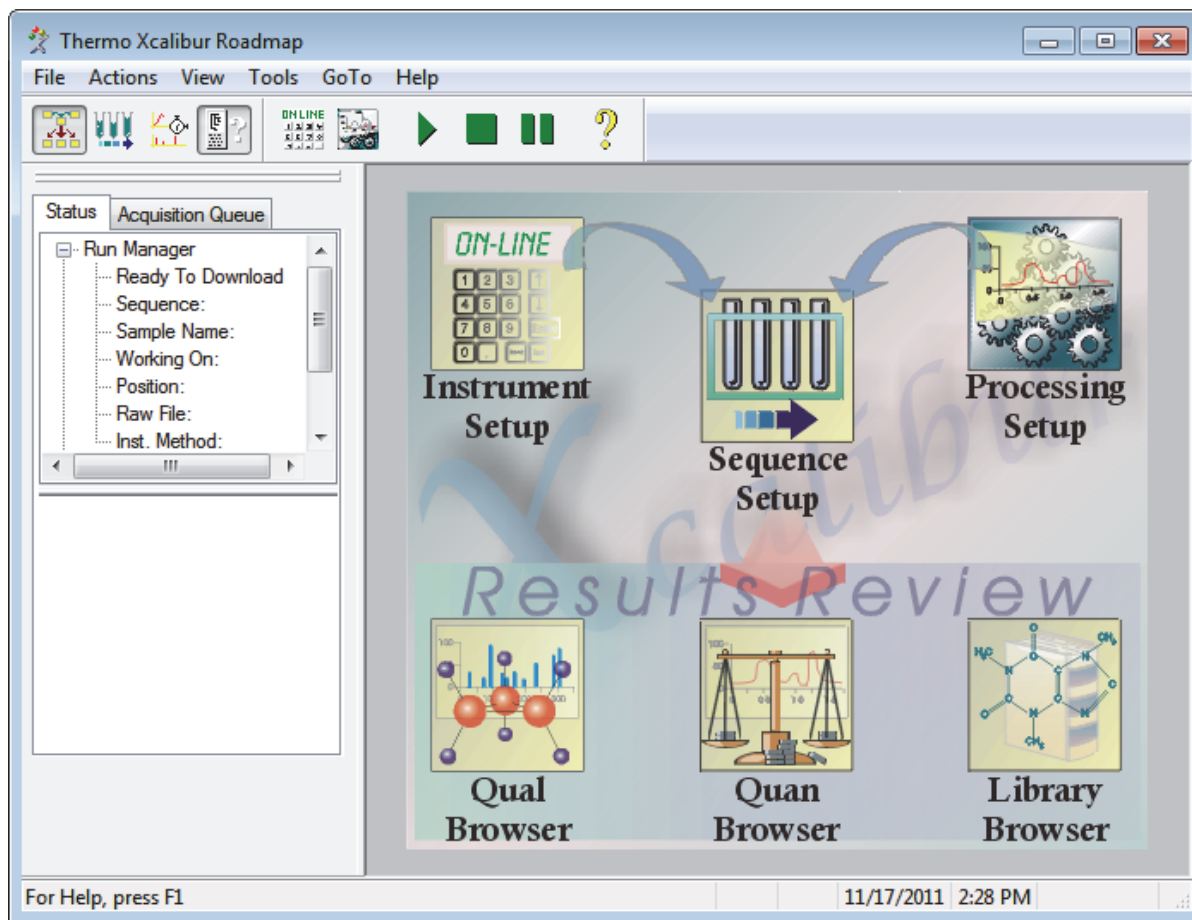
2. Choose **Tools > Library Manager** from the main menu.

The Thermo Library Manager dialog box opens, showing the NIST Libraries list.
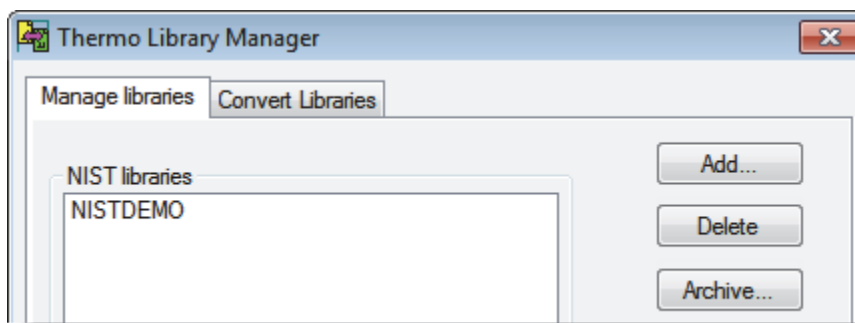
3. Click **Add**.

The Add Library dialog box opens.
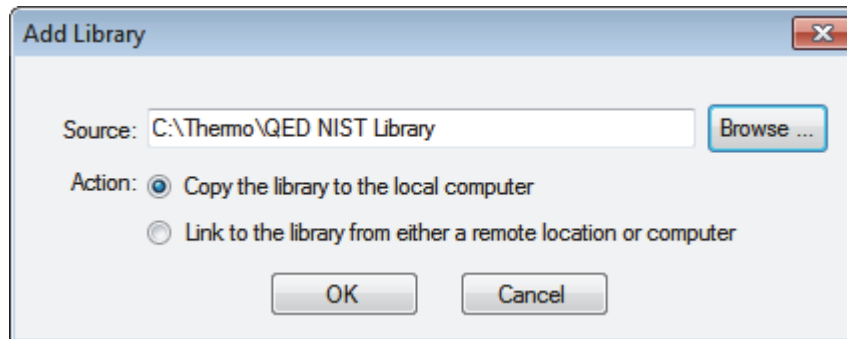
4. Click **Browse**, and locate your QED library in the C:\Thermo folder.

5. Click **OK**.

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

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

The Xcalibur application adds the QED library to the NIST Libraries list in the Library Manager dialog box.
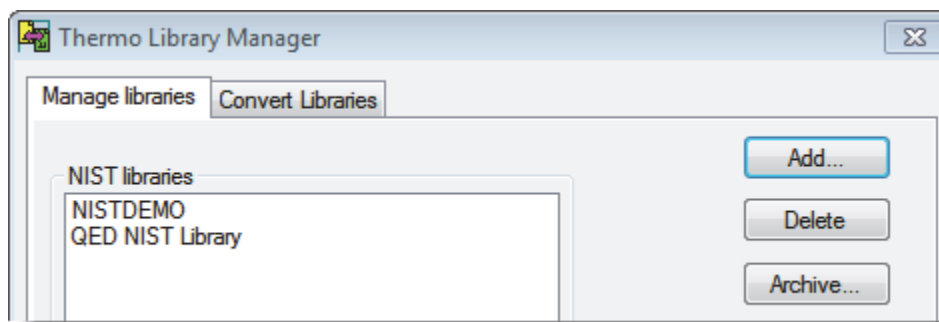
7. Click **Exit** in the Thermo Library Manager dialog box.

8. To confirm the library installation, do the following:

   a. Start the TraceFinder application.

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

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

   d. Choose **File > New > Method Template** from the main menu.

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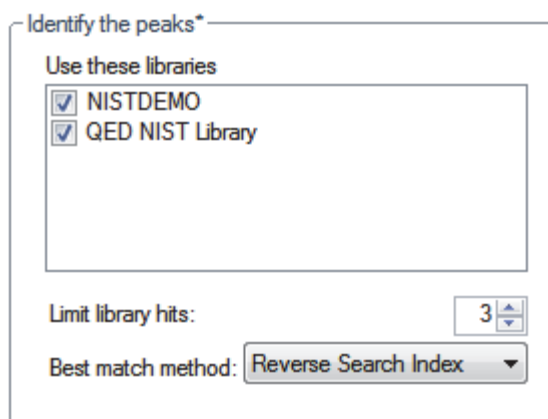
Launching the NIST Library Browser

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

❖ **To open the NIST library browser**

Choose **Go > Launch Library Browser** from the TraceFinder main menu.
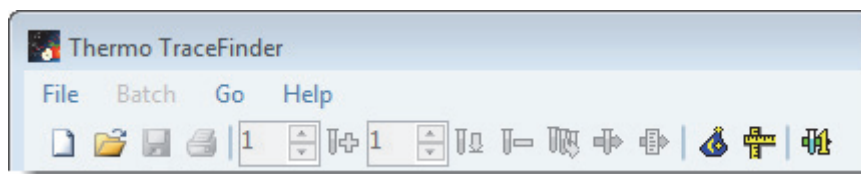
The NIST MS Search window opens.
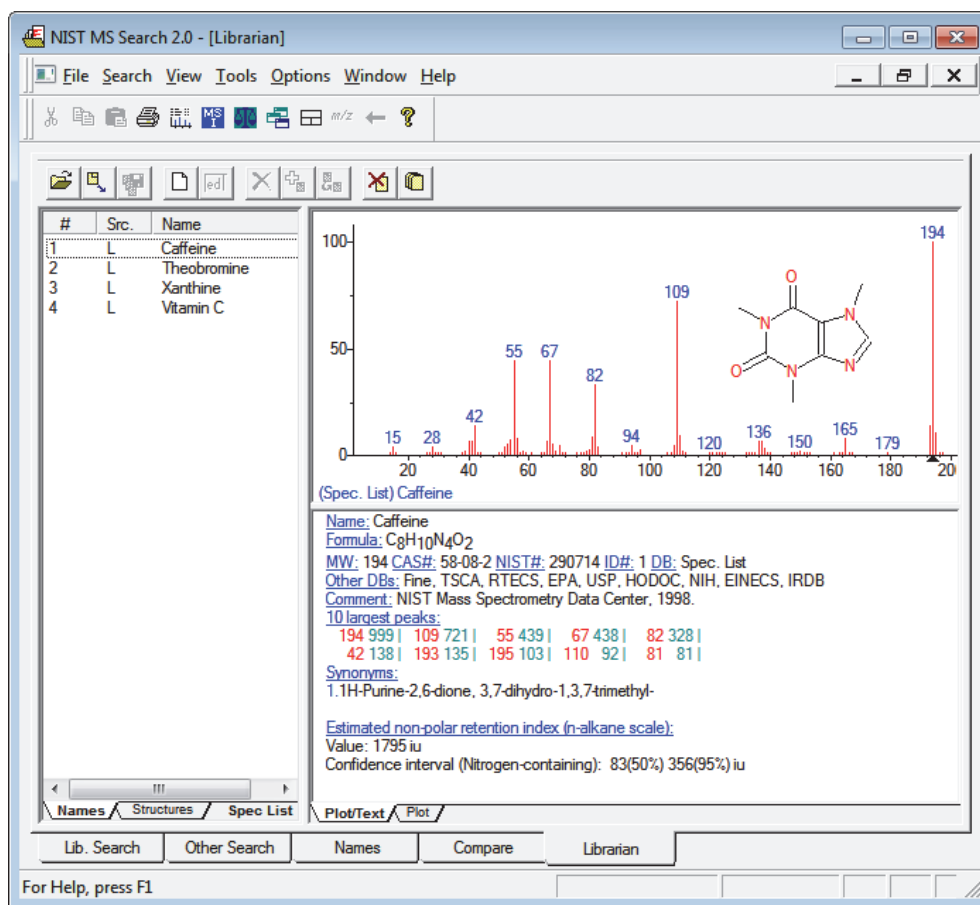
For detailed instructions about using the library browser, refer to the Help in the NIST MS Search window.

Launching the Qual Browser

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

❖ **To open the Qual Browser**

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

The Thermo Xcalibur Qual Browser opens.
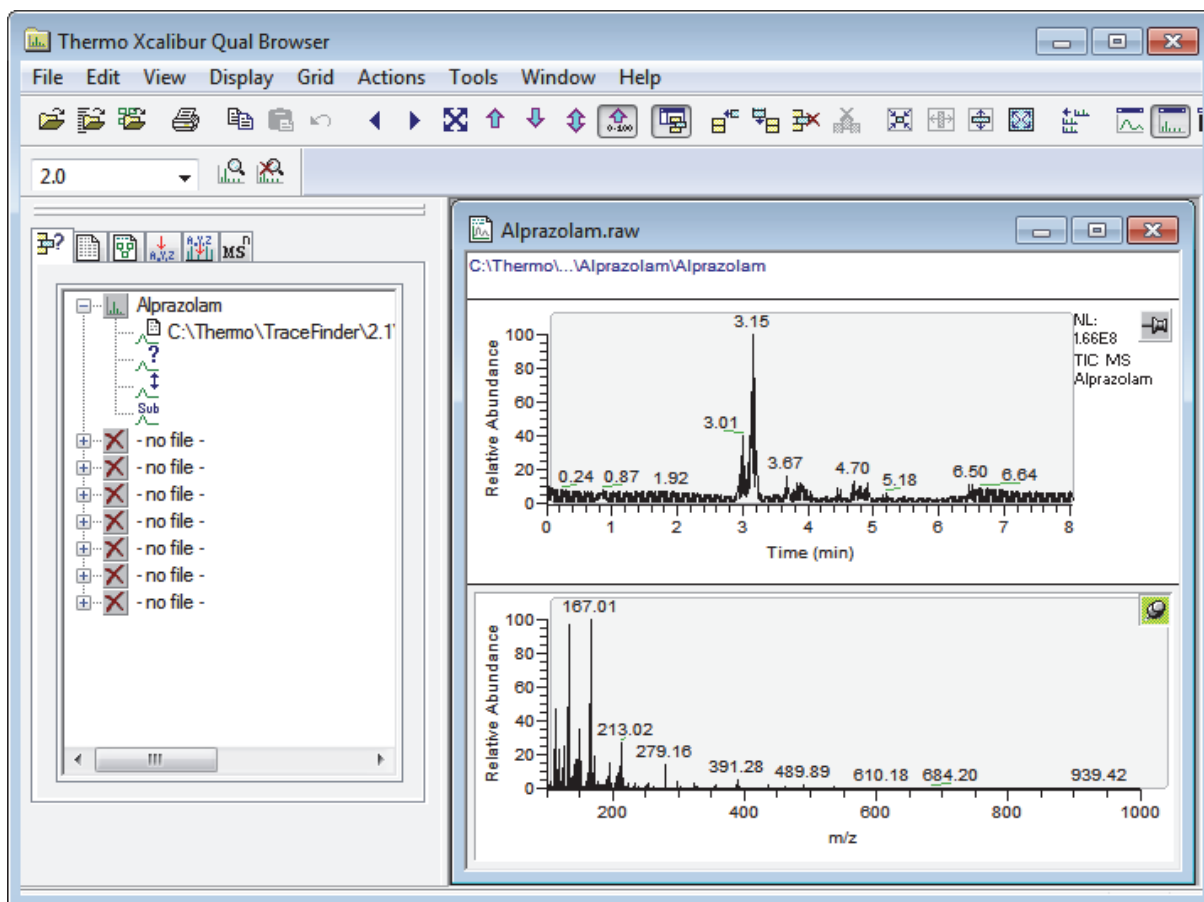
For detailed instructions about using the Qual Browser, refer to the Help in the Qual Browser window.

Converting Legacy Data

Use the TraceFinder Legacy Data Converter to convert methods, batches, method templates, or batch templates from the source versions to compatible TraceFinder 3.1 target configurations. See Version Compatibility.

- You can convert legacy data from TraceFinder versions 1.0.1, 1.1, 2.0, 2.1, or 3.0.

- You can convert data from EnviroLab Forms, QuanLab Forms, or ToxLab Forms.

- You can convert data from TraceFinder 3.1 for general quantitation to another installed configuration of TraceFinder 3.1.

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

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

The TraceFinder Legacy Data Converter window opens.
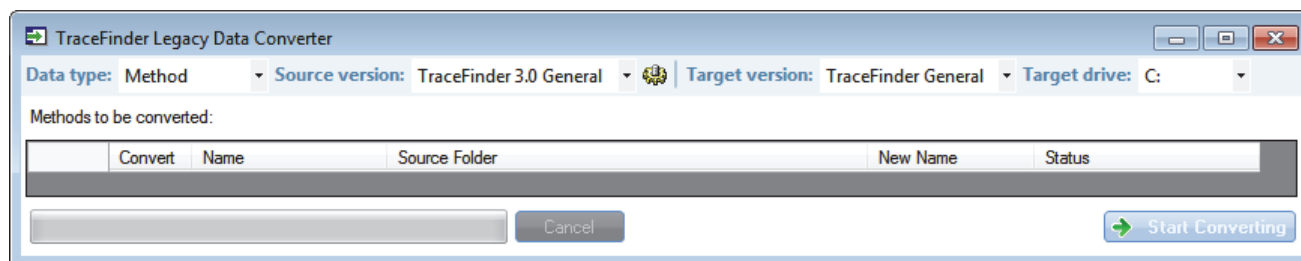
This section includes the following topics:

- Version Compatibility

- Converting Methods

- Converting Batches

- Converting Method Templates

- Converting Batch Templates

Version Compatibility

This table shows which source versions of methods, batches, method templates, or batch templates are compatible with TraceFinder 3.1 target configurations.

Table 2. Version compatibility

Source	TraceFinder 3.1 target			
	General	**EFS**	**Clinical Research**	**Forensic Toxicology**
TraceFinder 3.1 General		✓	✓	✓
TraceFinder 3.0 General	✓	✓	✓	✓
TraceFinder 2.1 General	✓	✓	✓	✓
TraceFinder 2.1 EFS		✓		
TraceFinder 2.1 Clinical Research			✓	✓
TraceFinder 2.1 Forensic Toxicology			✓	✓
TraceFinder 2.0 General	✓	✓	✓	✓
TraceFinder 2.0 EFS		✓		
TraceFinder 2.0 Clinical Research			✓	✓
TraceFinder 1.1 General	✓	✓	✓	✓
TraceFinder 1.1 EFS		✓		
TraceFinder 1.0.1		✓		
EnviroLab Forms 3.1		✓		
QuanLab Forms 3.1	✓	✓	✓	✓
ToxLab Forms 3.1			✓	✓
EnviroLab Forms 2.5.2		✓		
QuanLab Forms 2.5.2	✓	✓	✓	✓
ToxLab Forms 2.5.2			✓	✓

Converting Methods

Use the data converter to convert legacy methods to TraceFinder 3.1 methods.

❖ **To convert a method**

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

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

   The following example shows that you can convert methods from the TraceFinder 3.0 General configuration to the current General configuration. For a complete list of version compatibilities, see "Version Compatibility" on page 21.
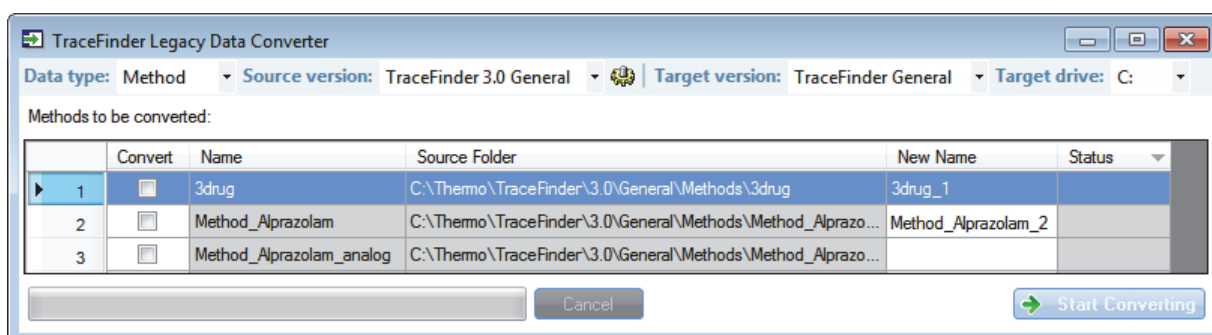
2. In the Source Version list, select the version of the method that you will convert.

   The Methods to be Converted 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 the **Change Default Source Folder** icon, 🛠.

      The application adds a Source Folder box to the window.
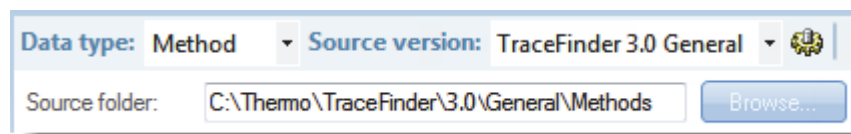
   b. Click **Browse** and locate a method folder.

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

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

   The application displays the selected folder in the Methods to be Converted table.

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

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

   The list displays only TraceFinder configurations with compatible data. See "Version Compatibility" on page 21.

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

   You cannot write the converted files to a mapped drive.

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

   When you populate the Methods to be Converted table, the application checks each method to see if a method with this name exists in the target folder.

   • If the method name already exists in the target folder, the default new name is the original name with "_1" appended.

   • If the method name does not exist in the target folder, 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.

7. Select the check box for each method that you will convert,

   and click [→ Start Converting].

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

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

   When the Status column reports that a method is successfully converted, the application writes the converted file to the …\TraceFinderData\Methods folder.

   > **Note** If a method conversion is unsuccessful, the Status column displays an error icon. Hold your cursor over the icon to display the error message.

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

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

Figure 4. Sample log file for converting a method

```
===== Start Converting Method from TraceFinder 3.0 General to TraceFinder General ==
--- Converting master method from
    'C:\Thermo\TraceFinder\3.0\General\Methods\Alprazalom1\Alprazalom1.mmx'
--- Creating master method
--- Importing properties of object 'MethodData' from XML file
    'C:\Thermo\TraceFinder\3.0\General\Methods\Alprazalom1\Alprazalom1.mmx'
--- Saving master method
--- Copying instrument method
--- Successfully converted master method from
    'C:\Thermo\TraceFinder\3.0\General\Methods\Alprazalom1\Alprazalom1.mmx'
    to 'C:\TraceFinderData\Methods\Alprazalom1_4\Alprazalom1_4.mmx'
-----------------------------------------------------------------------------
--- Converting master method from
    'C:\Thermo\TraceFinder\3.0\General\Methods\XC_method\XC_method.mmx'
--- Creating master method
--- Importing properties of object 'MethodData' from XML file
    'C:\Thermo\TraceFinder\3.0\General\Methods\XC_method\XC_method.mmx'
--- Saving master method
--- Copying instrument method
--- Successfully converted master method from
    'C:\Thermo\TraceFinder\3.0\General\Methods\XC_method\XC_method.mmx'
     to 'C:\TraceFinderData\Methods\XC_method_4\XC_method_4.mmx'
-----------------------------------------------------------------------------
======== Conversion completed. 2 total, 2 successful, 0 failed. ==========
=============================================================================
```

Converting Batches

Use the data converter to convert legacy batches to TraceFinder 3.1 batches.

❖ **To convert a batch**

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

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

   The following example shows that you can convert batches from the TraceFinder 3.0 General configuration to the current General configuration. For a complete list of version compatibilities, see "Version Compatibility" on page 21.
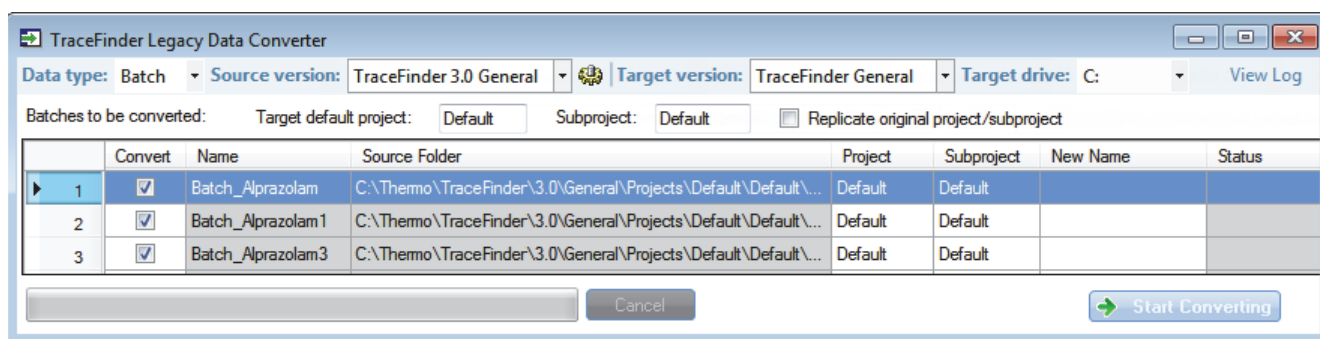
2. In the Source Version list, select the version of the batch that you will convert.

   The Batches to be Converted table displays all batches in the Projects folder for the selected source version.

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

   a. Click the **Source Folder** icon, .

      The application adds a Source Folder box to the window.
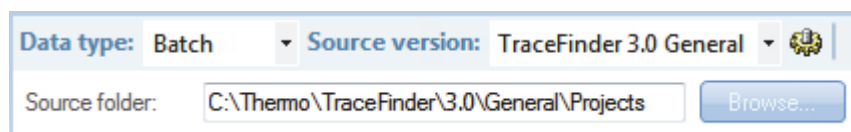
   b. Click **Browse** and locate a batch folder.

      You can select a specific batch folder or a project or subproject folder that contains multiple batches.

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

   The application displays the selected folder and all batches in that folder in the Batches to be Converted table.

   When you select a project or subproject folder that contains multiple batch folders, the application displays all the batches.

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

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

   The list displays only TraceFinder configurations with compatible data. See "Version Compatibility" on page 21.

5. In the Target Drive list, select a drive.

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

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

   –or–

   Select the **Replicate Original Project/Subproject** check box.

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

   When you populate the Batches to be Converted table, the application checks each batch to see if a batch with this name exists in the target folder.

   • If the batch name already exists in the target folder, the default new name is the original name with "_1" appended.

   • If the batch name does not exist in the target folder, the application keeps the original batch name.

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

8. 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 an error icon. Hold your cursor over the icon to display the error message.

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

Figure 5.   Sample log file for converting a batch

```
======== Start Converting Batch from TraceFinder 3.0 General to TraceFinder General ==========
--- Converting batch
from 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\BatchData.btd'
Loading data from source batch database
--- Copying raw file
from 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\Data\UnknownA1.raw'
to 'C:\TraceFinderData\Projects\Default\Default\Batch_alprazolam\Data\UnknownA1.raw'
--- Copying chrospec file
from 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\Data\UnknownA1.chrospec
to 'C:\TraceFinderData\Projects\Default\Default\Batch_alprazolam\Data\UnknownA1.chrospec'
--- Copying raw file
from 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\Data\UnknownA2.raw'
to 'C:\TraceFinderData\Projects\Default\Default\Batch_alprazolam\Data\UnknownA2.raw'
--- Copying chrospec file
from 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\Data\UnknownA2.chrospec
to 'C:\TraceFinderData\Projects\Default\Default\Batch_alprazolam\Data\UnknownA2.chrospec'
--- Copying raw file
from 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\Data\UnknownA3.raw'
to 'C:\TraceFinderData\Projects\Default\Default\Batch_alprazolam\Data\UnknownA3.raw'
--- Copying chrospec file
from 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\Data\UnknownA3.chrospec
to 'C:\TraceFinderData\Projects\Default\Default\Batch_alprazolam\Data\UnknownA3.chrospec'
--- ---------- Completed sample import ----------
--- Importing local method for 'Batch_alprazolam'
--- Importing properties of object 'MethodData'
from XML file 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\Methods\...|
--- Saving local method data for 'Batch_alprazolam_Alprazolam'
--- Copying reference files method
--- Copying instrument method
--- Saving batch data for 'Batch_alprazolam'
--- Successfully converted batch
from 'C:\Thermo\TraceFinder\3.0\General\Projects\Default\Default\Batch_alprazolam\BatchData.btd'
to 'C:\TraceFinderData\Projects\Default\Default\Batch_alprazolam'
--------------------------------------------------------------------------------
========== Conversion completed. 1 total, 1 successful ==========
================================================================================
```

Converting Method Templates

Use the data converter to convert legacy method templates to TraceFinder 3.1 method templates.

❖ **To convert a method template**

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

   The TraceFinder Legacy Data Converter displays the interface for converting method templates.
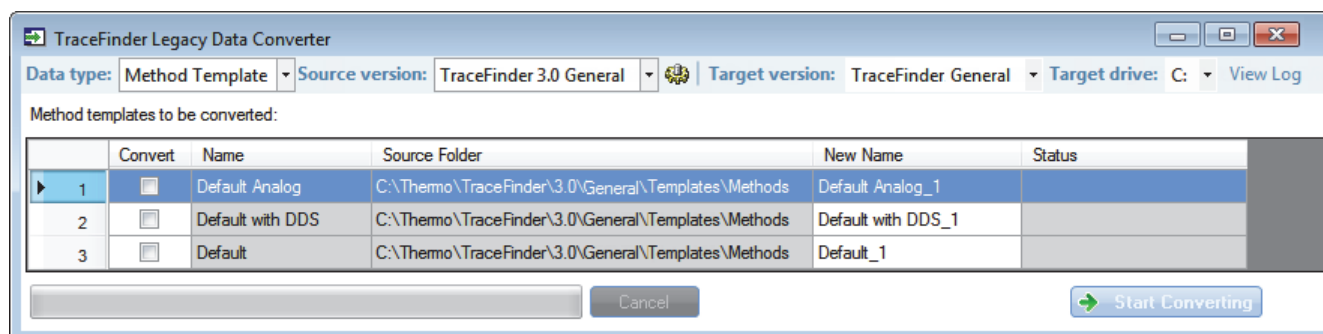
2. In the Source Version list, select the version of the method template that you will convert.

   The Method Templates to be Converted 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 the **Source Folder** icon, .

      The application adds a Source Folder box to the window.
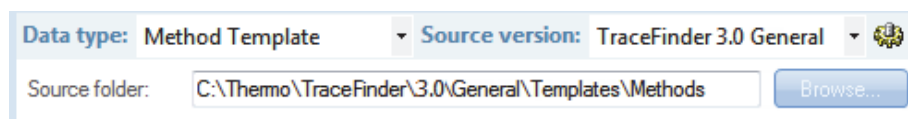
   b. Click **Browse** and locate a template folder.

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

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

   The application displays the selected folder in the Method Templates to be Converted table.

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

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

   The list displays only TraceFinder configurations with compatible data. See "Version Compatibility" on page 21.

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

   You cannot write the converted files to a mapped drive.

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

   When you populate the Method Templates to be Converted table, the application checks each method template to see if a method template with this name exists in the target folder.

   • If the method template name already exists in the target folder, the default new name is the original name with "_1" appended.

   • If the method template name does not exist in the target folder, 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.

7. Select the check box for each method template that you will convert,

   and click → Start Converting .

   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 following folder:

   …\TraceFinderData\Templates\Methods\Forensic folder

   > **Note** If a template conversion fails, the Status column displays an error icon. Hold your cursor over the icon to display the error message.

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

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

Figure 6.   Sample log file for converting a method template

```
=== Start Converting Method Template from TraceFinder 3.0 General to TraceFinder General ===
- Converting method template
  from 'C:\Thermo\TraceFinder\3.0 \General\Templates\Methods\Default Analog.pmtx'
- Importing properties of object 'ProcMethodTemplateData'
  from XML file 'C:\Thermo\TraceFinder\3.0 \General\Templates\Methods\Default Analog.pmtx'
- Saving the method template
- Successfully converted method template
  from 'C:\Thermo\TraceFinder\3.0 \General\Templates\Methods\Default Analog.pmtx'
  to 'C:\Thermo\TraceFinder\3.1\General\Templates\Methods\Default Analog_1.pmtx'
--------------------------------------------------------------------------------
====== Conversion completed. 1 total, 1 successful, 0 failed.  ==========
================================================================================
```

Converting Batch Templates

Use the data converter to convert legacy batch templates to TraceFinder 3.1 batch templates.

❖ **To convert a batch template**

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

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

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

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

   The Batch Templates to be Converted 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 the **Source Folder** icon, ⚙.

   The application adds a Source Folder box to the window.
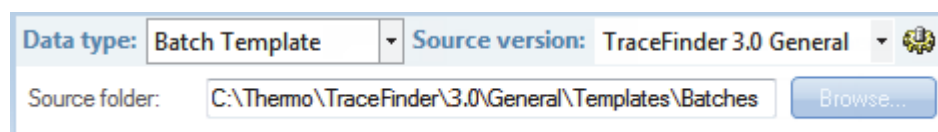
   b. Click **Browse** and locate a template folder.

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

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

   The application displays the selected folder in the Batch Templates to be Converted table.

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

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

   The list displays only TraceFinder configurations with compatible data. See "Version Compatibility" on page 21.

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

   You cannot write the converted files to a mapped drive.

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

   When you populate the Batch Templates to be Converted table, the application checks each batch template to see if a batch template with this name exists in the target folder.

- If the batch template name already exists in the target folder, the default new name is the original name with "_1" appended.

- If the batch template name does not exist in the target folder, 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.

7. Select the check box for each batch template that you will convert,

   and click [→ Start Converting] .

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

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

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

   > **Note** If a template conversion fails, the Status column displays an error icon. Hold your cursor over the icon to display the error message.

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

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

Figure 7. Sample log file for converting a batch template

```
= Start Converting Batch Template (LabForm type) from TraceFinder 3.0 General to TraceFinder Gener
- Converting batch template from 'C:\Thermo\TraceFinder\3.0\General\Templates\Batches\Batch_Templa
- Importing properties of object 'BatchTemplateData' from XML file
  'C:\Thermo\TraceFinder\3.0\General\Templates\Batches\Batch_Template_Alpraz.btmp'
-- Saving batch template to 'C:\Thermo\TraceFinder\3.1\General\Templates\Batches\Batch_Template_Al
- Successfully converted batch template from 'C:\Thermo\TraceFinder\3.0\General\Templates\Batches\
  to 'C:\Thermo\TraceFinder\3.1\General\Templates\Batches\Batch_Template_Alpraz.btmp'
=== Conversion completed. 1 total, 1 successful, 0 failed. =========|
```

Choosing a Mode or Console

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

Table 3. User roles and default access

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

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

Follow these procedures:

- To choose a mode

- To open the Configuration console

- To open the Administrator Console

- To display a log of instrument errors

- To monitor instrument status

- To watch acquisition and processing in real time

❖ **To choose a mode**

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

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

Mode	Description
Acquisition	Opens the Acquisition mode where you can create and review batches, batch data, reports, and local methods. See Chapter 5, "Using the Acquisition Mode." This mode is available only when you select the Acquisition Batch Wizard style in the Configuration mode. See "Batch Wizard Style" on page 66.
Analysis	Opens the Analysis mode where you can review batches, batch data, reports, and local methods. See Chapter 6, "Using the Analysis Mode."
Method Development	Opens the Method Development mode where you can create a master method, an instrument method, or a development batch. See Chapter 4, "Using the Method Development Mode."

❖ **To open the Configuration console**

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

When user security is activated, only users with Configuration permissions can access the Configuration console. See Chapter 3, "Using the Configuration Console."

❖ **To open the Administrator Console**

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

When user security is activated, only users with Administrator permissions can access the Administrator Console. Refer to the *TraceFinder Administrator Console User Guide*.

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

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

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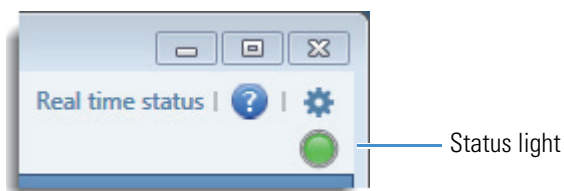
The Instrument Log dialog box opens.
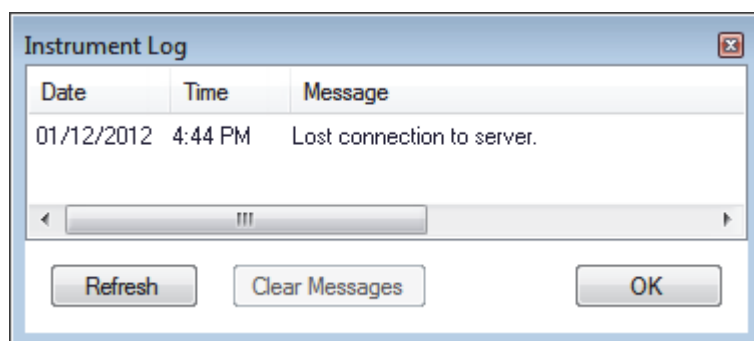
The Instrument Log displays all instrument errors that have occurred since the TraceFinder application started or since the last time that you cleared the message log.

2. Do any of the following:

- Click **Refresh** to display errors that occur after you open the Instrument Log dialog box.

- Click **Clear Messages** to remove messages from the Instrument Log display.

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

  C:\Thermo\TraceFinder\3.1\Forensic\Logs\TraceFinder.log

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

❖ **To monitor instrument status**

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

Green indicates that the instrument is ready.

Yellow indicates that the instrument is in standby mode.

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

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

Click **Real Time Status** in the upper right corner of the TraceFinder window.
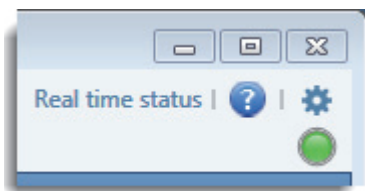
The application displays the Real Time Status pane at the bottom of the window.
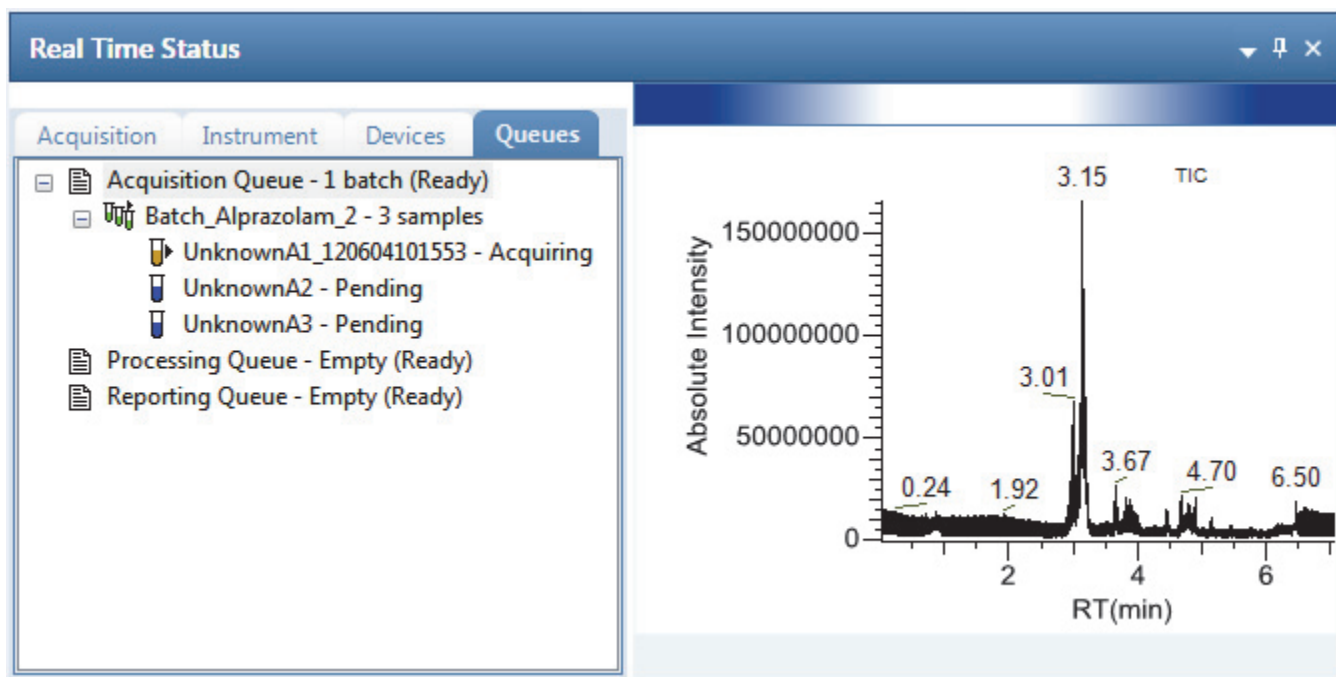
For descriptions of all the features of the Real Time Status pane, see "Real Time Status Pane" on page 368.

TraceFinder Window Features

A TraceFinder window with user security for a user in the default LabDirector role has these functions.
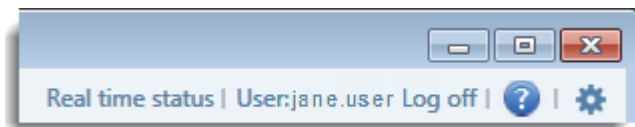
Table 4. TraceFinder window parameters

Parameter	Description
Real Time Status	Opens the Real Time Status pane for the current acquisition. The acquisition progress is displayed within the current mode window.
CurrentUserName	Displays the name of the current user. This is displayed only when user security is activated.
Log Off	Logs off the current user and displays the login screen. This function is available only when user security is activated.
Help	Opens the TraceFinder Help.
Configuration Console ⚙	Opens the Configuration console where you can configure several options for using the TraceFinder application. See Chapter 3, "Using the Configuration Console."

Using the Configuration Console

This chapter discusses the features of the Configuration console. When user security is activated, this console is available for a user with Configuration permissions. When user security is not activated, all users have access to all features in the Configuration console.

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

Using the features on the Configuration console, you can activate features such as available reports, user security, reporting defaults, multiplexing, detection algorithms, and target screening. You can also choose the reports that are available to users, the application defaults, and the defaults used for peak detection.

Contents

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

❖ **To access the Configuration console**

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

The TraceFinder Configuration console opens.
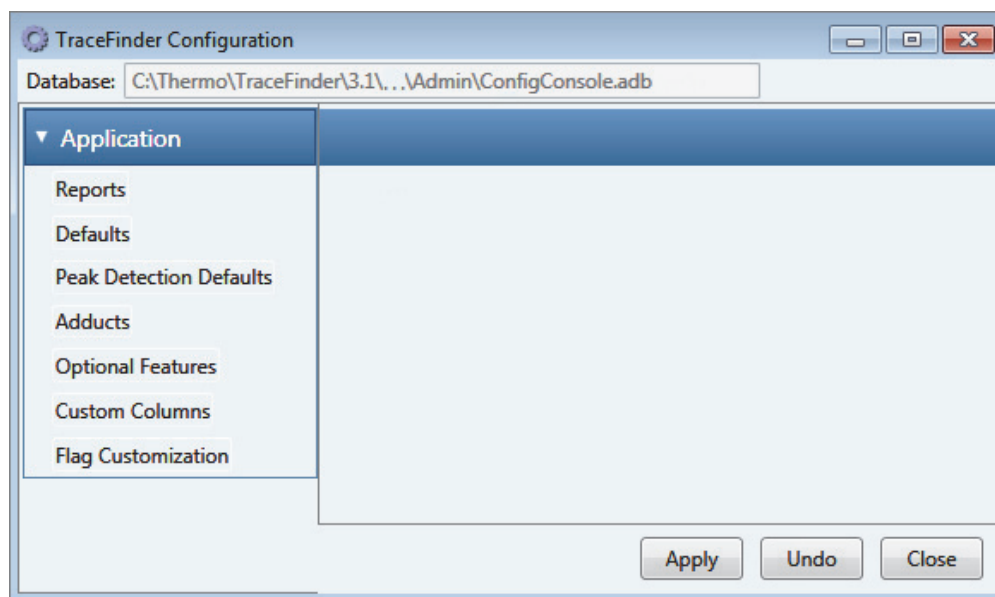
Table 5. Navigation pane functions in the Configuration console (Sheet 1 of 2)

Function	Description
Reports	Use the Reports view to configure standard, custom, ToxID, or target screening reports. See "Specifying the Reports" on page 40.
Defaults	Use the Defaults view to specify the default laboratory and instrument names, the displayed mass precision, and the intensity scale to use for reporting. See "Specifying Application Defaults" on page 45.
Peak Detection Defaults	Use the Peak Detection Defaults view to specify a peak detection algorithm and its options and to determine the area under a curve. See "Specifying Default Peak Detection Parameters" on page 47.
Adducts	Use the Adducts view to specify the adducts that will be available for use in method development. See "Specifying Adducts" on page 61.
Optional Features	Use the Optional Features view to enable features such as ToxID, quick acquisition, batch wizard styles, multiplexing, intelligent sequencing, and screening libraries. See "Activating Optional Features" on page 64.

Table 5. Navigation pane functions in the Configuration console (Sheet 2 of 2)

Function	Description
Custom Columns	Use the Custom Columns view to add six additional columns to the samples list in batches. See "Creating Custom Columns" on page 72.
Flag Customization	Use the Flag Customization view to customize error flags and conditions to indicate compound errors in Data Review for quantitation batches. See "Creating Custom Flags" on page 75.

Specifying the Reports

When user security is activated, as a user in either the default LabDirector or default ITAdmin role, you can configure a list of reports that are available to all users when they generate reports from the Method Development, Analysis, or Acquisition modes. From the Reports view, you can configure standard, custom, ToxID, or target screening reports.

When you first open the report configuration, all reports are included in the Displayed Reports pane and are available for use in any method you create. By default, the Intelligent Sequencing Report is not included in the Displayed Reports pane.

> **Note** The Intelligent Sequencing Report is available only when you install the Intelligent Sequencing power module and enable the Intelligent Sequencing features. See "Installing the Power Modules" on page 14 and "Intelligent Sequencing" on page 71.

> **Note** ToxID reports are available only when you activate the ToxID features. See "ToxID" on page 65.

Example PDF files of report formats are located in the following folder:

C:\Thermo\TraceFinder\3.1\Forensic\ExampleReports

Follow these procedures:

- To open the Reports view
- To specify which reports are available
- To import custom reports

❖ **To open the Reports view**

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

The Application - Reports view opens. For a list of all reports for the forensic toxicology market, see "Reports" on page 42.

❖ **To specify which reports are available**

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

   In the Method Development, Analysis, and Acquisition modes, users can access all reports that are selected for display.

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

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

> **Note** Only reports that can aggregate data at the batch level have the **Batch Level** check box activated. By default, the application selects the Batch Level feature for all these reports.

3. Do one of the following:

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

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

  Your report settings are immediately available in the TraceFinder application.

❖ **To import custom reports**
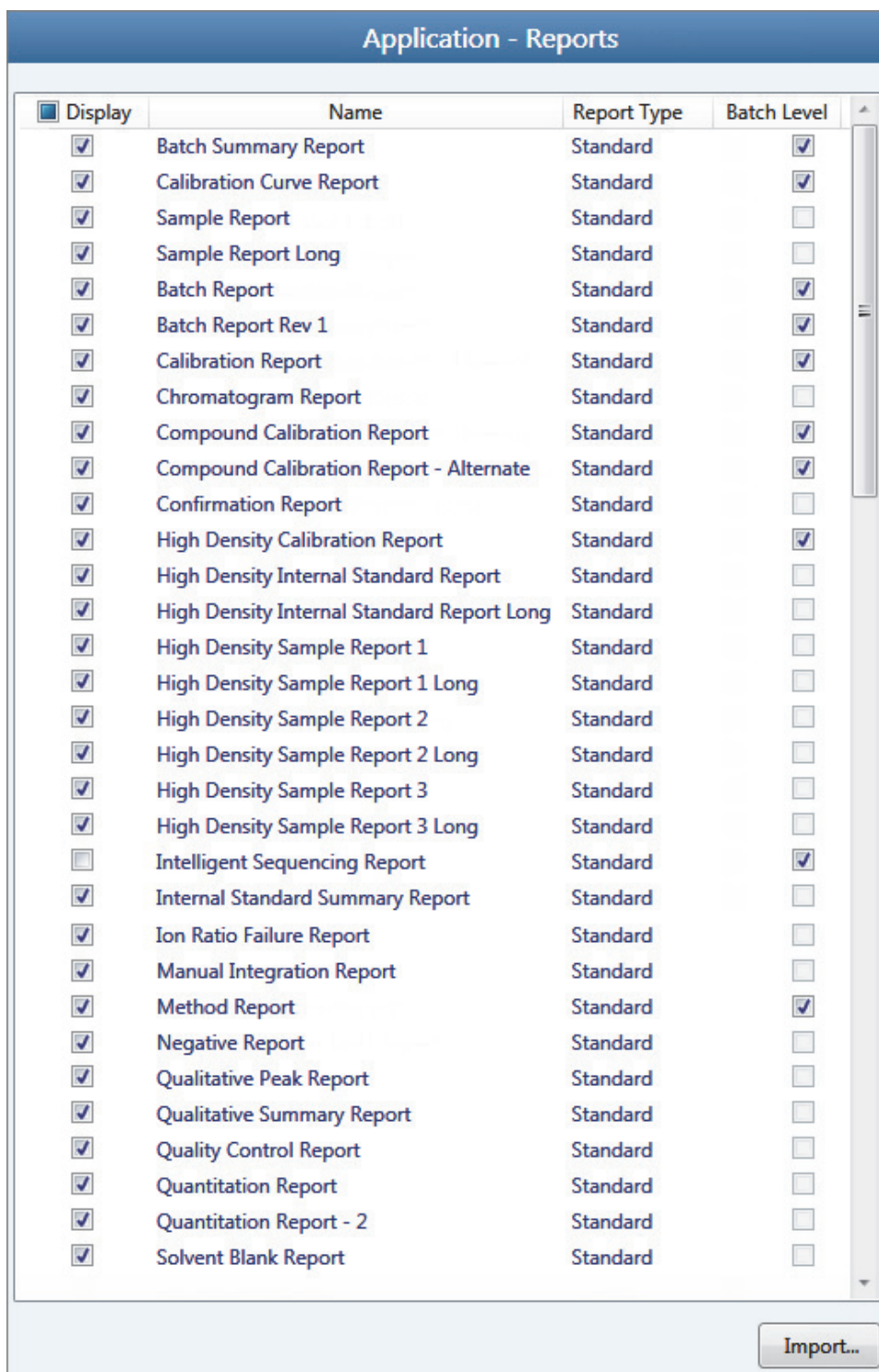
1. Click **Import**.

2. Locate a custom report (.xltm) and click **Open**.

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

  The application adds the custom reports to the list of available custom reports.

Reports

The application uses the following standard, custom, target screening, and ToxID reports. For descriptions of the parameters in the Reports view, see "Reports view parameters" on page 44.

Figure 8.   Reports view showing standard reports

Figure 9. Reports view showing custom reports

Figure 10. Reports view showing target screening reports

Figure 11. Reports view showing ToxID reports
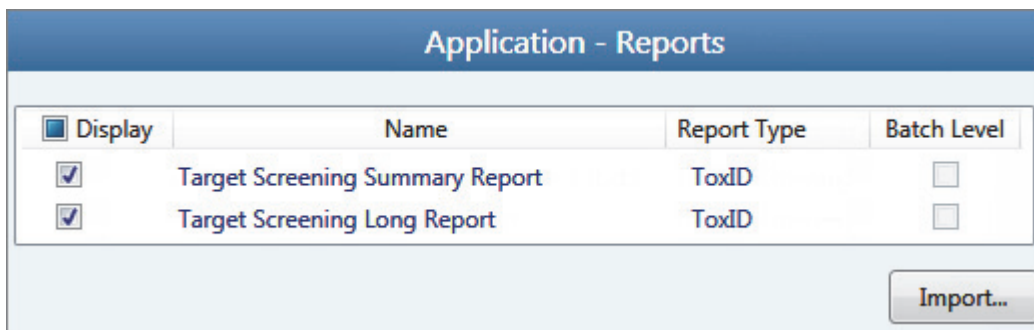
> **Note** ToxID reports are available only when you install the ToxID™ software and activate the ToxID features. For a detailed procedure for activating ToxID features, see "ToxID" on page 65.

Table 6. Reports view parameters

Parameter	Description
Display	Specifies reports that are selected for use in the application.
Name	Displays all reports that are available for this application.
Report Type	Specifies the report type: Standard, Custom, Target Screening, or ToxID.
Batch Level	By default, the application selects the Batch Level feature for all reports that can aggregate data at the batch level.
Import	Opens a browser where you can locate a custom report to add to the list of available custom reports.

Specifying Application Defaults

Use the Application - Defaults view of the Configuration console to specify the default laboratory and instrument names, the displayed mass precision, and the chromatogram intensity scale to use for reporting. When user security is activated, you can access these features only in the default LabDirector or default ITAdmin role.
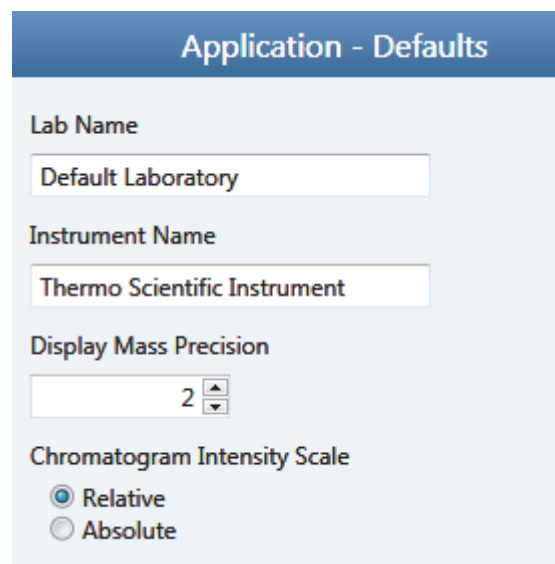
Follow these procedures:

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

❖ **To open the Defaults view**

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

The Application - Defaults view opens.

❖ **To specify a default laboratory name and instrument name**

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

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

   The application does not apply this default laboratory name to previously created methods. By default, the laboratory name is Default Laboratory.

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

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

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

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

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

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

The default number of digits to display is 2. The TraceFinder application uses this mass precision value to display mass values in the following locations:
  • Reports:
    – Blank Report
    – Confirmation Report (data spectra, library spectra, quantitation ion display, and qualitative ion display)
    – All High Density reports (*m/z* values)
    – Ion Ratio Failure Report (quantitation ion and qualitative ion)
    – Manual Integration Report (*m/z* value)
    – Qualitative Summary Report (all *m/z* values)
    – Quantitation Report (QIon)
  • All peaks on the Detection pages in the Method Development mode
  • The spectrum display in the Analysis mode
  • The spectrum display in the Method Forge dialog box

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

2. Select either the **Relative** or **Absolute** option for the Chromatogram Intensity Scale.

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

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

Specifying Default Peak Detection Parameters

When user security is activated, as a user in either the default LabDirector or default ITAdmin role, you can specify default peak detection parameters for the Genesis, ICIS, or Avalon detection algorithms. Use the Peak Detection Defaults view to specify a peak detection algorithm and its options and to determine the area under a curve. These parameters are available for quantitation methods only.

This section includes procedures for specifying common peak detection parameters and the parameters used for each of the following detection algorithms:

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

❖ **To open the Peak Detection Defaults view**

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

The Application – Peak Detection Defaults view opens.

- For detailed descriptions of detection parameters used for all detection algorithms, see "Common Peak Detection Parameters" on page 49.

- For detailed descriptions of detection parameters used for the Genesis detection algorithm, see "Genesis peak detection parameters" on page 51.

- For detailed descriptions of detection parameters used for the ICIS detection algorithm, see "ICIS peak detection parameters" on page 54.

- For detailed descriptions of detection parameters used for the Avalon detection algorithm, see "Avalon peak detection parameters" on page 57.

❖ **To specify common detection parameters**

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

   For detailed descriptions of the available detector types, see "Common Peak Detection Parameters" on page 49.

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

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

3. In the Retention Time area, do the following:

   a. In the Window box, specify the width of the window (in seconds) to indicate how far around the expected retention time the system will look for a peak apex.

   b. In the View Width box, specify the viewable size (in minutes) of the ion chromatogram display.

4. In the Ion Ratio Parameters area, do the following:

   a. In the Window Type list, select **Absolute** or **Relative** as the calculation approach for determining the acceptable ion ratio range.

   b. In the Window box, select the acceptable ion ratio range.

   c. In the Ion Coelution box, select the maximum difference in retention time between a confirming ion peak and the quantification ion peak.

5. In the Peak Detection Parameters area, select one of the detection algorithms: **Genesis**, **ICIS**, or **Avalon**.
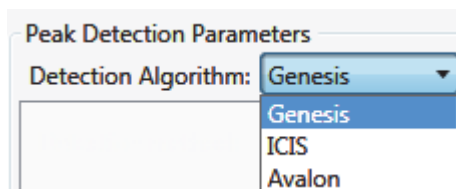
6. Specify the parameters for the selected detection algorithm.

   For detailed parameter descriptions, see one of the following:

   - Genesis Detection Method

   - ICIS Detection Method

   - Avalon Detection Method

Common Peak Detection Parameters

The Detector Type, Mass Tolerance, Retention Time, and Ion Ratio detection parameters are used for all detection algorithms.

Figure 12. Common peak detection areas

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

Parameter	Description
Detector Type	MS: Mass spectrometer that ionizes sample molecules and then separates the ions according to their mass-to-charge ratio (m/z). PDA: Photodiode array detector providing a linear array of discrete photodiodes on an integrated circuit chip. It is placed at the image plane of a spectrometer so that a range of wavelengths can be simultaneously detected. Analog: Supplemental detectors (for example, FID, ECD). When you select this detector, any reports that display a QIon value show the value as **Analog** and any reports that display spectra show the spectra as **Not Available**. A/D card: If your detector is not under data system control, you can capture the analog signal and convert it to digital using an interface box (for example, SS420X) for storage in the raw data file. UV: A UV spectrophotometer (for variable-wavelength detection) or photometer (for single-wavelength detection) equipped with a low-volume flow cell. This detector detects analytes that readily absorb light at a selected wavelength.

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

Parameter	Description
Mass Tolerance	
Units	• (Default) MMU (millimass units) MMU is a static calculation to the extracted mass. • PPM (parts per million) PPM is a variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.
Value	Upper limit of MMU or PPM. Default: 500 Range: 0.1 through 50 000
Retention Time	
Window (sec)	Width of the window (in seconds) to indicate how far around the expected retention time the system will look for a peak apex.
View Width (min)	Viewable size (in minutes) of the ion chromatogram display. Changing the view width does not affect the process of peak detection; the TraceFinder application uses it only for graphical display.
Ion Ratio Parameters	
Window Type	The absolute or relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	The acceptable ion ratio range.
Ion Coelution (min)	The maximum difference in retention time between a confirming ion peak and the quantification ion peak.

Genesis Detection Method

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

Figure 13. Genesis peak detection

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

Parameter	Description
Detection Algorithm	Specifies the Genesis peak detection algorithm.
Detection Method	Highest peak: Uses the highest peak in the chromatogram for component identification.
	Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value.
	Default: 1
	Range: Any odd integer from 1 through 15 points

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

Parameter	Description
S/N threshold	Current signal-to-noise threshold for peak integration. Peaks with signal-to-noise values less than this value are not integrated. Peaks with signal-to-noise values greater than this value are integrated. Range: 0.0 to 999.0
Enable Valley Detection	Uses the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Expected Width (sec)	The expected peak width parameter (in seconds). This parameter controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the *expected width*/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the TraceFinder application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. Range: 0.0 to 999.0
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a threshold and a tailing factor. Selecting the Constrain Peak Width check box activates the Peak Height (%) and Tailing Factor options.
Peak Height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when you select the Constrain Peak Width check box. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

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

Parameter	Description
Peak S/N Cutoff	The peak edge is set to values below this signal-to-noise ratio.
	This test assumes it has found an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio.
	When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the TraceFinder application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 10 000.0
Valley Rise (%)	The peak trace can rise above the baseline by this percentage after passing through a minimum (before or after the peak). This criteria is useful for integrating peaks with long tails.
	This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
	When the trace exceeds rise percentage, the TraceFinder application applies valley detection peak integration criteria. This test is applied to both the left and right edges of the peak. Range: 0.1 to 500.0
Valley S/N	Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher. Default: 2.0 Range: 1.0 to 100.0
# Background Scans	Number of background scans performed by the TraceFinder application.
Report Noise As	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or peak-to-peak resolution threshold. Options are RMS or Peak To Peak.

ICIS Detection Method

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

Figure 14. ICIS peak detection

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

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

Table 9. ICIS peak detection parameters (Sheet 2 of 3)

Parameter	Description
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value. Range: Any odd integer from 1 through 15 points Default: 1
Area Noise Factor	The noise level multiplier used to determine the peak edge after the location of the possible peak. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 5
Peak Noise Factor	The noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value. Range: 1 through 1000 Default: 10
Baseline Window	The TraceFinder application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 40
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box activates the Peak Height (%) and Tailing Factor options.
Peak Height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when you select the Constrain Peak Width check box. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

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

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

Avalon Detection Method

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

Figure 15. Avalon peak detection

Table 10. Avalon peak detection parameters

Parameter	Description
Detection Algorithm	Specifies the Avalon peak detection algorithm.
Detection Method	Highest peak: Uses the highest peak in the chromatogram for component identification.
	Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value. Default: 1 Range: Any odd integer from 1 through 15 points
Time/Event/Value	Displays the events specified in the Avalon Event List dialog box. Initially displays only the default events that cannot be edited or deleted.
Autocalc Initial Events	Automatically calculates the events in the Event list.
Edit	Opens the Avalon Event List dialog box where you can edit the Time/Event/Value parameters. See "Avalon Event List."

Avalon Event List

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

Figure 16. Avalon Event List dialog box
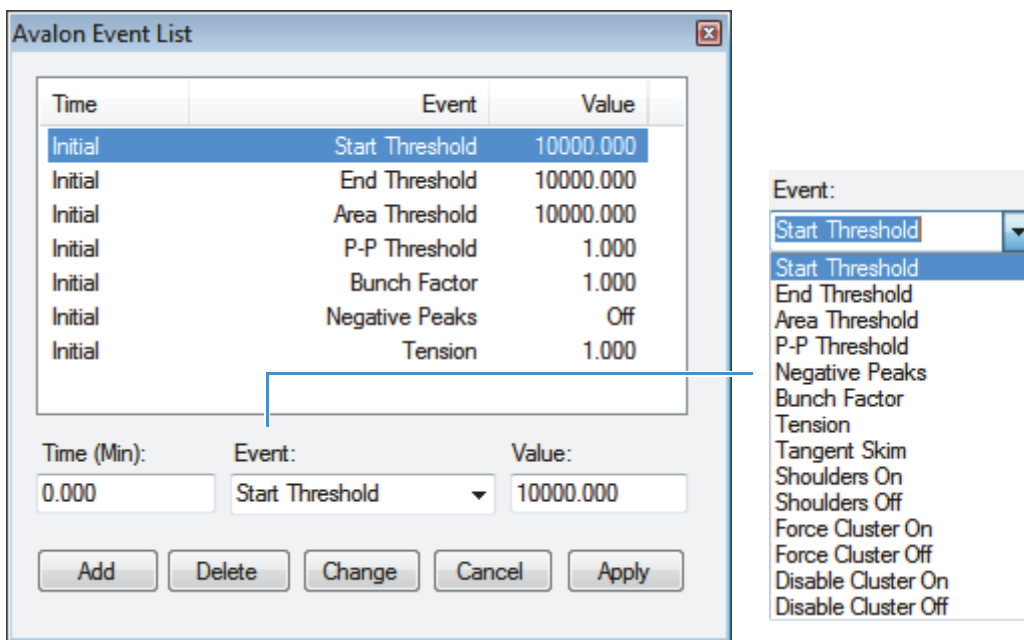
Table 11. Avalon Event List dialog box parameters

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

Figure 17. Event types

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

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

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

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

Specifying Adducts

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

Use the Application - Adducts view to specify the adducts that will be available for you to use in method development.

Follow these procedures:

- To open the Adducts view
- To add an adduct
- To remove an adduct

❖ **To open the Adducts view**

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

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

Application - Adducts

Positive Adducts

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

Negative Adducts

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

❖ **To add an adduct**

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

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

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

   Positive Adducts

2. Type the formula for the new adduct ion.

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

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

   For example, a sodium adduct has [M+Na]+ as the expected charged ion (where M is the neutral molecule), so you would type "Na" for the formula. A water adduct has [M+H+H2O]+ as the expected charged ion, so you would type "H3O" for the formula.

   > **IMPORTANT** When you create an adduct formula, you can type both uppercase and lowercase letters; however, the TraceFinder application interprets all uppercase input as single-letter elements and all lowercase input as two-letter elements.
   >
   > For example, it interprets the string "inau" as In Au and "COSI" as C O S I.

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

	New Adduct	NH3	Gain	1.01

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

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

4. Press Return.

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

These adducts are available for you to select in the Compound Database view of the Method Development mode when you specify parameter values for target peaks. See "Editing Compounds in the Database" on page 285.

❖ **To remove an adduct**

1. In the Positive Adducts or Negative Adducts pane, select the adduct that you want to remove.

2. Press DELETE and confirm that you want to delete the selected adduct.

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

Activating Optional Features

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

- ToxID

- Quick Acquisition

- Delay Calibration

- User Peak Detection Settings

- Auto Sampler Tray Configuration

- Batch Wizard Style

- Multiplexing

- Intelligent Sequencing

- Acquisition Submission Options

- Screening Libraries

❖ **To open the Optional Features page**

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

The Application - Optional Features page opens.

ToxID

You must activate the ToxID option before you can generate ToxID reports.

❖ **To activate ToxID**

1. Select the **ToxID** check box.

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

   The application immediately applies this feature change.

For a list of available ToxID reports, see "Reports" on page 42.

Quick Acquisition

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

> **Note** The Quick Acquisition feature is not available when you activate Multiplexing. See "Multiplexing" on page 70.

❖ **To activate quick acquisition**

1. Select the **Quick Acquisition (EnviroLab/ToxLab/QuanLab Forms)** check box.

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

   The application immediately applies this feature change.

For a description of the Quick Acquisition features, see "Working with Master Methods" on page 85.

Delay Calibration

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

❖ **To delay calculation of a calibration curve**

1. Select the **Delay Calibration** check box.

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

   The application immediately applies this feature change.

User Peak Detection Settings

Use the User Peak Detection Settings Allowed option to let users modify the method integration settings for specific compounds in Data Review. For instructions about modifying the peak detection parameters, see "To modify the peak detection settings" on page 510.

❖ **To allow users to modify peak detection settings**

1. Select the **User Peak Detection Settings Allowed** check box.

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

   The application immediately applies this feature change.

Auto Sampler Tray Configuration

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

❖ **To disallow automatic tray configuration**

1. Select the **Allow Auto Sampler to Automatically Determine Tray Configuration** check box.

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

   The application immediately applies this feature change.

Batch Wizard Style

Use the Batch Wizard Style option to choose one of two styles for your batch wizard.

❖ **To select a wizard style**

1. In the Batch Wizard Style list, select a wizard style:

   • **Acquisition Batch Wizard**: Adds the Acquisition mode to the navigation pane. This mode is similar to the Acquisition mode in the TraceFinder 1.1 application. See Chapter 5, "Using the Acquisition Mode."

     When you activate multiplexing, the application automatically activates this wizard style.

   • **Batch Template Wizard**: The default wizard style that is similar to the acquisition wizard in the EnviroLab Forms, ToxLab Forms, and QuanLab Forms applications. See "Creating a Batch Using the Batch Wizard" on page 435.

     Note The Batch Template Wizard is not available when you activate Multiplexing. See "Multiplexing" on page 70.

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

The application immediately applies this feature change.

Acquisition Submission Options

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

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

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

❖ **To specify acquisition submission features**

1. Select either the **Full Sequence Submission** or the **Single Sample Submission** option:

   - Full Sequence Submission: Supports look-ahead features of the autosampler. When the instrument method specifies the look-ahead feature, the TraceFinder application functions like a multiplex driver and feeds the autosampler the next vial position.

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

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

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

     > **Note** The Single Sample Submission feature is not available when you activate Multiplexing. See "Multiplexing" on page 70.

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

The application immediately applies this feature change.

Screening Libraries

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

When you specify the Library Search Type on the General page for a screening method, you choose either the Library Manager search type or the NIST search type. See "Editing the General Page" on page 225.

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

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

❖ **To specify a Library Manager screening library**

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

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

❖ **To specify a NIST screening library**

1. Click **Select**.

   The Select NIST Libraries dialog box opens, listing the libraries you installed for the application.
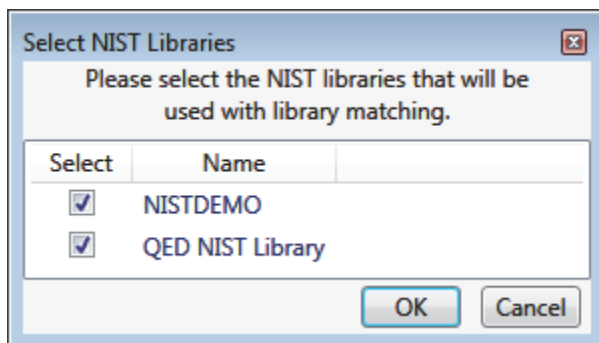
2. Select the check box for each NIST library that you want to use for screening and click **OK**.

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

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

   The application immediately applies this feature change.

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

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

Screening Libraries in a Quantitation Method

In a quantitation master method, you can enable library matching and set a score threshold to minimize poor matches. See "Library" on page 171. To match a compound, the resulting score from a library search must be higher than the specified threshold value.

Screening Libraries in a Target Screening Method

In a target screening master method, you can specify the library search to either identify or confirm library matches and set a score threshold to minimize poor matches. See "Specifying Identification and Confirmation Settings" on page 235.

- Identify or Confirm: The application identifies or confirms the sample compound by searching the specified search library and returning the highest score (as a percentage value) for the fragment ion spectrum in that library that matches the compound's ion spectrum.

- Score Threshold: To identify or confirm the presence of a compound, the resulting score from a library search must be higher than the specified threshold value.

> **IMPORTANT** To use a library search for identification or confirmation, the application requires meeting these conditions:
>
> - The raw data file must contain higher energy collision-induced dissociation (HCD), source collision-induced dissociation (CID), or all ions fragmentation (AIF) ion spectra.
>
> - The spectra must exist at a time point within the compound's elution time range.

Multiplexing

The Multiplexing options are available only when you install the Multiplexing Power Module. See "Installing the Power Modules" on page 14.

> **Note** Multiplexing is not available when you activate Intelligent Sequencing. See Intelligent Sequencing.

❖ **To specify multiplexing features**

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

2. Select the check box for each channel that you want to use for acquisition.

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

   The application immediately applies this feature change.

The application uses multiplexing features in the Acquisition mode when you specify channels for a sample in a batch (see "Defining the Sample List" on page 340) or monitor an acquisition (see "Devices Page" on page 371).

> **Note** When you activate multiplexing, the following optional features are not available:
> - Quick Acquisition
> - Batch Template Wizard
> - Single Sample Submission (Intelligent Sequencing)

Intelligent Sequencing

The Intelligent Sequencing option is available only when you install the Intelligent Sequencing Power Module. See "Installing the Power Modules" on page 14.

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

❖ **To activate the intelligent sequencing feature**

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

   > **Note** Intelligent Sequencing is not available when you activate Multiplexing. See "Multiplexing" on page 70.

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

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

   The application immediately applies this feature change.

Creating Custom Columns

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

You can use the Modify Columns dialog box to display and change the order of these columns in the sample list (see "Column Display" on page 393).

You can use the Field Chooser to display and change the order of these columns in the Data Review Samples pane (see "Samples Pane" on page 453).

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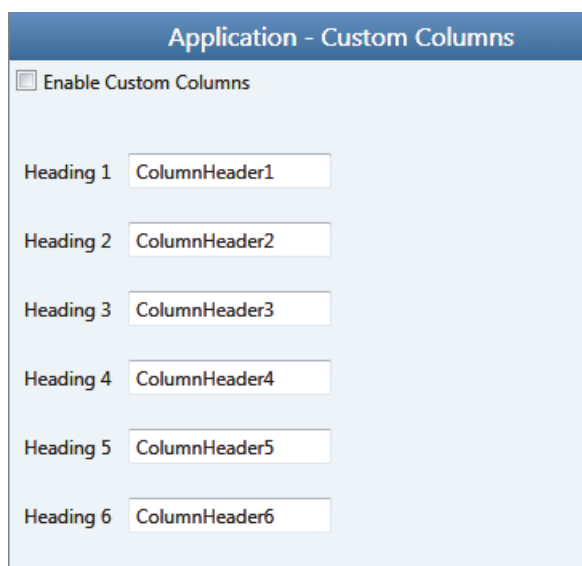
Follow these procedures:

- To open the Custom Columns page
- To add custom columns to new batches
- To create new batches without custom columns
- To control the display of custom columns

❖ **To open the Custom Columns page**

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

The Application – Custom Columns page opens.

Application - Custom Columns

☐ Enable Custom Columns

Heading 1 ColumnHeader1

Heading 2 ColumnHeader2

Heading 3 ColumnHeader3

Heading 4 ColumnHeader4

Heading 5 ColumnHeader5

Heading 6 ColumnHeader6

❖ **To add custom columns to new batches**

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

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

2. For each custom column, select the default column name and type your custom name.

   Example:

3. Click **Apply**.

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

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

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

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

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

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

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

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

Do one of the following:

- To make custom columns available for all batches, select the **Enable Custom Columns** check box and click **Apply**.

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

Creating Custom Flags

Use the Flag Customization view to customize error flags and conditions that indicate compound errors in Data Review for quantitation batches. You can edit the priority assigned to an error condition (flag rule) and the shape and color of the icon used to indicate the error. You can also delete an error condition or create a new one.

❖ **To open the Flag Customization view**

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

The Application - Flag Customization view opens.

Follow these procedures:

- To edit priority groups

- To create a new priority group

- To edit flag rules

- To create a new flag rule

- To remove all customization

❖ **To edit priority groups**

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

Do any of the following:

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

- Double-click the Shape value and select a new shape from the list.

- Click the Color arrow and select a new color from the color palette.
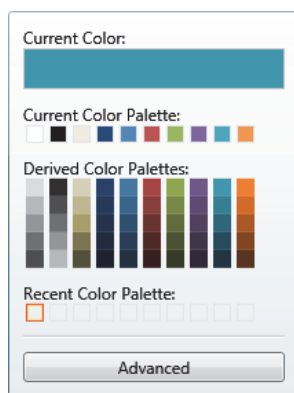
4. When you have completed all your changes, click **Apply** to save your changes.

❖ **To create a new priority group**
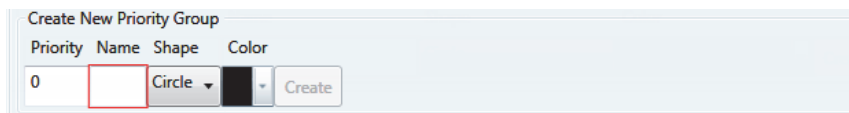
1. In the Priority box, type a value.

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

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

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

4. Click the Color list and select a color from the color palette.
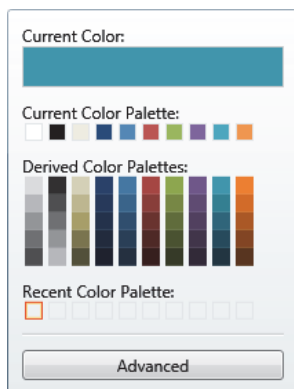
5. (Optional) Click **Advanced** and select a color based on RGB, HSL, or CMYK color palettes. See "Advanced Dialog Box" on page 79.

6. Click **Create**.

   The application adds the new flag to the Priority Groups list.

   Example:
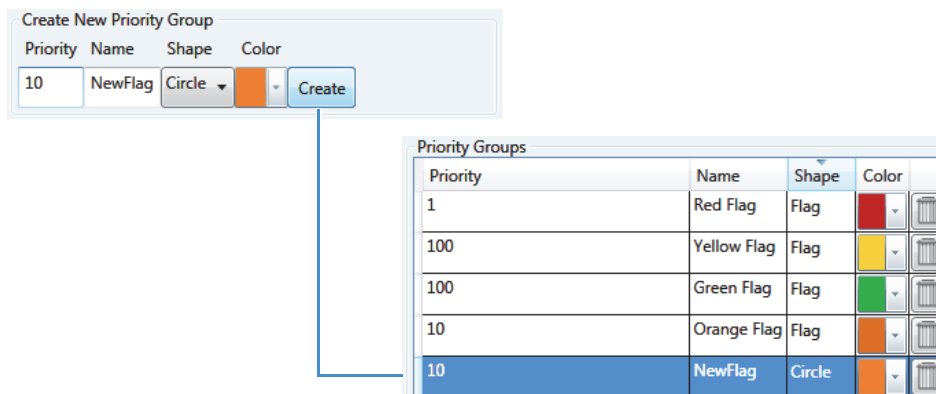
❖ **To edit flag rules**

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

1. Do any of the following:

   - In the Description column, select the current text and type a new description.

   - Double-click the PriorityGroup value and select a new group from the list.

   - Click **Delete**.

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

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

❖ **To create a new flag rule**

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

   Keep the name short and make it intuitive.

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

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

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

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

   This list includes both the default priority groups and any priority groups that you created. See "To create a new priority group" on page 77.

5. Click **Create**.

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

❖ **To remove all customization**

   Click **Reset to Factory Defaults**.

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

Advanced Dialog Box

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

Figure 18. Advanced RGB colors
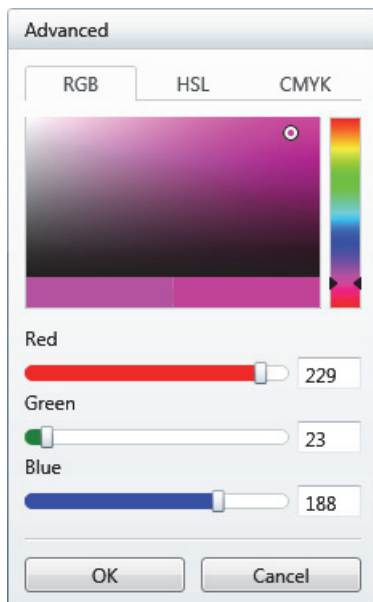
With the Red/Green/Blue (RGB) color palette, you can select a color with a specific RGB value, as displayed on a computer monitor.

Figure 19. Advanced HSL colors
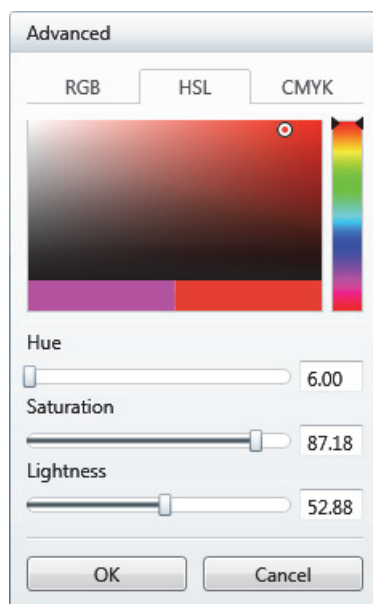
With the Hue/Saturation/Lightness (HSL) color palette, you can select a color with a specific HSL value, as is commonly used in computer graphics.

Figure 20. Advanced CMYK Colors
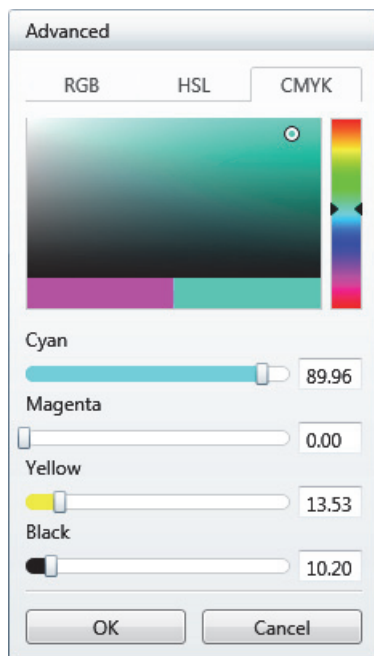
With the Cyan/Magenta/Yellow/Key (CMYK) color palette, you can select a color with a specific CMYK value, as you might specify in a color printer. The key (K) color used on printers is always black.

Using the Method Development Mode

This chapter includes method development tasks assigned to the default Supervisor or LabDirector role when user security is activated.

Contents

- Working with Master Methods
- Working with the Compound Database
- Working with Instrument Methods
- Working with Development Batches
- Using Quick Acquisition

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

You can also use the Quick Acquisition feature to quickly submit a single sample from any view in the Method Development mode.

❖ **To access the Method Development mode**

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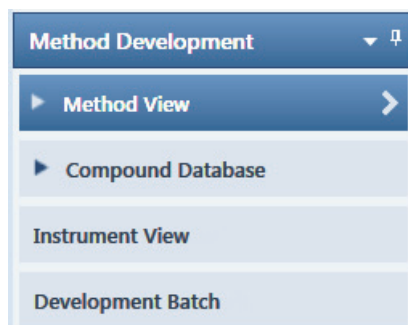
The Method Development navigation pane opens.

For descriptions of all the features on the Method Development navigation pane for a quantitation method, see "Method Development navigation pane for quantitation methods."

For descriptions of all the features on the Method Development navigation pane for a screening method, see "Method Development navigation pane for screening methods" on page 84.

Figure 21. Method Development navigation pane for quantitation methods

Available only when you select the Acquisition Batch Wizard
as your wizard style in the Configuration console.
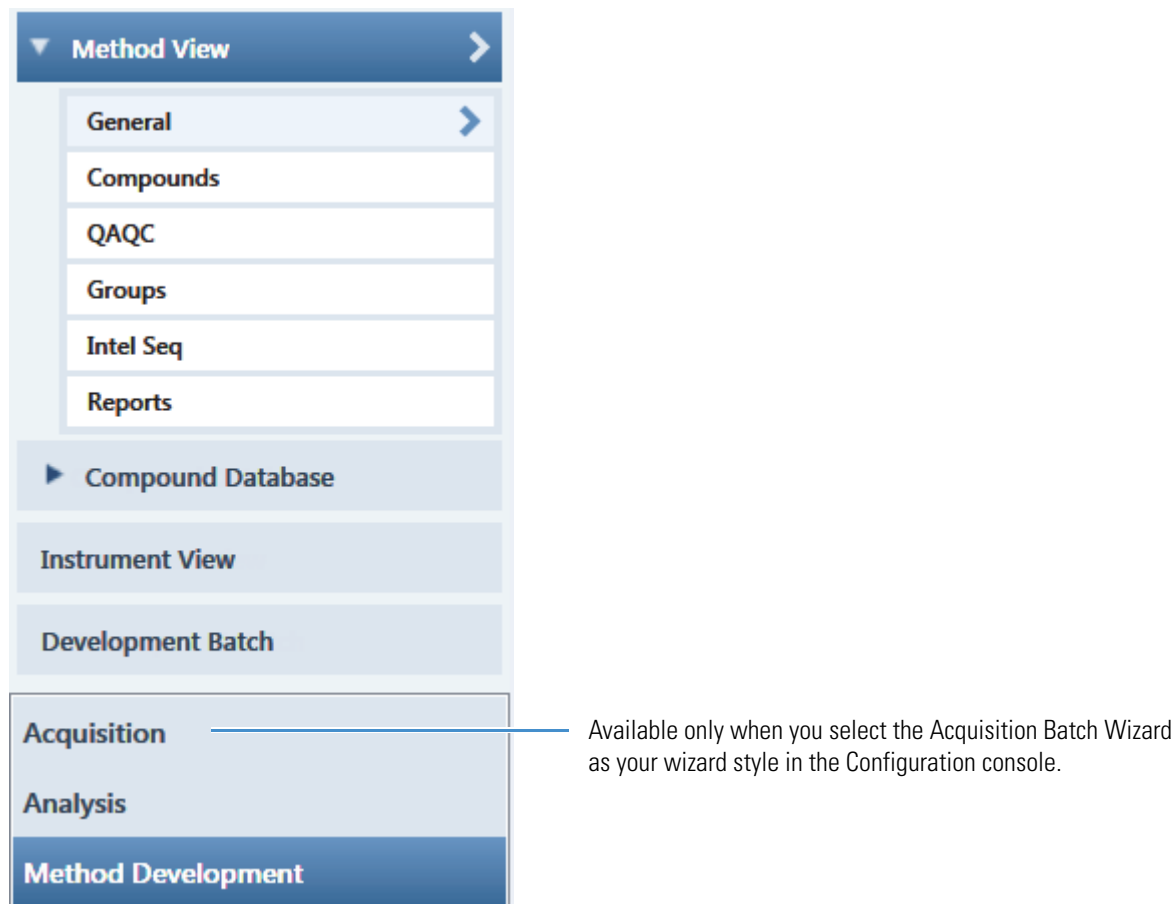
Table 13. Method Development navigation pane commands for quantitation methods

Command	Description
Method View	Displays the Method View for the master method. See "Working with Master Methods" on page 85.
General	Displays the General page of the Method View. See "Editing the General Page" on page 113.
Compounds	Displays the Compounds page of the Method View. See "Editing the Compounds Page" on page 120.
QAQC	Displays the QAQC page of the Method View. See "Editing the QAQC Page" on page 190.
Groups	Displays the Groups page of the Method View. See "Editing the Groups Page" on page 201.
Intel Seq	Displays the Intelligent Sequencing page of the Method View. See "Editing the Intelligent Sequencing Page" on page 204.
Reports	Displays the Reports page of the Method View. See "Editing the Reports Page" on page 208.
Compound Database	See "Working with the Compound Database" on page 269.
Instrument View	See "Working with Instrument Methods" on page 309.
Development Batch	See "Working with Development Batches" on page 315.

Figure 22. Method Development navigation pane for screening methods

Available only when you select the Acquisition Batch Wizard as your wizard style in the Configuration console.
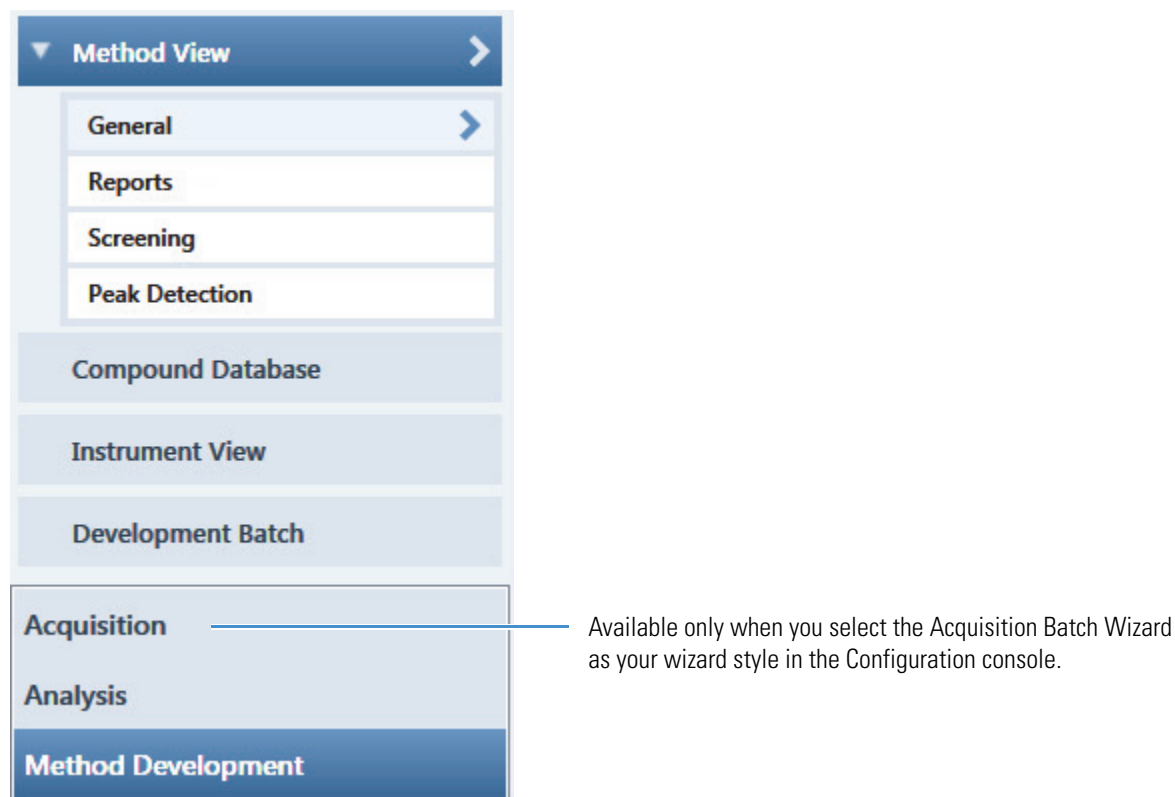
Table 14. Method Development navigation pane commands for screening methods

Command	Description
Method View	Displays the Method View for the master method. See "Working with Master Methods" on page 85.
General	Displays the General page of the Method View. See "Editing the General Page" on page 225.
Reports	Displays the Reports page of the Method View. See "Editing the Reports Page" on page 208.
Screening	Displays the Screening page of the Method View. See "Editing the Screening Page" on page 232
Peak Detection	Displays the Peak Detection page of the Method View. See "Editing the Peak Detection Page" on page 250
Compound Database	See "Working with the Compound Database" on page 269.
Instrument View	See "Working with Instrument Methods" on page 309.
Development Batch	See "Working with Development Batches" on page 315.

Working with Master Methods

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

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

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

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

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

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

This section includes instructions for the following tasks:

- Creating a New Master Method

- Editing a Quantitation Master Method

- Editing a Target Screening Master Method

- Saving a Master Method to a New Name

- Creating a Method Template

- Importing Published Master Methods

- Exporting Mass Data

Creating a New Master Method

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

- Creating a New Method with Method Forge

- Importing an Xcalibur Master Method

- Creating a Blank Quantitation Method

- Selecting Compounds from the Compound Database

- Creating a Screening Method

Then, use the common features of the Method View to complete and save it as a master method.

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

Figure 23. Create Master Method dialog box
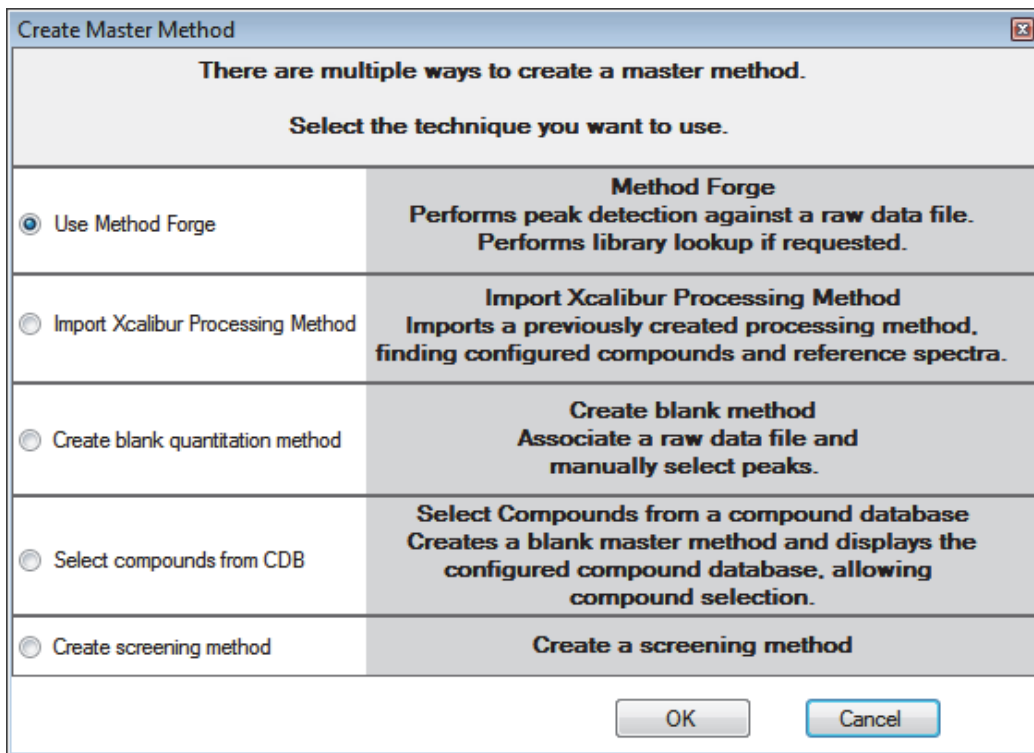
Creating a New Method with Method Forge

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

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

- Reviews your raw data file and identifies compounds that are present in your sample.

- Uses your mass spectral reference libraries to assign compound names and CAS numbers.

- Uses mass spectral information to select potential quantification and confirming ions and a reference mass spectrum for the compound.

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

Follow these procedures:

- To automatically select compounds to create a new method

- To manually select compounds to create a new method

❖ **To automatically select compounds to create a new method**

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

   The Create Master Method dialog box opens. To view all available ways to create a master method, see "Create Master Method dialog box" on page 86.

2. Select the **Use Method Forge** option and click **OK**.
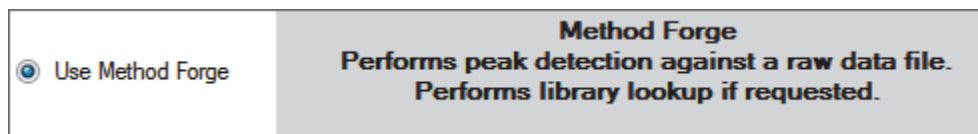
   The Method Forge dialog box opens. For detailed descriptions of all the features on the Method Forge dialog box, see "Method Forge Dialog Box" on page 96.

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

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

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

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

     See "Creating a Method Template" on page 254.

   • Select a method template from the template list, and click **Open Method Template Editor** to edit and save the method template.

   • Select a method template from the template list.

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

Figure 24. Example method template parameters
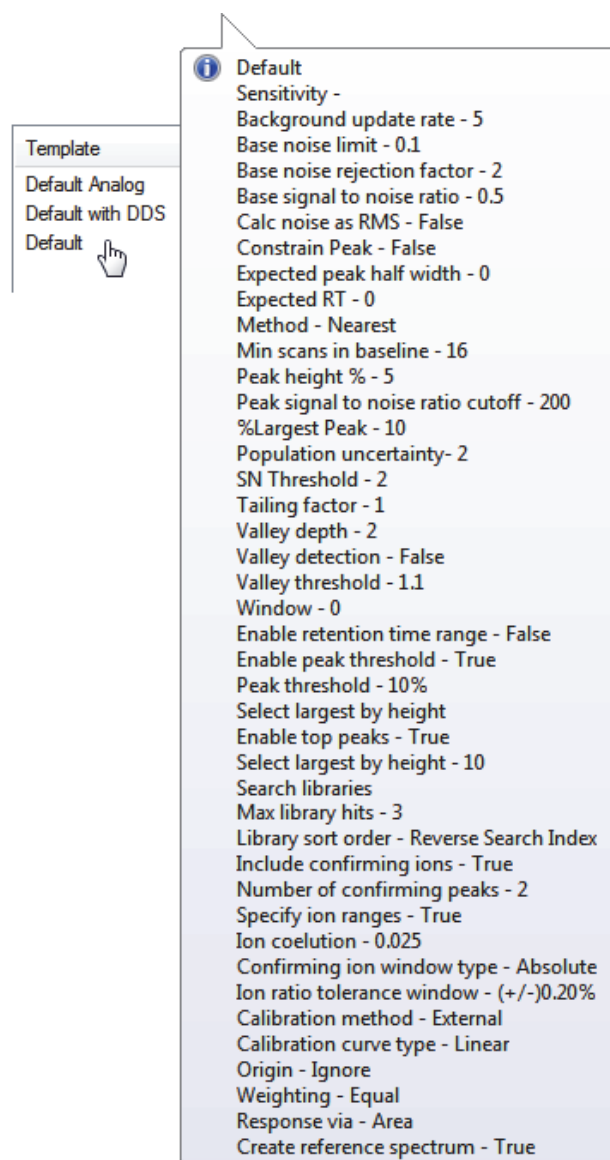
4. Select the **Name the Master Method** check box and type a name for your master method.

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

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

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

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

    a. In the Raw File Selection area, choose **Use an Existing Raw Data File**.

    b. Click the browse button and locate a raw data file to use for the method.

    c. Go to step 8.

    –or–

    a. In the Raw File Selection area, choose **Acquire a New Raw Data File**.

    b. From the Instrument method list, select a method (.meth) file to use for acquiring the data.

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

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

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

7. To acquire a new raw data file, do one of the following:

    Select **Manual Injection**.

    –or–

    Specify the autosampler settings:

    a. Select **Use Autosampler**.

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

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

    Range: 0.1 to 2000 µL

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

As the Method Forge creates the method, it displays the following status bars:
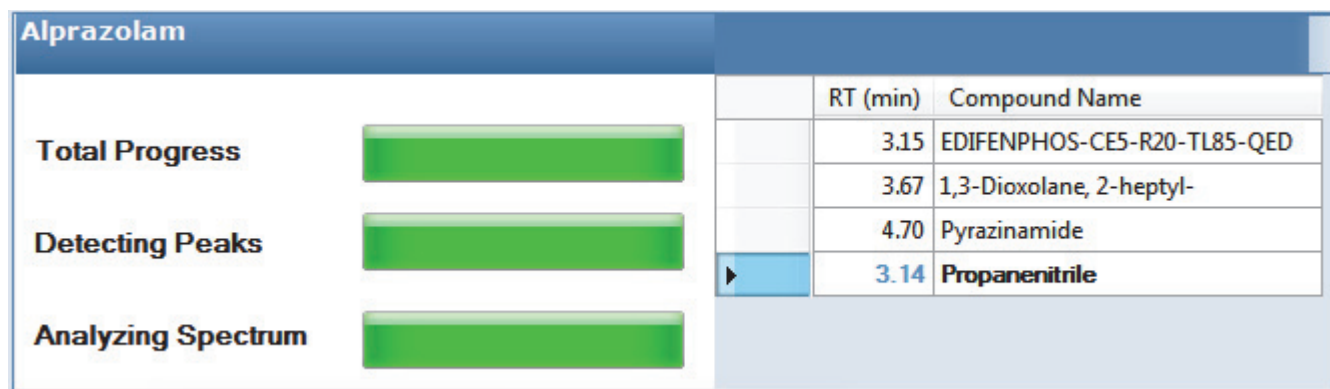
- For analog peaks, the Method Forge displays the detected peak as *Peak@(RT)Analog*. The Method Forge does not perform a library search for peaks found in analog traces.

- For mass spectral peaks, the Method Forge process searches the associated libraries and displays the identified compound names instead of the peak times.
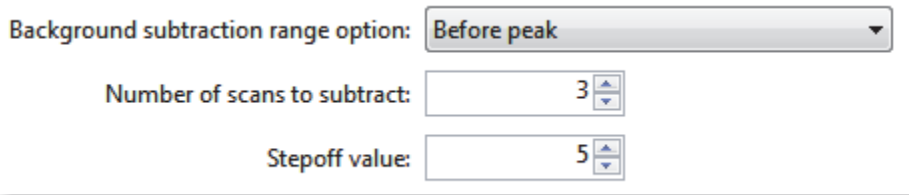
When the acquisition is completed, Method Forge performs peak detection, library searching (except for analog peaks), and identification of characteristic ion and reference spectra. Method Forge then loads this information into a new master method. This process occurs immediately if you selected a previously acquired raw data file.

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

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

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

- **Before Peak**: Averages and subtracts a specified number of scans before the apex of the peak.

- **After Peak**: Subtracts a specified number of scans following the apex of the peak.

- **Both Sides of Peak**: Subtracts a specified number of scans from each side of the apex of the peak.

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

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

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

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

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

For a detailed description of how to modify all the parameters in a master method, see "Editing a Quantitation Master Method" on page 109.

❖ **To manually select compounds to create a new method**

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

   The Create Master Method dialog box opens. See "Create Master Method dialog box" on page 86.

2. Select the **Use Method Forge** option and click **OK**.
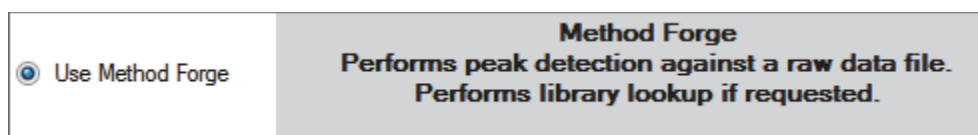
   The Method Forge dialog box opens. For detailed descriptions of all the features on the Method Forge dialog box, see "Importing an Xcalibur Master Method" on page 98.

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

Template	Libraries	
Default Analog	1	
Default	1	

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

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

     See "Creating a Method Template" on page 254.

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

     …\TraceFinderData\Templates\Methods\Forensic folder

   • Select a method template from the template list.

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

To view the parameters for each available method template, hold your cursor over the template name. For example:

Template

Default Analog
Default with DDS
Default

ℹ Default
Sensitivity -
Background update rate - 5
Base noise limit - 0.1
Base noise rejection factor - 2
Base signal to noise ratio - 0.5
Calc noise as RMS - False
Constrain Peak - False
Expected peak half width - 0
Expected RT - 0
Method - Nearest
Min scans in baseline - 16
Peak height % - 5
Peak signal to noise ratio cutoff - 200
%Largest Peak - 10
Population uncertainty- 2
SN Threshold - 2
Tailing factor - 1
Valley depth - 2
Valley detection - False
Valley threshold - 1.1
Window - 0
Enable retention time range - False
Enable peak threshold - True
Peak threshold - 10%
Select largest by height
Enable top peaks - True
Select largest by height - 10
Search libraries
Max library hits - 3
Library sort order - Reverse Search Index
Include confirming ions - True
Number of confirming peaks - 2
Specify ion ranges - True
Ion coelution - 0.025
Confirming ion window type - Absolute
Ion ratio tolerance window - (+/-)0.20%
Calibration method - External
Calibration curve type - Linear
Origin - Ignore
Weighting - Equal
Response via - Area
Create reference spectrum - True

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

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

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

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

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

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

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

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

Best match compound spectra

Peaks found in raw data file   Best match compound name   Possible matches

8. (Optional) To use a library compound other than the compound chosen by the TraceFinder application, do the following:

   a. Select the peak in the RT column.

   b. In the Libraries pane, scroll to the spectrum for the compound that you want to use.

   c. Select the check box in the header of the spectrum pane.
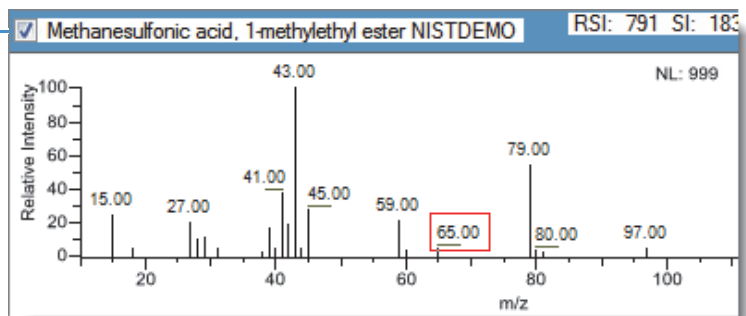
   d. Repeat these steps for each peak that you want to replace.

9. In the Compound Name list, use the CTRL or SHIFT keys to select each compound that you want to include in the method compound.

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

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

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

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

11. Click **Create**.

    The TraceFinder application uses all selected compounds to create the method and displays the General page of the Method View. For detailed descriptions of all the features on the General page, see "General page for a quantitation method" on page 118.

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

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

    For a detailed description of how to modify a master method, see "Editing a Quantitation Master Method" on page 109.

Method Forge Dialog Box

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

Figure 25. Method Forge dialog box

Table 15. Method Forge dialog box parameters (Sheet 1 of 2)

Parameter	Description
Method template selection	
Open Method Template Editor	Opens the Method Template Editor, where you can edit the currently selected method template. See "Creating a Method Template" on page 254.
Template	Method template to use to create this master method. All methods require a method template. To view the parameters of each template, hold your cursor over the method name. See the Method Template Parameters example in "To automatically select compounds to create a new method" on page 87.
Name the Master Method	The name for the new master method. If you do not specify a method name, the application uses the raw data file name for the method.
Automatically Create the Master Method	When the acquisition is completed, Method Forge performs peak detection, library searching, and identification of characteristic ion and reference spectra. This information is loaded into a new master method. This process occurs immediately when you specify an existing raw data file.

Table 15. Method Forge dialog box parameters (Sheet 2 of 2)

Parameter	Description
Raw file selection	
Use an Existing Raw Data File	Activates the Raw Filename box where you can select a raw data file used in creating the master method.
Acquire a New Raw Data File	Activates functions to acquire data to create a raw data file used in creating the master method.
Instrument Method	The saved method (.meth) file used for acquiring the data.
Raw Filename	The file name where the TraceFinder application writes the raw data.
Path	The location where the TraceFinder application saves the raw data file.
Sample Comment	(Optional) A comment about the acquired sample or the data file.
Manual Injection	Performs a manual acquisition.
Use Autosampler	Performs an autosampler acquisition.
Vial Position	The tray vial number used for the autosampler acquisition.
Injection Amount	The volume (in milliliters) injected by the autosampler acquisition.
Check Instruments	Opens the Submit to Acquisition dialog box that prompts you to prepare the instrument before you acquire the sample used to create a method. Available only when you select the Acquire a New Raw Data File option.
Function button	
Overwrite	Overwrites the specified master method name. This function is activated only when the specified master method name already exists.
OK	Creates a master method using the data and parameters that you specified.
Cancel	Closes Method Forge and does not create a master method.

Importing an Xcalibur Master Method

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

❖ **To import an Xcalibur master method**

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

   The Create Master Method dialog box opens. To view all available ways to create a master method, see "Create Master Method dialog box" on page 86.

2. Select the **Import Xcalibur Processing Method** option and click **OK**.
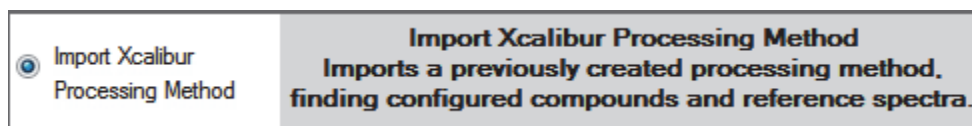
   The Import an Xcalibur Method dialog box opens.
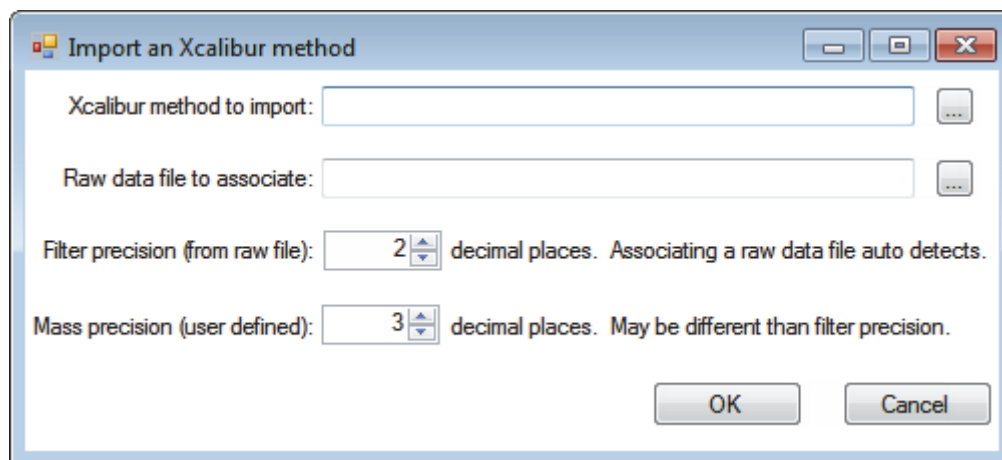
3. For the Xcalibur Method to Import box, browse to the location of the Xcalibur processing method file, and open the file.

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

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

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

   …\TraceFinderData\Methods*Methodname*

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

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

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

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

   You can set the number of mass precision decimal places to any integer between 2 and 6, inclusive.
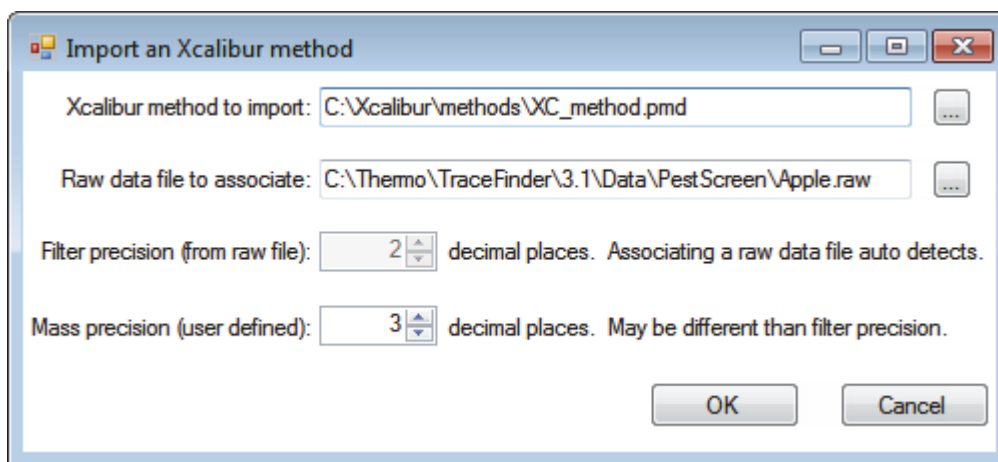
   > **Note** When you associate a raw data file, the application reads the filter precision from the associated file so that you cannot change the Filter Precision value.

7. Click **OK**.

   The TraceFinder application adds all compounds found in the imported Xcalibur method and displays the General page of the Method View. For detailed descriptions of the features on the General page, see "General Page for a Quantitation Method" on page 117.

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

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

   For a detailed description of how to modify a master method, see "Editing a Quantitation Master Method" on page 109.

Creating a Blank Quantitation Method

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

❖ **To create a blank quantitation method**

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

   The Create Master Method dialog box opens. To view all available ways to create a master method, see "Create Master Method dialog box" on page 86.

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

	Create blank method
◉ Create blank quantitation method	**Associate a raw data file and manually select peaks.**

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

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

   The Associate a Raw Data File dialog box opens.

   Browse to a data file

   Select a previously associated data file

Associate a raw data file			
Raw data file to associate:	C:\Thermo\TraceFinder\3.1\Data\Alprazolam.raw ▼		...
Update instrument/trace selections	○ No	◉ Yes	
Update target ion ratio values	◉ No	○ Yes	
Update scan filters for all peaks	○ No	◉ Yes	
Automatically set reference spectrum	◉ No	○ Yes	○ Yes, with background subtraction
		OK	Cancel
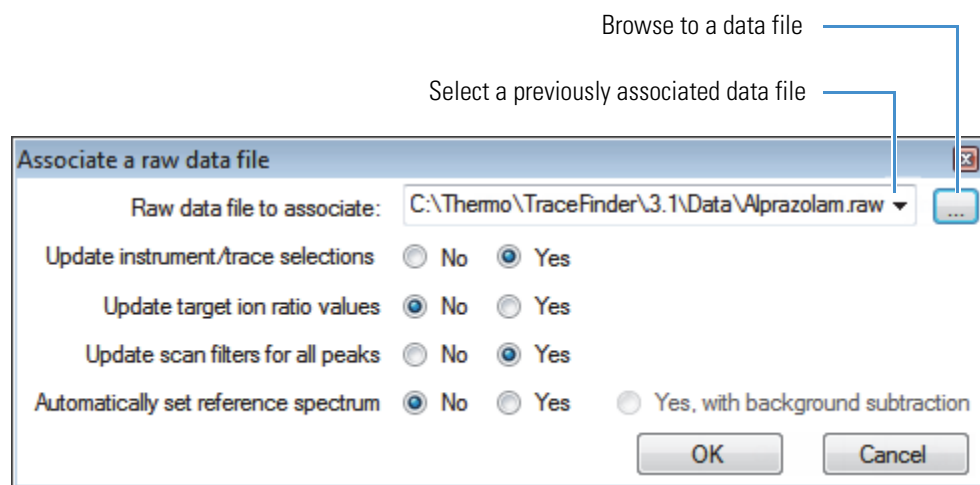
4. Browse to a raw data file to associate with the method (or select from the list of previously associated raw data files) and open the file.

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

   …\TraceFinderData\Methods*Methodname*

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

   • **Update Instrument/Trace Selections**: Reads the Detector and Trace options from the associated raw data file. On the Detection page, only detector types and traces that are defined in the raw data file are available. For detailed descriptions of the available Detector and Trace values, see "Signal" on page 141.

   • **Update Target Ion Ratio Values**: Reads the ion ratio values from the associated raw data file.

   • **Update Scan Filters for All Peaks**: Updates all peaks with scan filters from the associated raw data file.

   • **Automatically Set Reference Spectrum**: Reads a reference spectrum from the associated raw data file.

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

     > **Note** The background subtraction option is available only when you select a background subtraction method on the General page in the master method. See "Editing the General Page" on page 113.

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

6. Click **OK**.

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

7. Select a qualitative peak processing template from the list.

   The application uses the libraries in this template to identify compounds for the method. If there is no library selected in the method template, found peaks are identified as peak@*RT* on the Compounds page.

   To specify the libraries in the qualitative peak processing template, open the template in the Method Template Editor, and then follow the instructions "To identify the peaks" on page 256.

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

   The method must include at least one compound.

9. Click the **Detection** tab.

   The Detection page shows an empty Compound list and displays the chromatographic data for the compounds in the raw data file.
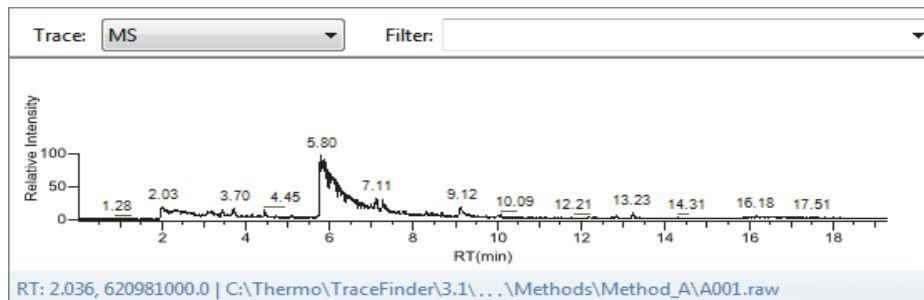
10. Select a filter from the Filter list.

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

12. Right-click and choose **Add This Peak as New Compound** from the shortcut menu.
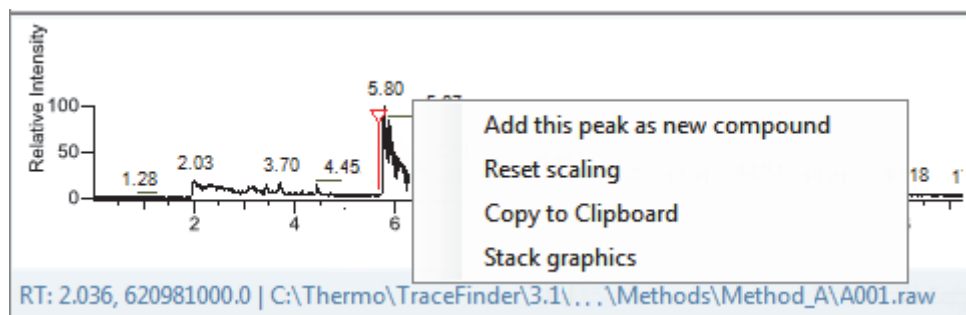
    The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quantitative peak, and the second and third largest ions as the confirming ion peaks.

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

If the name of the first match is already in the library, the Add New Compound dialog box opens.
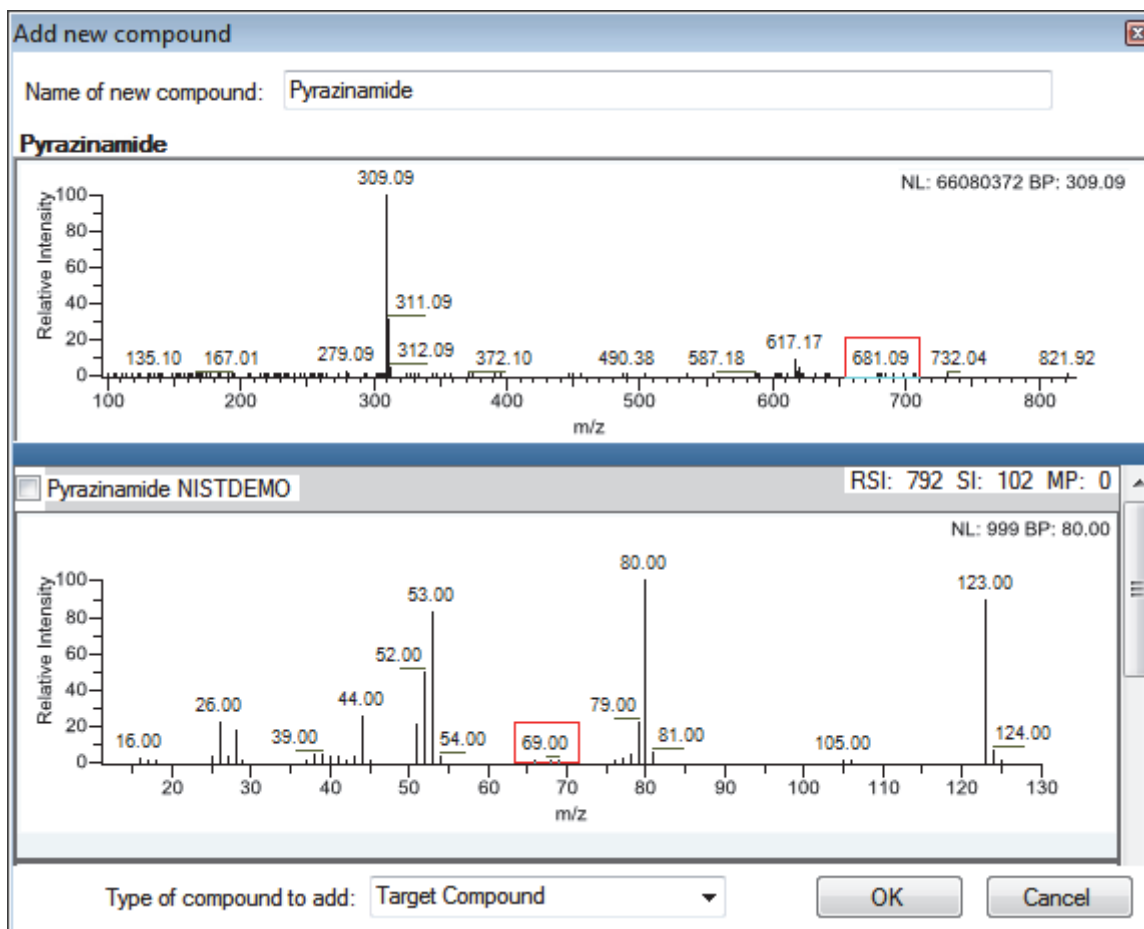
13. (Optional) Do the following:

    a. To use a compound other than the compound already in the library, scroll to the spectrum for that compound and select the compound name in the title bar of the spectrum pane.
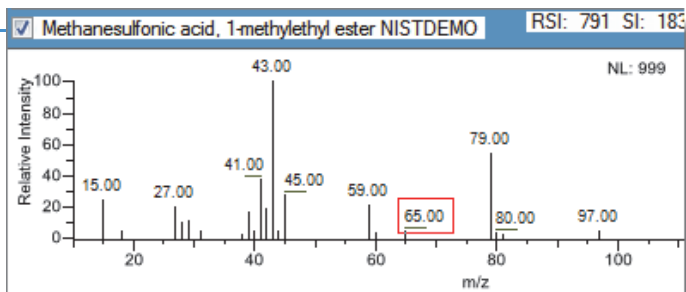
    b. In the Type of Compound To Add list, select a compound type.

    c. Click **OK**.

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

    For detailed descriptions of all the features on the Detection page, see "Editing the Compounds Page" on page 120.

15. Click **General** in the navigation pane.

    The General page for the method opens. For detailed descriptions of all the features on the General page, see "General page for a quantitation method" on page 118.

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

17. To save the new method, choose **File > Save** from the main menu and name the method.

    For a detailed description of how to modify the parameters in a master method, see "Editing a Quantitation Master Method" on page 109.

Selecting Compounds from the Compound Database

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

❖ **To select compounds from the compound database**

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

   The Create Master Method dialog box opens. To view all available ways to create a master method, see "Create Master Method dialog box" on page 86.

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

⦿ Select compounds from CDB	**Select Compounds from a compound database** Creates a blank master method and displays the configured compound database, allowing compound selection.

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

3. Select the check box for each of the compounds that you want to add to the method.

4. To select all compounds in the database, select the **Compound** check box at the top of the list.

5. Click **Apply**.

   The TraceFinder application adds the selected compounds to the method.

6. Click **General** in the navigation pane.

   The General page for the method opens. For detailed descriptions of all the features on the General page, see "General Page for a Quantitation Method" on page 117.

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

8. To save the new method, choose **File > Save** from the main menu and name the method.

   For a detailed description of how to modify a master method, see "Editing a Quantitation Master Method" on page 109.

Creating a Screening Method

You can create a new master method specifically for target screening.

❖ **To create a target screening method**

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

   The Create Master Method dialog box opens. To view all available ways to create a master method, see "Create Master Method dialog box" on page 86.

2. Select the **Create Screening Method** option and click **OK**.
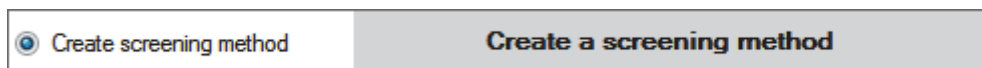
   The Method View for a target screening method includes General, Reports, Screening, and Peak Detection pages.
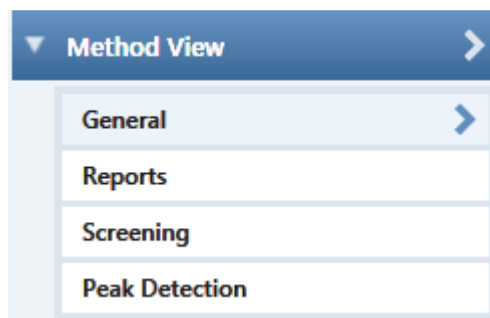
   These instructions demonstrate the minimum parameters you must define to create and save a screening master method. For a detailed description of how to modify all parameters in a screening master method, see "Editing a Target Screening Master Method" on page 222.

   The General page for the screening method opens.

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

4. Click **Screening** in the Method View navigation pane.

   The Screening page for the screening method opens.

   The Target Screening Settings pane displays the compound databases stored in the following folder:

   …\Thermo\TraceFinder\3.1\Forensic\Databases

5. Select the **Enabled** check box for at least one compound database.

   You must select at least one compound database before you can save the method.

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

7. In the Save Master Method dialog box, type a name for the method and click **OK**.

   For a detailed description of how to modify a master method, see "Editing a Target Screening Master Method" on page 222.

Editing a Quantitation Master Method

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

This section includes instructions for the following tasks:

- Opening a Quantitation Master Method
- Editing the General Page
- Editing the Compounds Page
- Editing the QAQC Page
- Editing the Groups Page
- Editing the Intelligent Sequencing Page
- Editing the Reports Page

Opening a Quantitation Master Method

Use the TraceFinder application to open a master method that was created and saved in the current TraceFinder application or converted from these legacy applications: previous versions of TraceFinder, EnviroLab Forms, QuanLab Forms, or ToxLab Forms. To convert legacy methods, see "Converting Legacy Data" on page 20.

Follow these procedures:

- To open a saved master method
- To modify retention times in a method

❖ **To open a saved master method**

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

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

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

The Open Master Method dialog box opens, displaying all available methods.

Figure 26. Open Master Method dialog box

Table 16. Open Master Method dialog box parameters (Sheet 1 of 2)

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan or Screening.
Date Changed	Date the method was last updated.
Size	Size in megabytes.
Domain	TraceFinder domain for which the method was created: General, EFS, Clinical, or Forensic.

Table 16. Open Master Method dialog box parameters (Sheet 2 of 2)

Parameter	Description
Type	Type of method to display: Quan, Screening, or Any.
Path	Path to the selected method in the TraceFinderData\Methods folder.

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

Type: Quan ▾
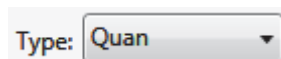
The method list displays all quantitation methods.

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

The General page for the selected method opens. For detailed descriptions of all the features on the General page, see "General Page for a Quantitation Method" on page 117.

❖ **To modify retention times in a method**

1. Do one of the following from any page in the Method View or Local Method view:

   • Choose **Method View > Adjust Retention Times** from the main menu of the Method View in the Method Development mode.

   • Choose **Local Method > Adjust Retention Times** from the main menu of the Local Method view in the Analysis mode.

The Adjust Retention Times dialog box opens.

Adjust Retention Times

Adjustment all compounds by
- ⦿ Absolute (minutes)   0.00
- ○ Relative (%)   0.00
- ○ By file...   Select

OK   Cancel
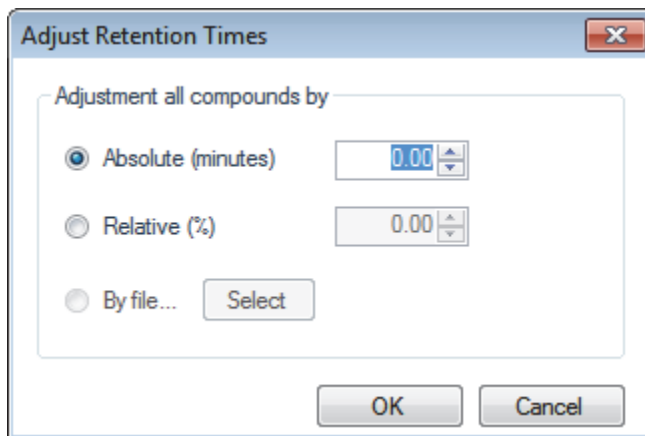
2. Do one of the following:

   a. Select the **Absolute** option.

   b. Specify a positive or negative value to increase or decrease the expected retention times.

      Valid values: –100.00 through 100.00

c. Click **OK**.

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

–or–

a. Select the **Relative** option.

b. Specify a positive or negative value to increase or decrease the expected retention times.

Valid values: –100.00 through 100.00

c. Click **OK**.

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

–or–

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

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

b. Click **Select**.

The Adjust Retention Time by File dialog box opens, displaying all processed samples.
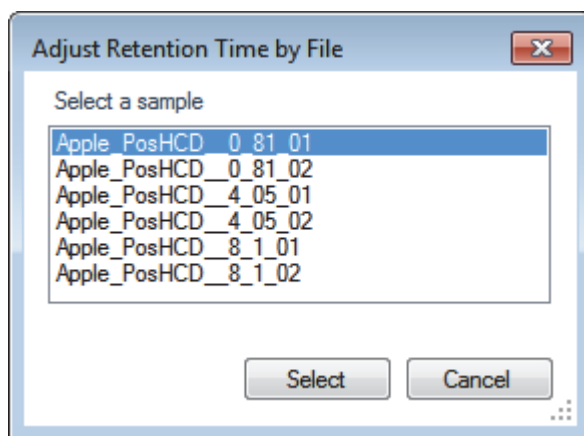
c. Select the sample whose retention times you want to use in the method.

d. Click **Select**.

e. Click **OK**.

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

Editing the General Page

The General page defines basic information about the master method. For detailed descriptions of all the features, see "General Page for a Quantitation Method" on page 117.

Follow these procedures:

- To open the General page
- To specify general information for a master method
- To edit an instrument method
- To select a qualitative peak processing template
- To set automated background subtraction options
- To specify mass tolerance
- To include data-dependent filters
- To enter a note for the method

❖ **To open the General page**

Click **General** in the Method View navigation pane.
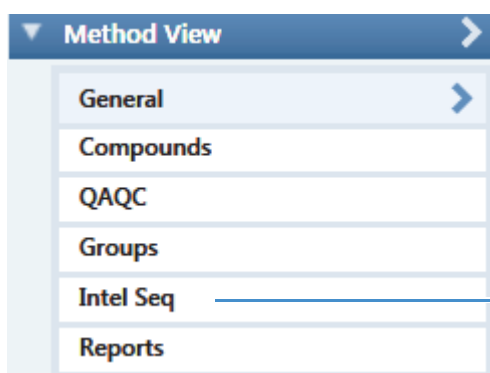
Available only when you activate Intelligent Sequencing in the Configuration console.

❖ **To specify general information for a master method**

1. In the Lab Name box, type the name to be displayed on the top of each printed, saved, or exported report.

   The default name is Default Laboratory.

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

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

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

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

4. From the Mass Precision box, select a precision value (between **2** and **6** inclusive) as the number of decimal places to be used in reports and in peak and spectrum displays.

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

   When you select Level, the TraceFinder application displays a Use Level list where you can choose a calibration level. To define the available calibration levels on the Compounds page, see "Editing the Compounds Page" on page 120.

❖ **To edit an instrument method**

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

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

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


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

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

   The TraceFinder application returns you to the General page. See "General Page for a Quantitation Method" on page 117.

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

   The Update Instrument Method? dialog box opens.
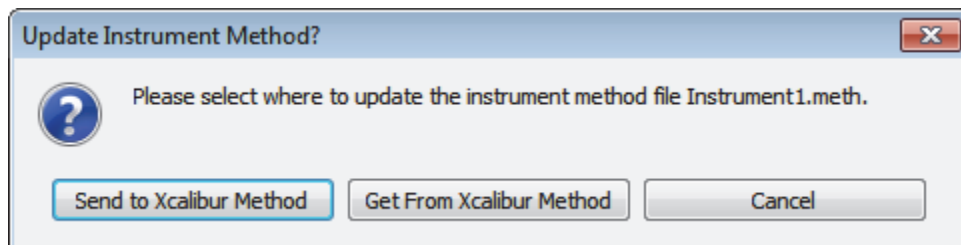
6. Choose one of the following options:

   • **Send to Xcalibur Method**: Overwrites the instrument method in the C:\Xcalibur\methods folder with the current instrument method.

   • **Get From Xcalibur Method**: Overwrites the current instrument method with the instrument method in the C:\Xcalibur\methods folder.

   • **Cancel**: Make no changes to the instrument method in the current master method.

❖ **To select a qualitative peak processing template**

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

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

…\TraceFinderData\Templates\Methods\Forensic folder

❖ **To set automated background subtraction options**

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

   • **Before Peak**: Averages and subtracts a specified number of scans before the apex of the peak.

   • **After Peak**: Subtracts a specified number of scans after the apex of the peak.

   • **Both Sides of Peak**: Subtracts a specified number of scans from each side of the apex of the peak.

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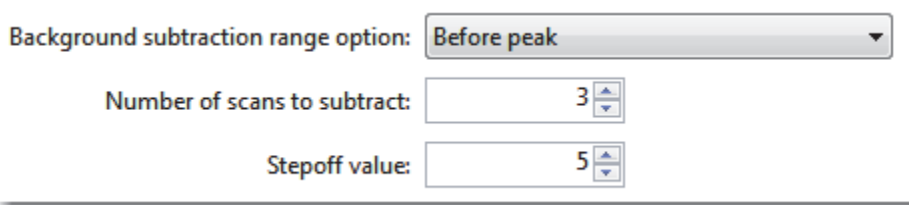
(indicated with BS in the scan heading) as the last scan for each compound on the Quantitation Report - 2 report. The application does not use background subtraction with qualitative processing.

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

   This is the number of scans that the TraceFinder application subtracts from the background after averaging. When you select the Both Sides of Peak option, the application subtracts this number of scans from **each** side of the peak.

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

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

Background subtraction range option:	Before peak ▼
Number of scans to subtract:	3 ⏶⏷
Stepoff value:	5 ⏶⏷

   Before Peak example:

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

   After Peak example:

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

   Both Sides of Peak example:

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

❖ **To specify mass tolerance**

1. Select the units of measure that you want to use.

2. Specify the number of millimass units or parts per million to use as the m/z ± tolerance value.

   The application applies this mass tolerance to the extracted chromatograms.

❖ **To include data-dependent filters**

Select the **Include Data Dependent Filters** option.

The application includes data-dependent filters when you specify filters in the method. See "Signal" on page 141.

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

Filter: + c d ESI Full ms [200.00-800.00] ▾

Data-dependent filter

When you process a sample using a data-dependent filter, the application uses the TIC trace to find all data-dependent full scans, lists them, and performs a library search against the data-dependent MS/MS or MS^n scan.

❖ **To enter a note for the method**

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

You can add a note to explain what makes this method unique.

General Page for a Quantitation Method

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

Figure 27. General page for a quantitation method

Table 17. General page parameters (Sheet 1 of 2)

Parameter	Description
Lab Name	The laboratory name to be displayed on the top of each printed, saved, or exported report. Default: Default Laboratory To specify this default laboratory name, see "Specifying Application Defaults" on page 45.
Assay Type	The name for the analysis type to be targeted by the method. The assay type associates the method with the analysis of a compound or specific class of compounds (for example, you might use an assay type of PAH for the analysis of Polynuclear Aromatic Hydrocarbons).

**Table 17.** General page parameters (Sheet 2 of 2)

Parameter	Description
Injection Volume	The system uses the injection volume (in μL) for sample injection. For a more detailed explanation, refer to the documentation for the autosampler.
	The injection volume in the master method overrides the injection volume in the instrument method. The injection volume in the batch overrides the injection volume in the master method.
	Range: 0.1 to 2000 μL
Mass Precision	Number of decimal places used in reports and in peak and spectrum displays. Valid values: Integers from 2 to 6, inclusive.
Ion Range Calc Method	The TraceFinder application uses the selected ion range calc method to calculate the ion ratio range windows: Manual (default), Average, Level, or Weighted average. When you select Level, an additional list is displayed where you can select a calibration level amount. To define these calibration levels on the Compounds page, see "Editing the Compounds Page" on page 120.
Instrument Method	Instrument method used for acquiring samples.
Edit	Opens the Thermo Xcalibur Instrument Setup dialog box where you can edit the instrument method.
Update	Choose one of the following:
	Send to Xcalibur Method: Overwrites the Xcalibur method with the current instrument method.
	Get From Xcalibur Method: Overwrites the current instrument method with the Xcalibur method.
Qualitative Peak Processing Template	The TraceFinder application uses the qualitative peak processing template to perform peak detection on quantitative samples following compound analysis.
Background Subtraction Range Option	Valid values: None, Before Peak, After Peak, Both Sides of Peak Default: None
Number of Scans To Subtract	Valid values: Even numbered integers Default: 0
Stepoff Value	Offset from the selected peak to the first subtracted peak.
Mass Tolerance	Upper limit of MMU or PPM. Default: 500 Range: 0.1 through 50 000 • (Default) MMU (millimass units): MMU is a static calculation to the extracted mass. • PPM (parts per million): PPM is a variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.
Include Data Dependent Filters	Available only for quantitation methods.
Notes	Optional notes about the method.

Editing the Compounds Page

Use the Compounds page to set all parameters for identifying, detecting, and quantifying the target compound list.

❖ **To open the Compounds page**

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

Available only when you activate
Intelligent Sequencing in
the Configuration console
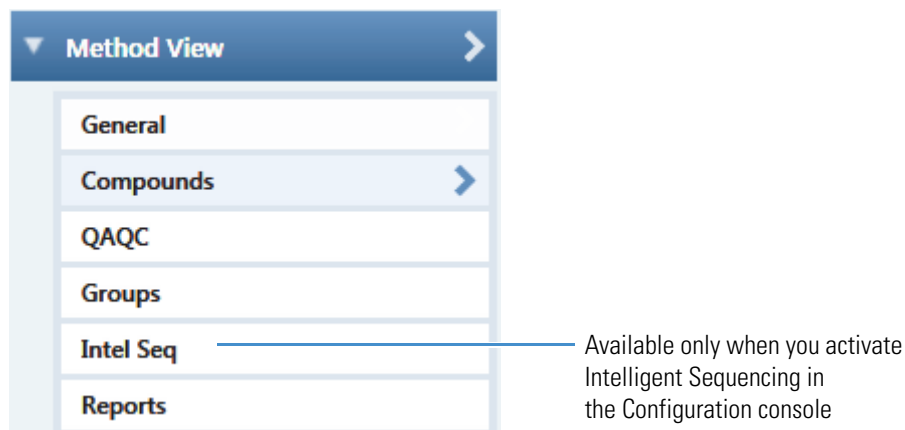
From the Compounds page of the Method View, you can access the following pages:

Acquisition List   See also Acquisition List.

Identification   See also "Identification page parameters" on page 123.

Detection   See also "Detection page panes" on page 138.

Calibration   See also "Calibration page parameters" on page 177.

Calibration Levels   See also "Calibration Levels page parameters" on page 180.

QC Check Levels page   See also "QC Check Levels page parameters" on page 182.

Real Time Viewer   See also "Real Time Viewer page parameters" on page 186.

Each page on the Compounds page (except the Acquisition List and Real Time Viewer pages) uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 188.

Acquisition List

The Acquisition List page displays all compounds defined for the current method in a display similar to the Compound Database view. From the Acquisition List page, you can add additional compounds from the Compound Database or delete compounds from the method.

For detailed descriptions of all the features in the Compound Database views, see "Working with the Compound Database" on page 269.

❖ **To remove a compound from the method**

1. Select the compound in the Compound list.

2. Click the **Remove Compound** icon, ▬.

3. To confirm that you want to delete the selected compound, at the prompt, click **OK**.

   The application removes the selected compound and all its peak information.

4. To remove multiple compounds, use the CTRL or SHIFT keys.

   The application confirms that you want to remove the selected compounds.

❖ **To add a compound to the method**

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

   The Select Compounds from Database dialog box opens, listing all the compounds defined in the compound database. This dialog box is identical to the Compound Database with the exception that you cannot edit the compound data from here; you can only choose which compounds you want to include in your method.

Figure 28. Select Compounds from Database dialog box
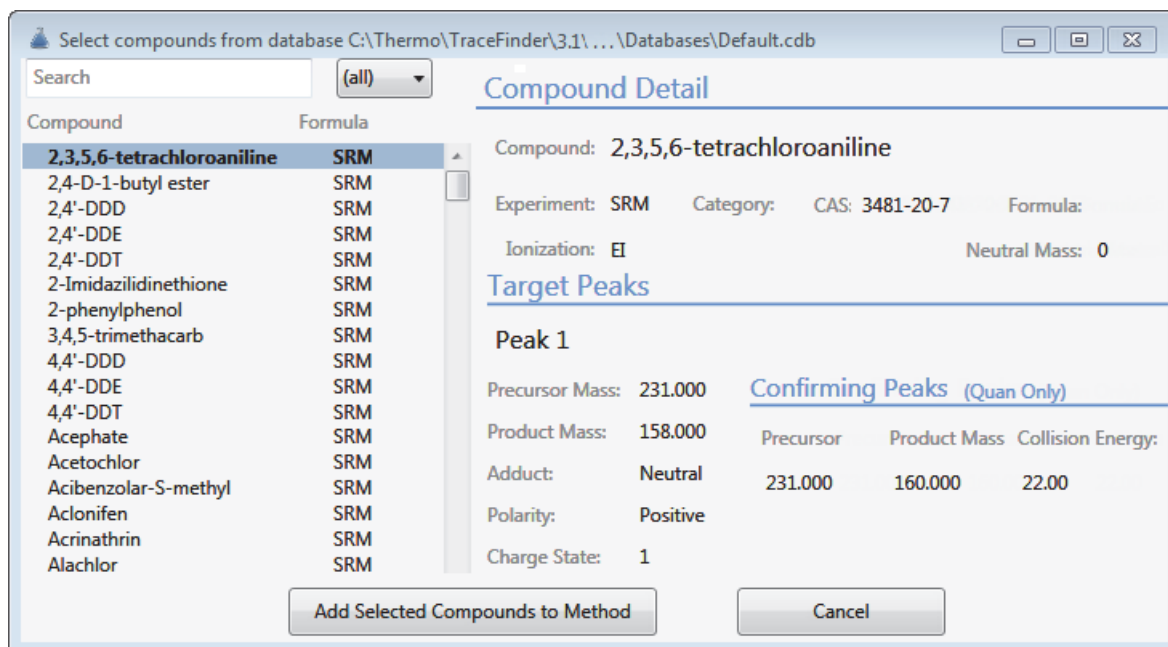
2. Select the compounds to add to the method.

   You can use the SHIFT or CTRL keys to select multiple compounds.

3. Click **Add Selected Compounds to Method**.

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

Identification

The Identification page lists the compounds that are targeted for analysis, reporting, and other compound-specific values. For descriptions of all values on the Identification page, see "Identification page."

❖ **To filter the displayed compounds**

From the Show list, select the type of compounds that you want to display in the compounds list.
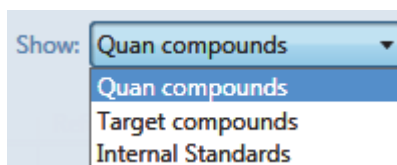
Compound type	Description
Quan Compounds	Displays only quantitation compounds, such as target compounds and internal standards.
Target Compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.

Figure 29. Identification page

Table 18. Identification page parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column. The TraceFinder application uses the RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Compound	A list of identified compounds. To customize the compound names, click the cell and type a new name. To display a filtered list of compounds, use the Show list.
Compound Type	Compound types are Target Compound and Internal Standard. The TraceFinder application uses target compounds and internal standards in quantitative analysis.

Table 18. Identification page parameters (Sheet 2 of 2)

Parameter	Description
Active	Identifies each compound to be included in data review and reporting. By default, all added compounds are set to active. This active or inactive setting populates the Batch View and Data Review view in the Analysis mode.
CAS No	The Chemical Abstract Service (CAS) number that the TraceFinder application matched with each compound. To change or add a number, click the CAS No cell and enter a new number.
Use as RT Reference	When performing peak detection with retention time standards, the TraceFinder application first identifies those compounds identified as retention time standards and then uses their observed retention times to adjust any associated target compound.
Reference Compound	To be used for retention time adjustment for a compound. This list includes all compounds that are selected in the Use as RT Reference column.
Shortcut menu	The Identification page uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 188.

Detection

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

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

Times   See also "Times page parameters" on page 139.

Signal   See also "Signal page parameters" on page 148.

Detect   See also "Detect page parameters for Genesis" on page 153.
See also "Detect page parameters for ICIS" on page 157.
See also "Detect page parameters for Avalon" on page 159.

Suitability   See also "System Suitability dialog box" on page 163.

Spectrum   See also "Spectrum page shortcut menu commands" on page 170.

Library   See also "Library page shortcut menu commands" on page 172.

Ratios   See also "Ratios page parameters" on page 174.

On the Detection page (see "Detection page" on page 137), you can configure how characteristic ions for targeted compounds are detected and integrated. You can also edit the list of characteristic ions for a specific compound. Refining these parameters in the master method for each compound and its ions can reduce the degree of manual integration that would otherwise be required.

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

Follow these procedures:

- To filter the displayed compounds
- To change the displayed information for detected peaks
- To add compounds to the method
- To change the compound reference spectrum
- To replace a quantitation mass
- To add a mass to the existing quantitation mass ranges
- To add a quantitative peak
- To add a spectral peak as a new compound
- To replace a quantitative peak with a confirming ion peak
- To set a confirming ion peak as an additional quantitative peak
- To add a trace to the Real Time Status pane
- To replace a confirming ion peak
- To add a mass as a new confirming ion peak
- To use the cut-and-paste feature on confirming ion peaks
- To save the new method

❖ **To filter the displayed compounds**

From the Show list, select the type of compounds that you want to display in the compounds list.
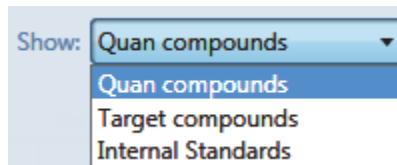
Compound type	Description
Quan Compounds	Displays only quantitation compounds, such as target compounds, internal standards, and surrogates.
Target Compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.

❖ **To change the displayed information for detected peaks**

1. Right-click the chromatogram plot for any of the quan or confirming peaks and hold the cursor over **Peak Labels**.

2. Choose to display labels for the peak area, peak retention time, peak height, or signal to noise.
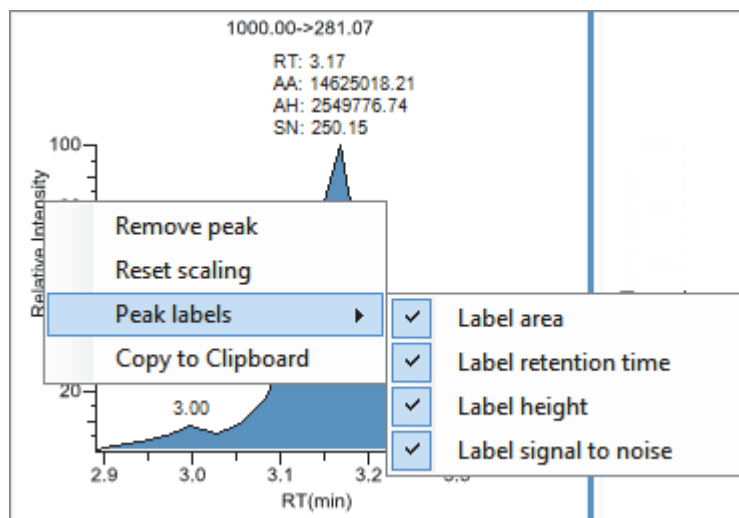
3. To remove a label, select the label type again and clear it.

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

❖ **To add compounds to the method**

> **Tip** You can add compounds from the current raw data file (begin at step 7), or you can associate another raw data file and add compounds from that file (begin at step 1).

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

   The Associate a Raw Data File dialog box opens.

   Browse to a data file. ————

   Select a previously associated data file. ————
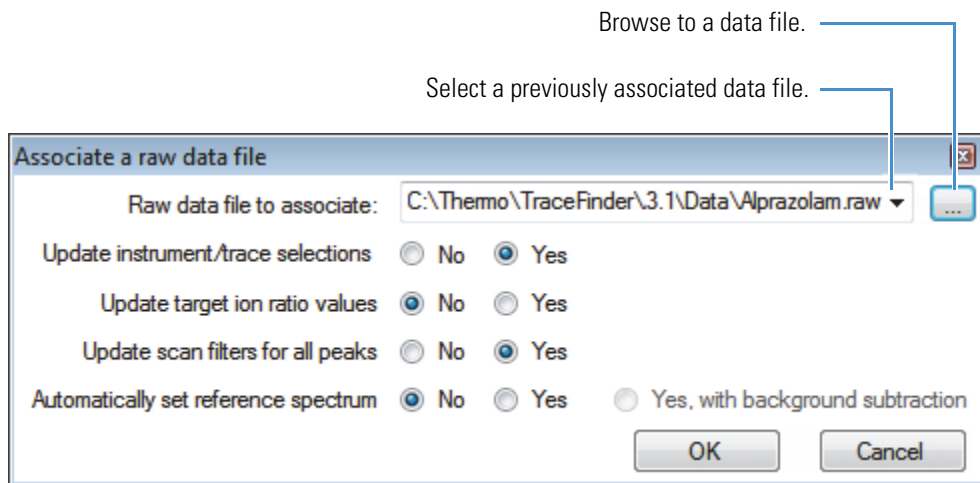
2. Browse to a raw data file to associate with the method (or click the arrow and select from the list of previously associated raw data files) and open the file.

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

   …\TraceFinderData\Methods*Methodname*

3. To update the target ion ratio values when you associate this raw data file, select the **Yes** option.

4. To update the scan filters when you associate this raw data file, select the **Yes** option.

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

   Select the **Yes** option.

   –or–

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

   The application uses the background-subtracted reference spectrum during quantitative processing and reports the background-subtracted reference spectrum (indicated with BS in the scan heading) as the last scan for each compound on the Quantitation Report - 2 report.

   > **Note** This option is available only when you select a background subtraction method on the General page in the master method. See "Editing the General Page" on page 113.

6. Click **OK**.

   The TraceFinder application displays the chromatographic and spectrum data for the
   compounds in the associated raw data file.
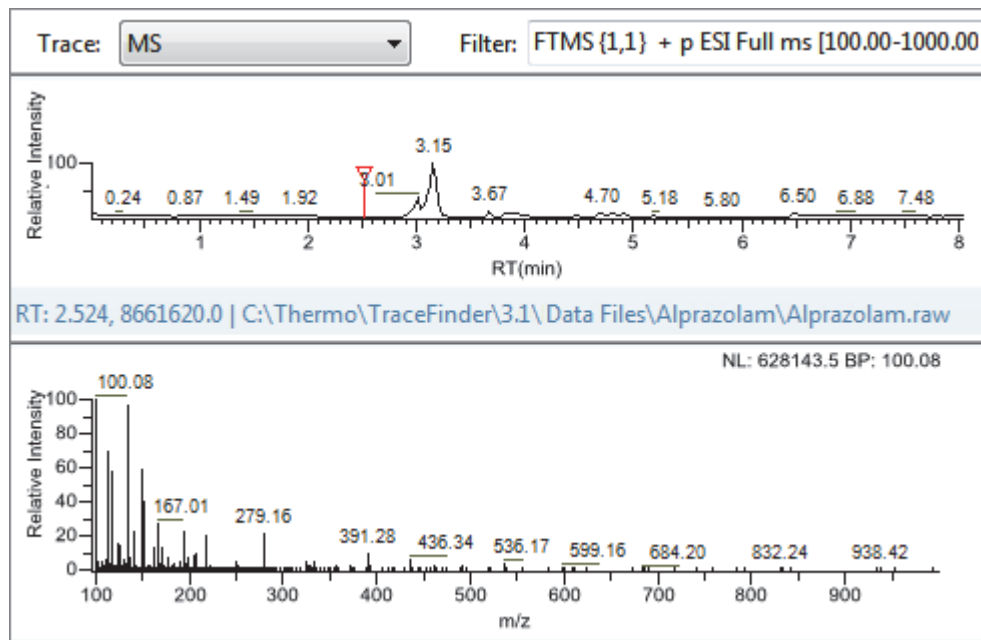
> **IMPORTANT** While the spectra pane displays the associated raw data file, you cannot
> display peak information for an original compound in the Compound list. You can
> display peak information only for compounds in the associated raw data file. To
> return the display functionality for all compounds in the method, save the method.

7. Select a filter from the Filter list.

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

9. Right-click and choose **Add This Peak as New Compound** from the shortcut menu.
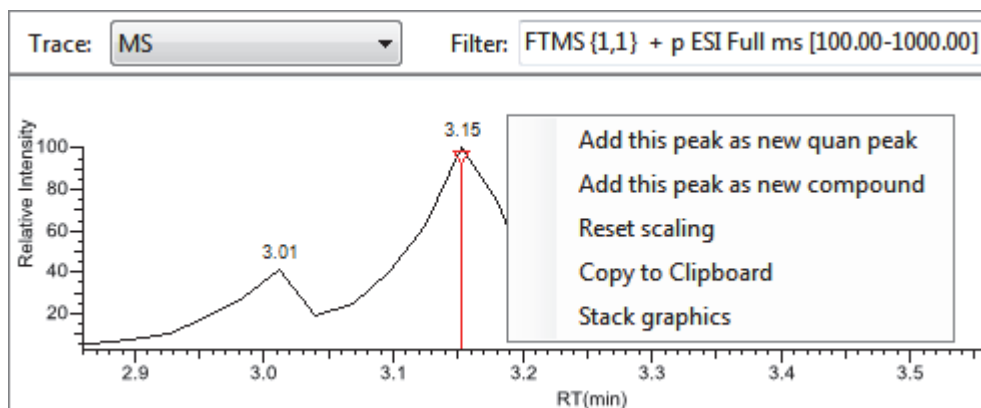
The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quantitative peak, and the second and third largest ions as the confirming ion peaks.

- When the name of the first match does not exist in the method, the application adds this compound to the method and displays the name in the Compound list. You can now view and edit the parameters for this compound.

- When the name of the first match is already in the method, the Add New Compound dialog box opens. You cannot overwrite a compound name in the method. If the selected peak already exists in the method, you must give it a new name to add it to the method. Or, you can select a different compound to add to the method, following step 10 through step 12.

Figure 30. Add New Compound dialog box
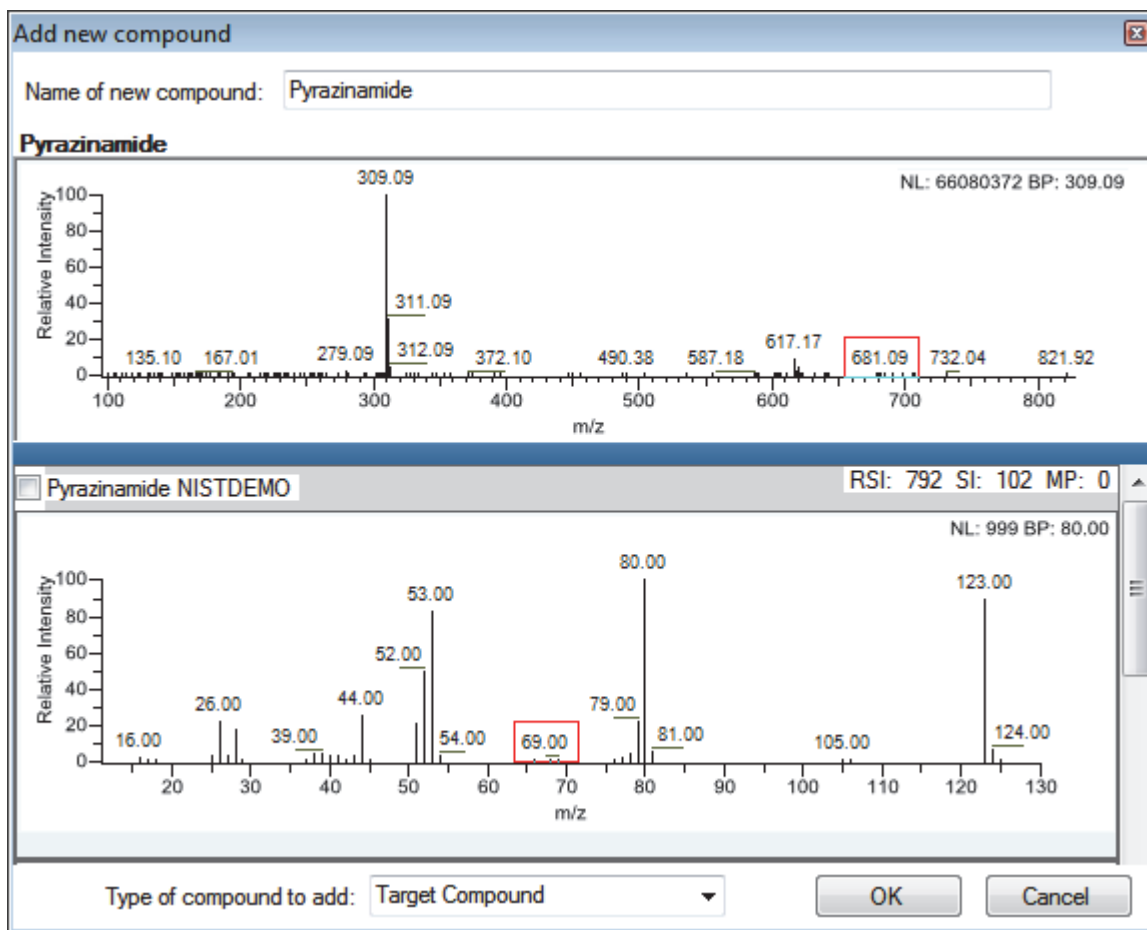
10. Do one of the following:

    • Type a new name for the first matched compound.

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

      Name of new compound: Pyrazinamide ⚠

    –or–

    • To use a compound other than the first matched compound, scroll to the spectrum for that compound and select its corresponding check box in the title bar of the spectrum pane.
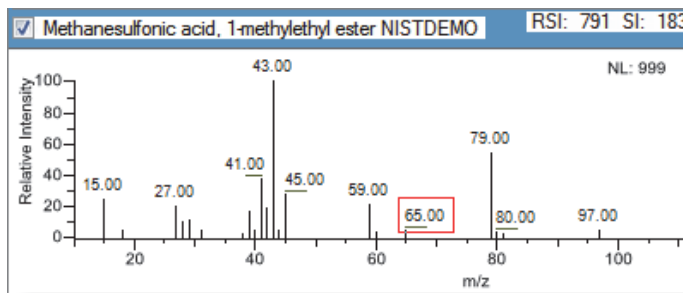
      Selected compound

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

12. Click **OK**.

❖ **To change the compound reference spectrum**

1. In the chromatogram pane, click a peak.

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

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

❖ **To replace a quantitation mass**

1. Click the data pane for the quantitation mass that you want to replace.

2. In the spectrum pane, hold the cursor over a peak.

   The red box indicates the selected peak.
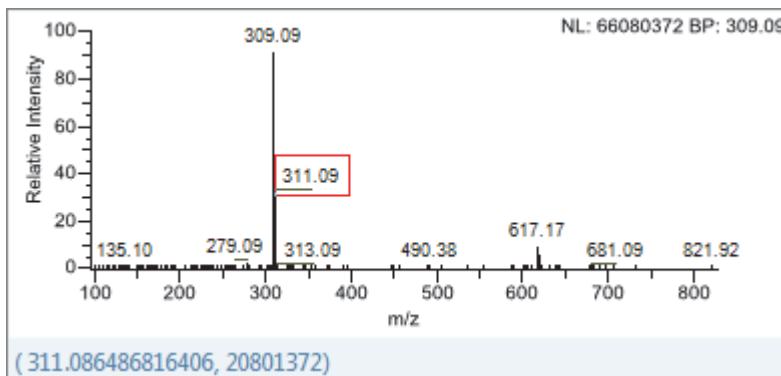
3. Right-click and choose **Set This Spectral Peak as Quan Value** from the shortcut menu.

4. Choose either **Don't Update Ion Ratios** or **Update Ion Ratios Using This Spectrum**.

   You can see the updated ion ratios on the Ratios page for the confirming ion peaks. See "Ratios" on page 173.

❖ **To add a mass to the existing quantitation mass ranges**

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

   The red box indicates the selected peak.

2. Right-click and choose **Add This Spectral Peak to Existing Quan Ranges** from the shortcut menu.

3. Choose either **Don't Update Ion Ratios** or **Update Ion Ratios Using This Spectrum**.

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

   If you chose to update the ion ratios, you can see the updated ion ratios on the Ratios page for the confirming ion peaks. See "Ratios" on page 173.

❖ **To add a quantitative peak**

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

   The red box indicates the selected peak.

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

   The application adds a new quantitative peak to the compound.
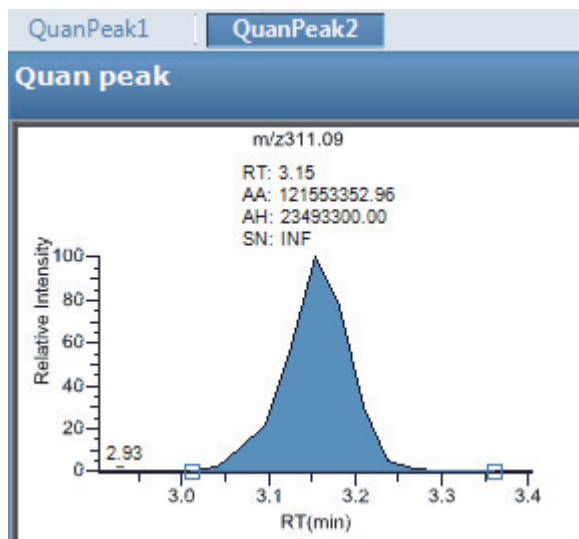
You can use the shortcut menu in the spectrum pane for this new quantitative peak to perform any of the tasks that you would perform on the original quantitative peak.

❖ **To add a spectral peak as a new compound**

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

   The red box indicates the selected peak.

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

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

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

Figure 31. Add New Compound dialog box
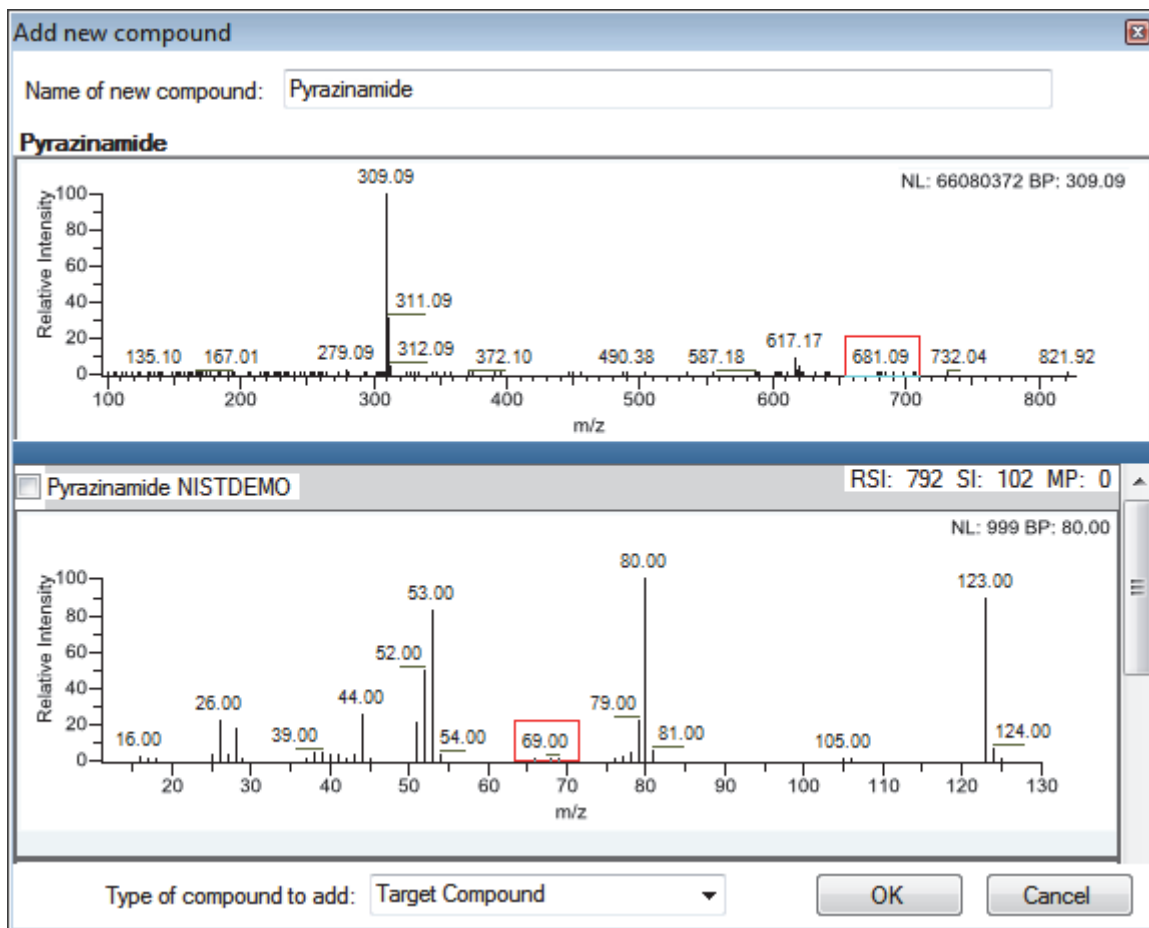
3. (Optional) Make any of the following changes:

- Change the name for the compound in the Name of New Compound box.

- Use a compound other than the compound chosen by the TraceFinder application by scrolling to the spectrum for that compound and selecting the compound name in the title bar of the spectrum pane.
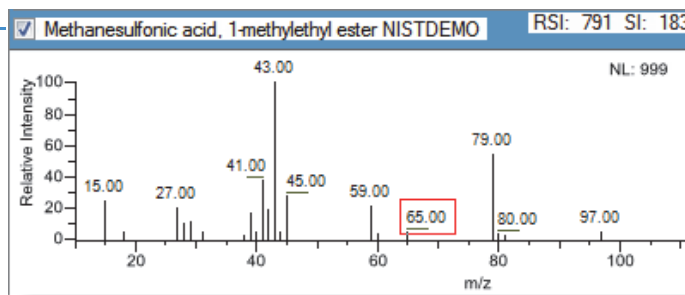
Selected compound

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

4. Click **OK**.

❖ **To replace a quantitative peak with a confirming ion peak**

1. When you have multiple quantitative peaks, select the quantitative peak that you want to replace.

2. Right-click the header bar for the confirming ion peak that you want to use as the quantitative peak, and choose **Swap with Quan Peak** from the shortcut menu.

The application swaps the quantitative peak and the confirming ion peak. The application replaces all information for the quantitative peak with information for the confirming ion. This includes the expected retention time that the confirming ion inherited from the original quantitative peak. The original quantitative peak replaces the confirming ion peak. The application recalculates the ratios for all confirming ion peaks.

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

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

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

❖ **To add a trace to the Real Time Status pane**

Right-click the header bar for the quantitative peak or confirming ion peak that you want to add to the Real Time Status pane and choose **Display in Real Time Viewer** from the shortcut menu.
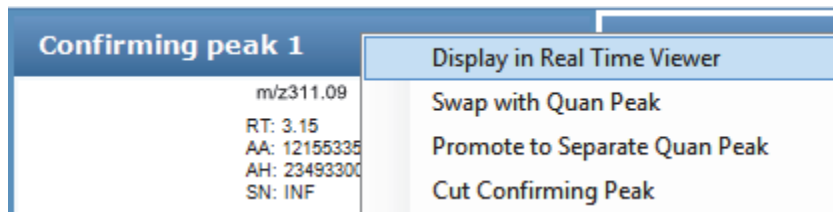
The application moves the peak to the Traces To Display in Real Time Viewer pane on the Real Time Viewer page. See "Real Time Viewer" on page 186.

Trace *m/z* 311.09 added to Real Time Viewer
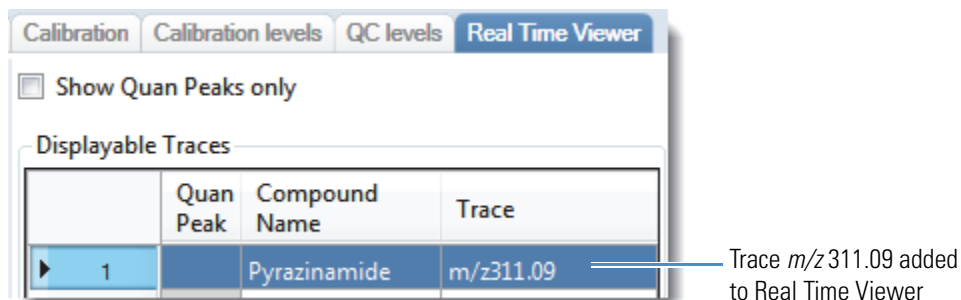
When you acquire samples with this method, the application displays the *m/z* 311.09 trace in addition to the TIC in the Real Time Status pane.
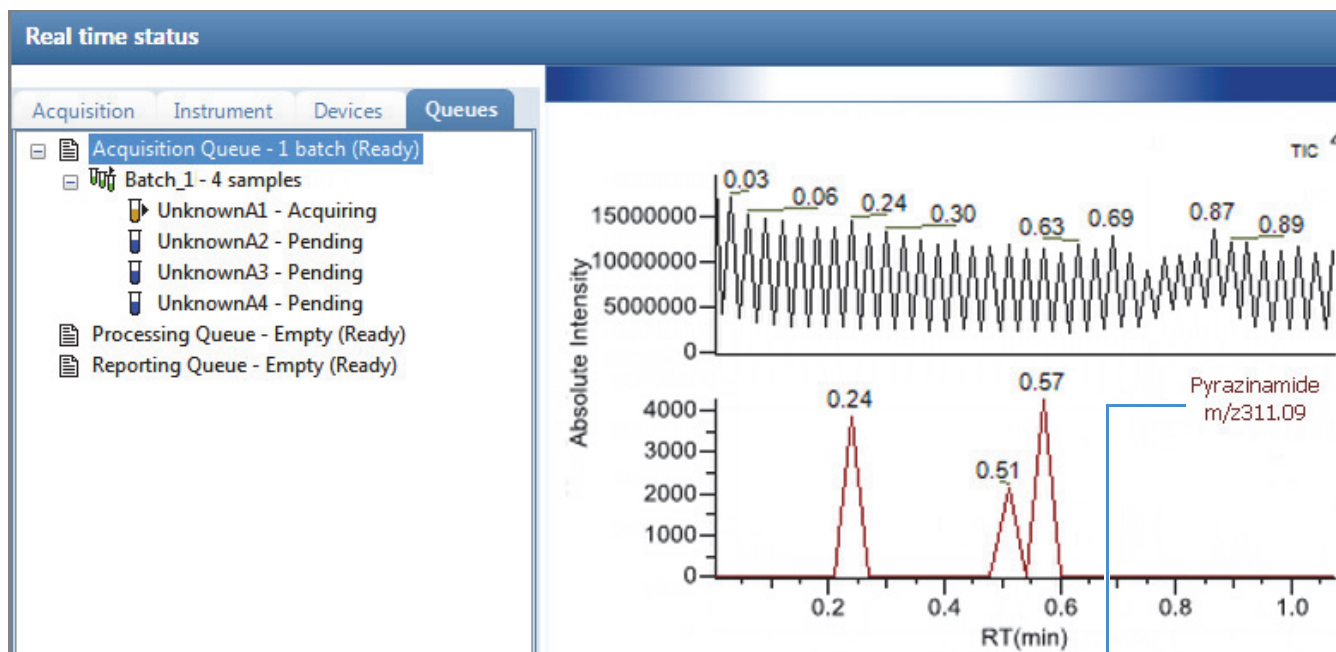
Trace *m/z* 311.09 added to Real Time Status display

❖ **To replace a confirming ion peak**

1. Click the pane for the confirming ion peak that you want to replace.

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

   The red box indicates the selected peak.

3. Right-click and choose **Set This Spectral Peak as Confirming** from the shortcut menu.

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

❖ **To add a mass as a new confirming ion peak**

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

   The red box indicates the selected peak.

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

   The TraceFinder application adds the confirming ion peak to the quantitative peak.
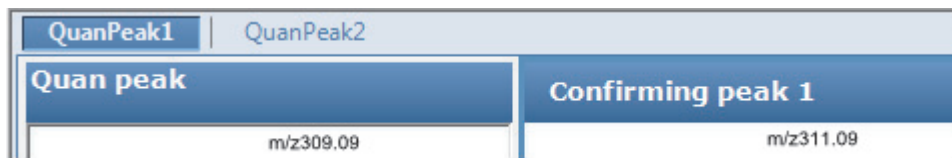
   You can use the shortcut menu in the spectrum pane for this new confirming ion peak to perform any of the tasks that you would perform on the original confirming ion peaks.

❖ **To use the cut-and-paste feature on confirming ion peaks**

1. Right-click the header bar for the confirming ion peak that you want to remove and choose **Cut Confirming Peak** from the shortcut menu.

2. Right-click the header bar for the confirming ion peak that you want to replace and choose **Paste Confirming Peak** from the shortcut menu.

   The application pastes the confirming ion peak that you removed. You can paste a deleted peak back to the quantitative peak from which it was removed, or you can paste the confirming ion peak that was deleted to another quantitative peak for this compound.

❖ **To save the new method**

1. Choose **File > Save**.

   The Save Master Method dialog box opens.

2. Type a new name for the master method and click **OK**, or select a method name to overwrite and click **Overwrite**.

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

   …\TraceFinderData\Methods

Detection Page

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

Figure 32. Detection page

Selected compound data

Chromatogram pane

Spectrum pane

Selected compound

Table 19. Detection page panes

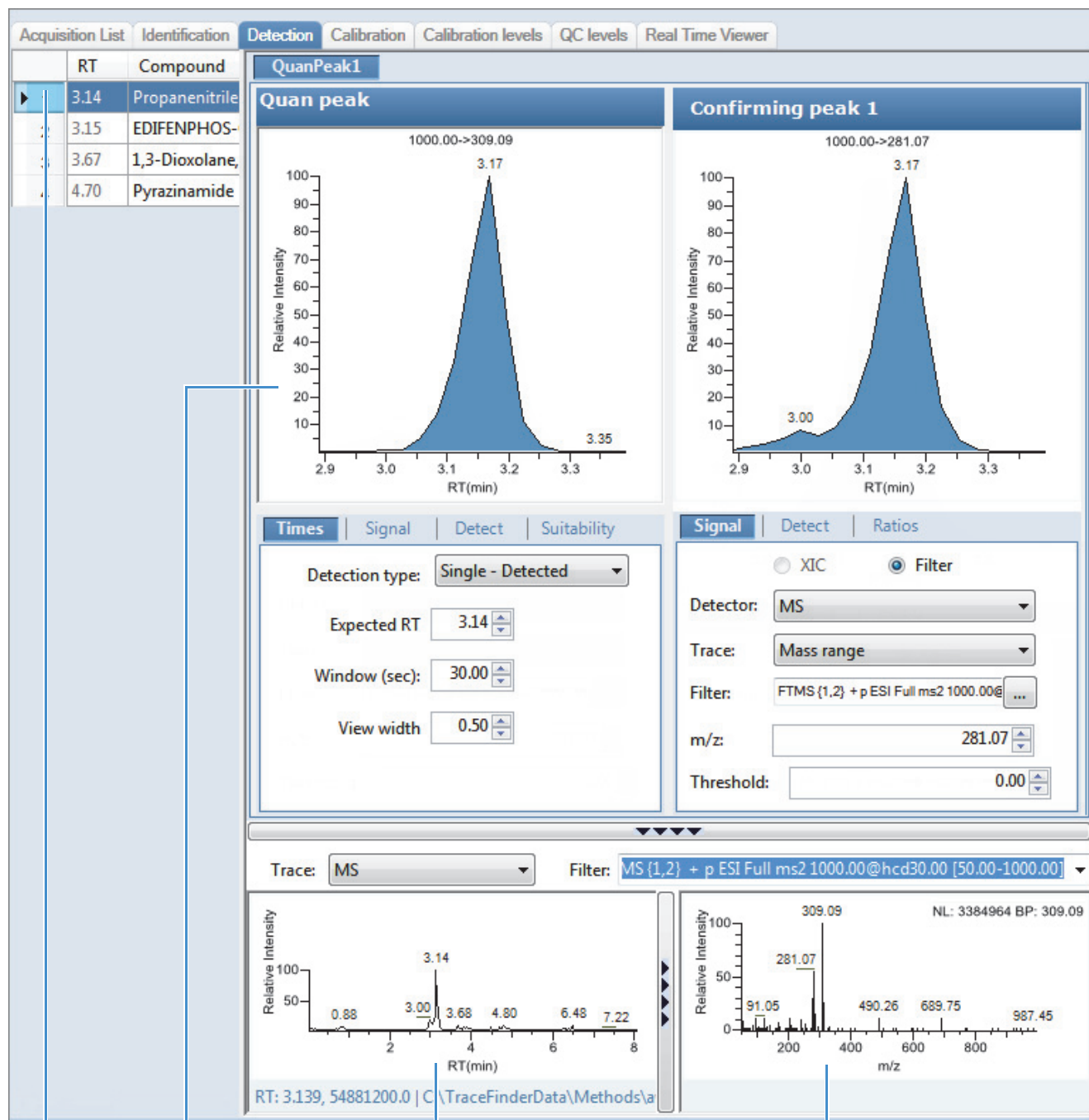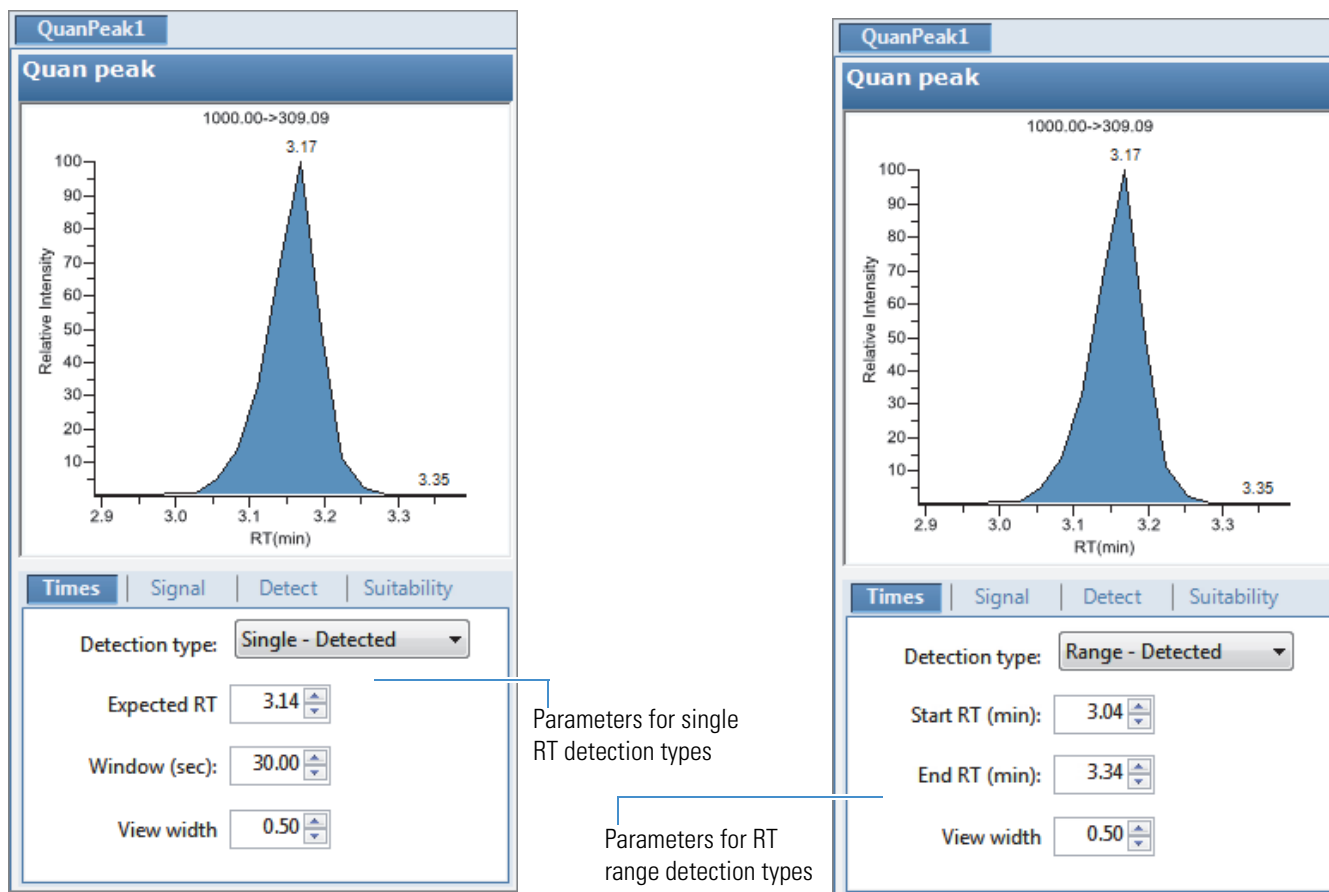| Pane	Description
Compound	Lists all compounds in the master method. The Compound list uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 188.
QuanPeak*n*	Displays a chromatogram for the quantitative peak and its confirming ion peaks. The quantitative peak and confirming peak panes include additional pages for retention time, signal, detection, spectrum, and ratio parameters for the selected compound.
Trace	Displays a combination of the Detector and Trace values used for the raw data file.
	Do not confuse this Trace parameter with the Trace parameter on the Signal page. This Trace parameter combines both the Detector and Trace values specified on the Signal page. See "Signal page for a mass spectrometer detector" on page 147.
	Note When you select a detector option other than MS or PDA, the spectrum pane reports "Not Available."
Filter	Displays the filter used for the raw data file. Available only when you set the Trace parameter to MS.
Reference Chromatogram and Spectra	Displays a reference chromatogram and spectra for the raw data file.
	When you view an analog trace, there is no spectra display. To close the spectra pane and use the full width to display the chromatogram, click ▸ .
Additional pages	
Times	Defines the retention time and window for a quantitative peak. See "Times" on page 139.
Signal	Defines the detector and detection parameters used to display each chromatogram trace. See "Signal" on page 141.
Detect	Defines the peak detection algorithm and its options. See "Detect" on page 151.
Spectrum	Defines a reference mass spectrum for a quantitative peak or compound. See "Spectrum" on page 165.
Ratios	Defines the criteria for evaluating, confirming, or qualifying ions. See "Ratios" on page 173.

Times

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

Figure 33. Times page

Parameters for single RT detection types

Parameters for RT range detection types

Table 20. Times page parameters (Sheet 1 of 2)

Parameter	Description
Detection Type	**Single - Detected**: (Default) Specified as a centered retention time window. The application integrates a distinct peak. In reports, the application displays the expected retention time and actual retention time values as Method RT and Detected RT, respectively. **Range - Detected**: Specified as a retention time start/end range. **Range - Integrated**: Specified as a retention time start/end range. The application integrates all peaks within the specified time range.
Expected RT (min)	Expected retention time for a single peak. Available only for the Single - Detected detection type.
Window (sec)	Width of the window (in seconds) to indicate how far around the expected retention time the system looks for a peak apex. Available only for the Single - Detected detection type.

Table 20. Times page parameters (Sheet 2 of 2)

Parameter	Description
Start/End RT (min)	Beginning and ending retention time window that can encompass multiple peaks. Available only for the Range - Detected and the Range - Integrated detection types. When you change from a Single - Detected detection type, these values default to the previous beginning and ending time calculated from the Expected RT and Window values.
View Width (min)	Viewable size of the ion chromatogram display. Changing the view width does not affect the peak detection process; the TraceFinder application uses it only for graphical display. When you select either Range - Detected or Range - Integrated as the detection type, you cannot select a View Width value less than the retention time range (*end time* minus *start time*).
Shortcut menu	
Set Peak Windows Settings to All Peaks in Compound	Copies the View Width and Window values to all quantitative peaks for the compound and updates the compound. Available only when a compound has multiple quantitative peaks.
Set Peak Windows Settings to All Peaks in Method	Copies the View Width and Window values to all quantitative peaks for the method and updates the method.

Signal

Use the Signal page to define the detector and filters as you display each chromatogram trace. For detailed descriptions of all the features on the Signal page, see "Signal Page" on page 147. The TraceFinder application can use both analog detectors and mass spectrometer detectors. See "Signal page for a mass spectrometer detector" on page 147 or "Signal page for an analog detector" on page 148.

Follow these procedures:

- To specify ranges of ions for detection and integration

- To specify an XIC filter

- To specify an MS filter

❖ **To specify ranges of ions for detection and integration**

1. Select **MS** from the Detector list.

2. Select **Mass Range** from the Trace list.

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

> **Note** The parameters in the Ranges area are available only when you set the Detector parameter to MS and the Trace parameter to Mass Range.

The Edit Mass Ranges dialog box opens where you can define mass ranges using a center of mass or start and end values.

Figure 34. Edit Mass Ranges dialog box
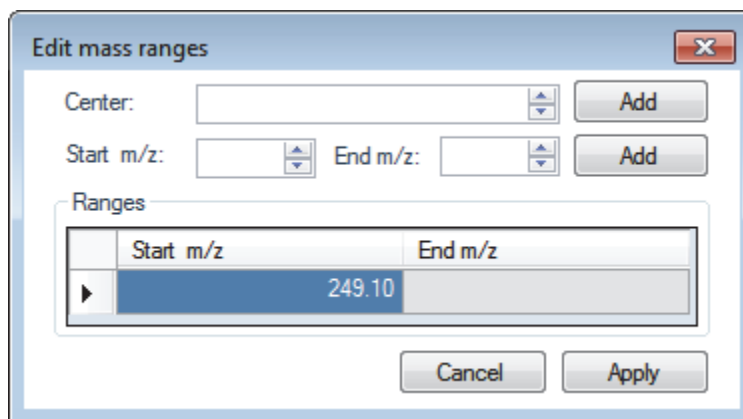
4. Enter a value in the Center Mass box and click **Add**.

A new row with this value opens under Ranges. Center mass values are listed in the Start *m/z* column. The application uses a range of one amu centered on this value.

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

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

6. Add as many ranges as you want.

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

7. Click **Apply**.

   The application applies the parameters to the list of ranges.

❖ **To specify an XIC filter**

1. Select **MS** from the Detector list.

2. Select **Mass Range** from the Trace list.

3. Select the **XIC** option.

   > **Note** The XIC option is available only when you set the Detector parameter to MS and the Trace parameter to Mass Range.
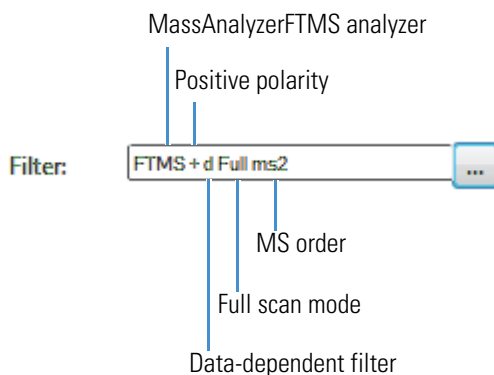
4. Click the Filter browse button.

   The XIC Filter dialog box opens. See XIC Filter dialog box.

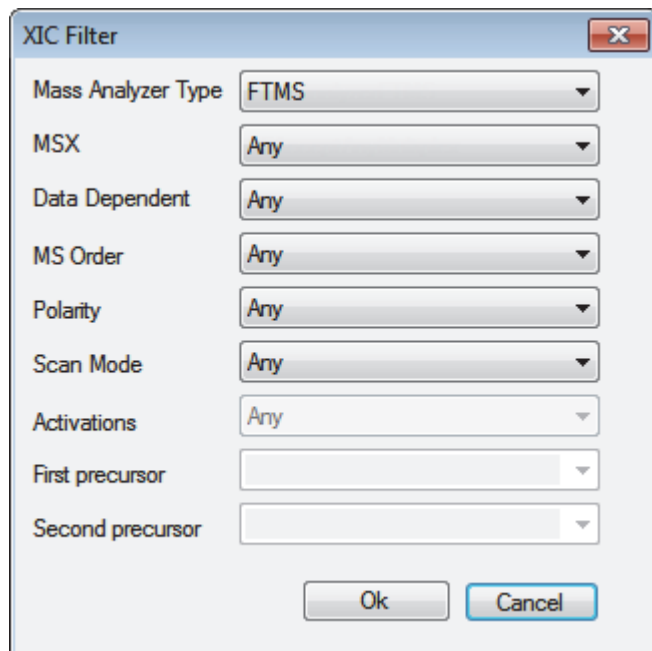5. Specify your filter options.

6. Click **OK**.

   The application updates the chromatogram data using the specified XIC filter options.

   The Filter box indicates the parameters of the specified XIC filter. For example:

Figure 35. XIC Filter dialog box

Table 21. XIC Filter dialog box parameters (Sheet 1 of 2)

Parameter	Description
Mass Analyzer Type	Any: Allows any mass analyzer. FTMS: Fourier Transform Mass Spectrometer ITMS: Ion Trap Mass Spectrometer Sector: Static electric or magnetic sectors, or a combination of the two SQMS: Single Quad Mass Spectrometer TOFMS: Time-of-Flight Mass Spectrometer TQMS: Triple Quad Mass Spectrometer
MSX	Any: Allows both MSX and non-MSX scans. On: Allows only MSX scans. Off: Allows only non-MSX scans.
Data Dependent	Any: Allows both data-dependent and non-data-dependent filters. On: Allows only data-dependent filters. Off: Allows only non-data-dependent filters.
MS Order	Any: Allows any MS order. MS: Single mass spec stage MS2-MS3: Multiple mass spec stages
Polarity	Any: Allows both positive and negative. Positive Negative

Table 21. XIC Filter dialog box parameters (Sheet 2 of 2)

Parameter	Description
Scan Mode	Any: Allows any scan mode. Full: Full-scan mode SIM: Selective ion monitoring SRM: Selective reaction monitoring CRM: Consecutive reaction monitoring Q1MS: MS using quadrupole 1 Q3MS: MS using quadrupole 3
Activations	Any: Allows any activation method. CID: Collision-induced dissociation MPD: Multiple photodissociation ECD: Electron capture dissociation PQD: Pulsed dissociation ETD: Electron transfer dissociation HCD: Higher energy collision-induced dissociation This parameter is available only when the MS Order is set to MS2 or MS3.
First Precursor	This parameter is available only when the MS Order is set to MS2 or MS3.
Second Precursor	This parameter is available only when the MS Order is set to MS3.

❖ **To specify an MS filter**

1. Select the **Filter** option.

2. Select **MS** from the Detector list.

3. Select a trace type from the Trace list.

4. Select a filter from the Filter list.
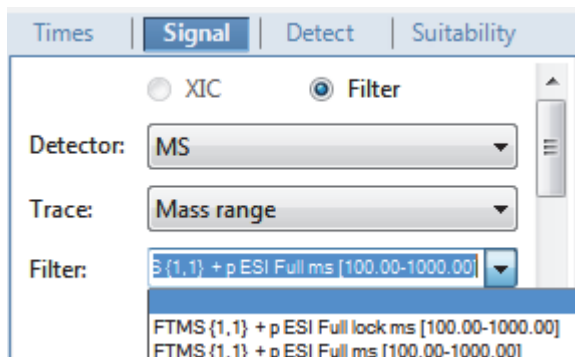
Filter types can be any of the following:

- MS

- MS2

- MS2 CID

- MS2 HCD

5. To update the new filter selection, click outside the Signal pane.

As long as the filter is highlighted blue, the new selection is not yet applied.

6. (Optional for quantitative peaks) To apply this same quantitative peak filter to other peaks, right-click and choose one of the following from the shortcut menu:

- **Set Filter Options on All Peaks in This Compound**: Applies this filter to all other peaks in the compound.

- **Set Filter Options on All Compounds**: Applies this filter to all peaks for all compounds in the method.

- **Set Quan Peak Filter Options on All Compounds**: Applies the filter specified for the quantitative peak to all quantitative peaks for all compounds in the method.

7. (Optional for confirming peaks) To apply this same confirming peak filter to other peaks, right-click and choose one of the following from the shortcut menu:

- **Set Filter Options on All Peaks in This Compound**: Applies this filter to all other peaks in the compound.

- **Set Filter Options on All Compounds**: Applies this filter to all peaks for all compounds in the method.

- **Set Confirm Peak Filter Options on All Compounds**: Applies the filter specified for the confirming peak to all confirming peaks for all compounds in the method.

- **Set Confirm Peak 1 Filter Options on All Compounds**: Applies the filter specified for confirming peak 1 to the first confirming peak for all compounds in the method.

Signal Page

Use the features on the Signal page to define the detector and filters as you display each chromatogram trace for either analog detectors or mass spectrometer detectors. For detailed descriptions of all the parameters on the Signal page, see "Signal page parameters" on page 148.

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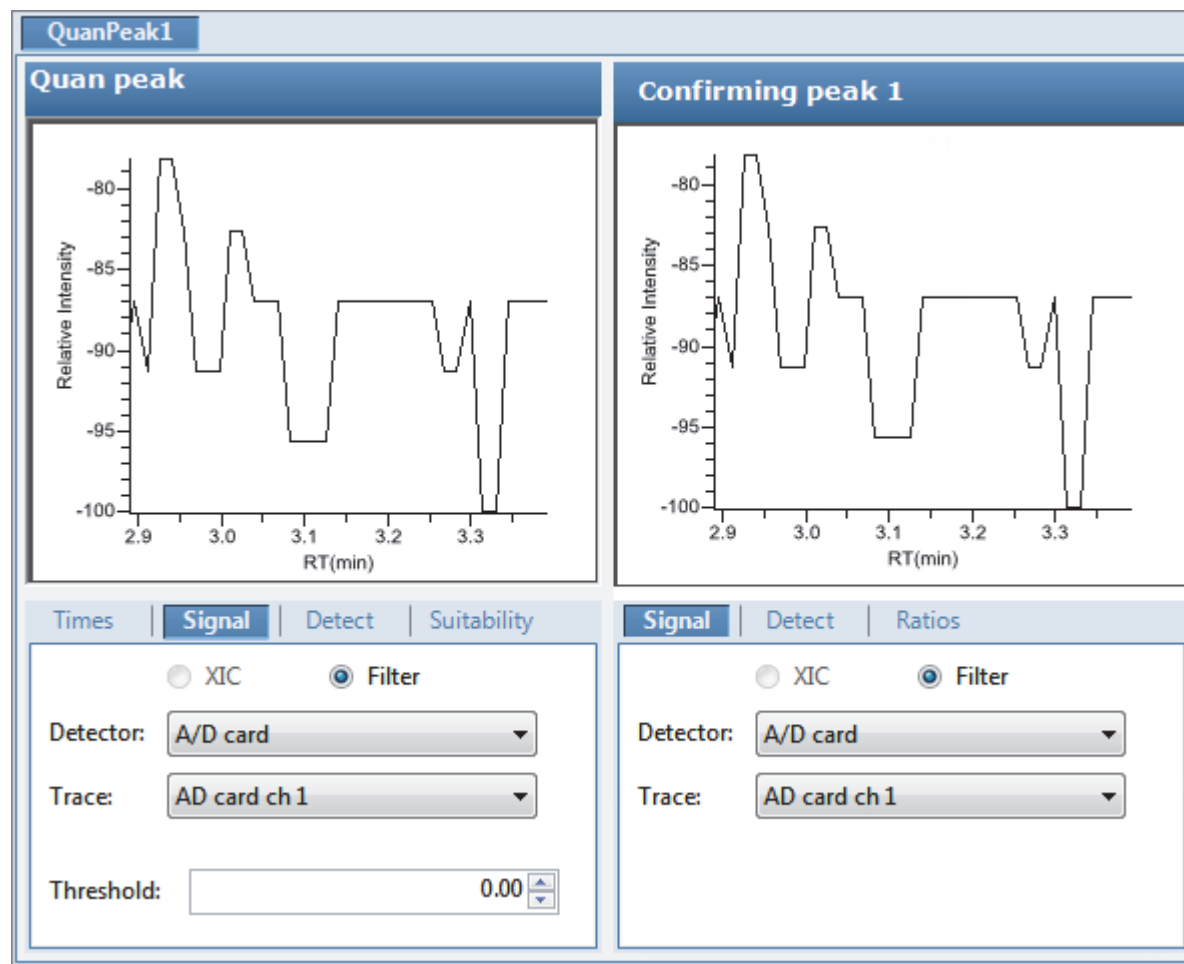- Signal page for an analog detector

Figure 36. Signal page for a mass spectrometer detector
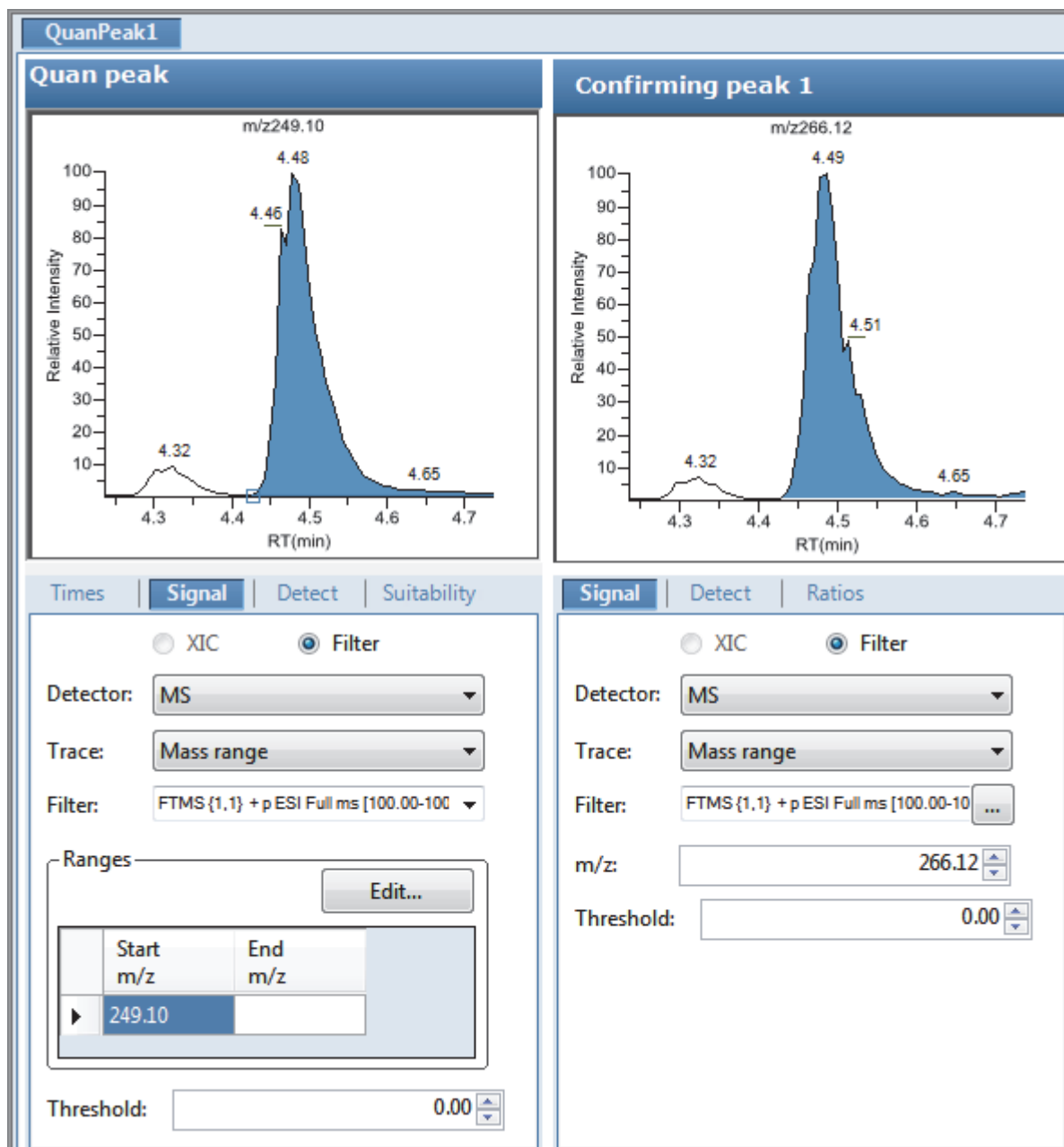
Figure 37. Signal page for an analog detector

Table 22. Signal page parameters (Sheet 1 of 3)

Parameter	Description
XIC	Available only when you select the MS detector. Specifies an Extracted Ion Chromatogram experiment type that uses a single, full-scan mass filter that is post-processed to extract a peak for the ions of interest.
Filter	Available only when you select the MS detector. Select from the list of mass filters to use for processing the compound.

Table 22. Signal page parameters (Sheet 2 of 3)

Parameter	Description
Detector	Options are determined by the detection options used to create the method. The method can use the standard options (all the listed options) or only the detection options used to acquire an associated raw data file.
	MS: Mass spectrometer that ionizes sample molecules and then separates the ions according to their mass-to-charge ratio (m/z).
	PDA: Photodiode array detector providing a linear array of discrete photodiodes on an integrated circuit chip. It is placed at the image plane of a spectrometer to allow a range of wavelengths to be simultaneously detected.
	Analog: Supplemental detectors (for example, FID, ECD). When you select this detector, any reports that display a QIon value show the value as **Analog** and any reports that display spectra show the spectra as **Not Available**.
	A/D card: If you have a detector not under data system control, you can capture the analog signal and convert it to digital using an interface box (for example, SS420X) for storage in the raw data file.
	UV: A UV spectrophotometer (for variable-wavelength detection) or photometer (for single-wavelength detection) equipped with a low-volume flow cell. This detector detects analytes that readily absorb light at a selected wavelength.
Trace	Represents a specific range of the data. The TraceFinder application uses the trace to identify the characteristic ions for a compound.
	MS detector options: Mass Range, TIC, or Base Peak. When you select Mass Range, you are prompted to enter the start and end *m/z* values for the ranges.
	PDA detector options: Spectrum Maximum, Wavelength Range, or Total Scan.
	Analog detector options: Analog 1, Analog 2, Analog 3, or Analog 4. You can configure these channel names in your instrument configuration.
	A/D Card detector options: AD Card ch1, AD Card ch2, AD Card ch3, or AD Card ch4. You can configure these channel names in your instrument configuration.
	UV detector options: Channel A, Channel B, Channel C, or Channel D. You can configure these channel names in your instrument configuration.
Filter	Available only when you select the MS detector. Represents a particular data acquisition channel. For example, the filter option + *c Full ms [35.00-500.00]* represents a positive ion centroid signal acquired in single-stage, full-scan mode from *m/z* 35 to 500.

Table 22. Signal page parameters (Sheet 3 of 3)

Parameter	Description
Ranges	Available only when you select the Mass Range trace for an MS detector.
Edit	Opens the Edit Mass Ranges dialog box where you can specify a range of ions for detection and integration. See "To specify ranges of ions for detection and integration" on page 141.
Start *m/z* End *m/z*	Specifies ranges of ions for detection and integration. The application sums the multiple ions specified by these ranges. Ranges specified by a center mass value are listed as a single value in the Start *m/z* column. The application uses a range of one amu centered on this value.

Detect

Use the Detect page to define the peak detection algorithm (sensitivity) and its options and to determine the area under a curve. There are three sensitivity modes: Genesis, ICIS, and Avalon. The Genesis and Avalon sensitivity modes are used for mass spectrometry detection. The ICIS sensitivity mode is used primarily for analog detection.

On this page, you can specify how you want each mode to run. See the following for detailed descriptions of all the features on the Detect page:

- For Genesis sensitivity, see "Detect page parameters for Genesis" on page 153.

- For ICIS sensitivity, see "Detect page parameters for ICIS" on page 157.

- For Avalon sensitivity, see "Detect page parameters for Avalon" on page 159.

Figure 38. Detect page for Genesis

Table 23. Detect page parameters for Genesis (Sheet 1 of 3)

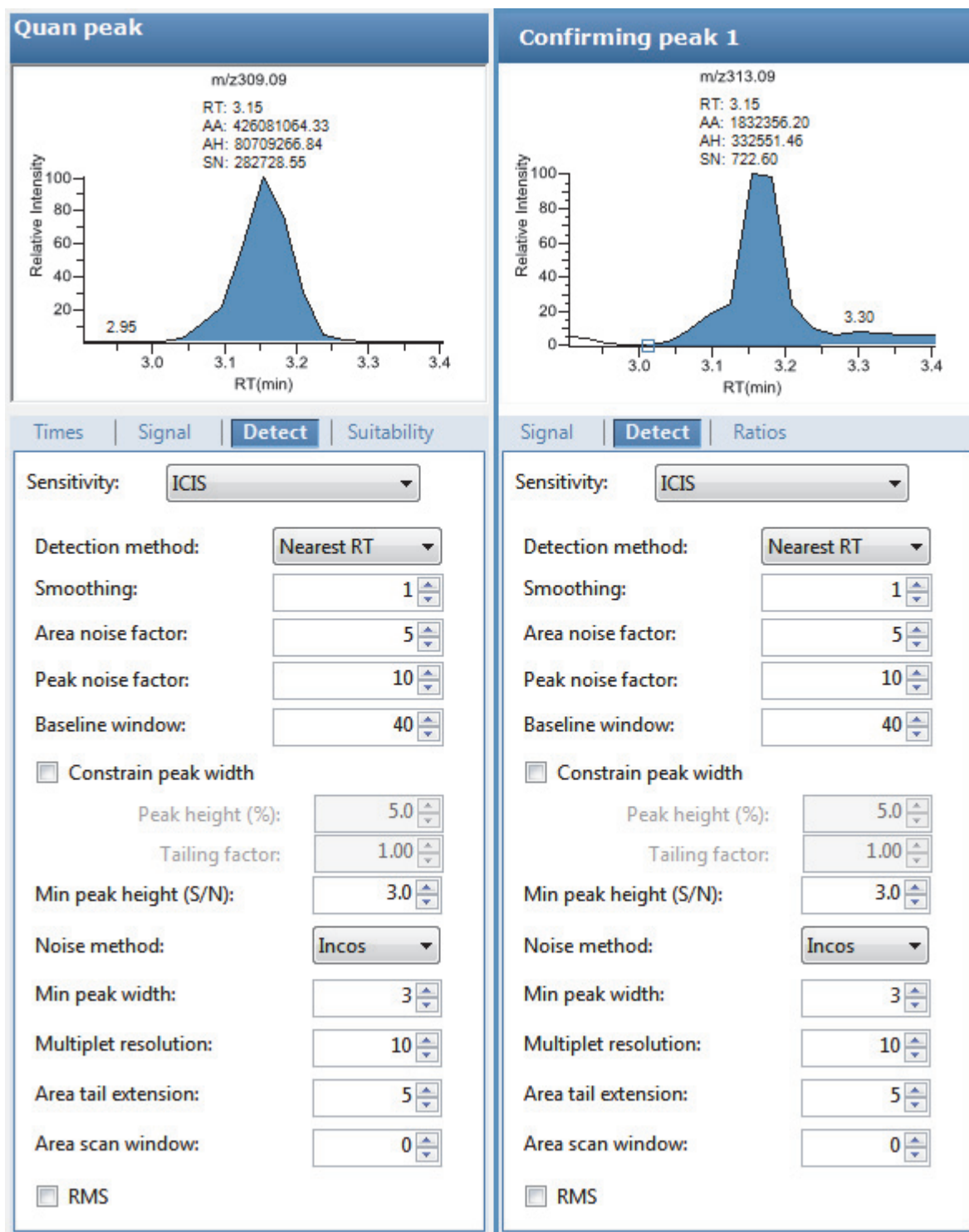| Parameter	Description
Sensitivity	Specifies the Genesis peak detection algorithm.
Detection Method	Highest peak: Uses the highest peak in the chromatogram for component identification. Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Default: 1 Range: Any odd integer from 1 through 15 points
S/N Threshold	Current signal-to-noise threshold for peak integration. Peaks with signal-to-noise values less than this value are not integrated. Peaks with signal-to-noise values greater than this value are integrated. Range: 0.0 to 999.0
Enable Valley Detection	Uses the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Expected Width (sec)	The expected peak width parameter (in seconds). This parameter controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the *expected width*/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the TraceFinder application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. Range: 0.0 to 999.0
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box activates the Peak Height (%) and Tailing Factor options.
Peak Height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when you select the Constrain Peak Width check box. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

Table 23. Detect page parameters for Genesis (Sheet 2 of 3)

Parameter	Description
Min Peak Height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0 Available only for quantitation methods.
Peak S/N Cutoff	The peak edge is set to values below this signal-to-noise ratio. This test identifies an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio. When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the TraceFinder application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 10 000.0
Valley Rise (%)	The peak trace can rise above the baseline by this percentage after passing through a minimum (before or after the peak). This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. When the trace exceeds rise percentage, the TraceFinder application applies valley detection peak integration criteria. The TraceFinder application applies this test to both the left and right edges of the peak. The rise percentage criteria is useful for integrating peaks with long tails. Range: 0.1 to 500.0
Valley S/N	Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher. Default: 2.0 Range: 1.0 to 100.0
# Background Scans	Number of background scans performed by the TraceFinder application.
Report Noise As	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or a peak-to-peak resolution threshold. Options are RMS or Peak to Peak.
Shortcut menu	
Apply to All Peaks in Method	Updates all compounds in the method with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.

Table 23. Detect page parameters for Genesis (Sheet 3 of 3)

Parameter	Description
Apply to All Peaks with Like Sensitivity Setting	Uses the current settings on the Detect page to update all compounds in the method that use the Genesis sensitivity mode. These updates apply to both quantitative and confirming ion peaks that use the Genesis sensitivity mode.
Apply to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.

Figure 39. Detect page for ICIS

Table 24. Detect page parameters for ICIS (Sheet 1 of 2)

Parameter	Description
Sensitivity	Specifies the ICIS peak detection algorithm, used primarily with analog detectors.
Detection Method	Highest peak: Uses the highest peak in the chromatogram for component identification. Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Default: 1 Range: Any odd integer from 1 through 15 points
Area Noise Factor	The noise level multiplier used to determine the peak edge after the location of the possible peak. Default: 5 Range: 1 through 500
Peak Noise Factor	The noise level multiplier used to determine the potential peak signal threshold. Default: 10 Range: 1 through 1000
Baseline Window	The TraceFinder application looks for a local minima over this number of scans. Default: 40 Range: 1 through 500
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box activates the Peak Height (%) and Tailing Factor options.
Peak Height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when you select the Constrain Peak Width check box. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0
Min Peak Height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0 Available only for quantitation methods.

Table 24. Detect page parameters for ICIS (Sheet 2 of 2)

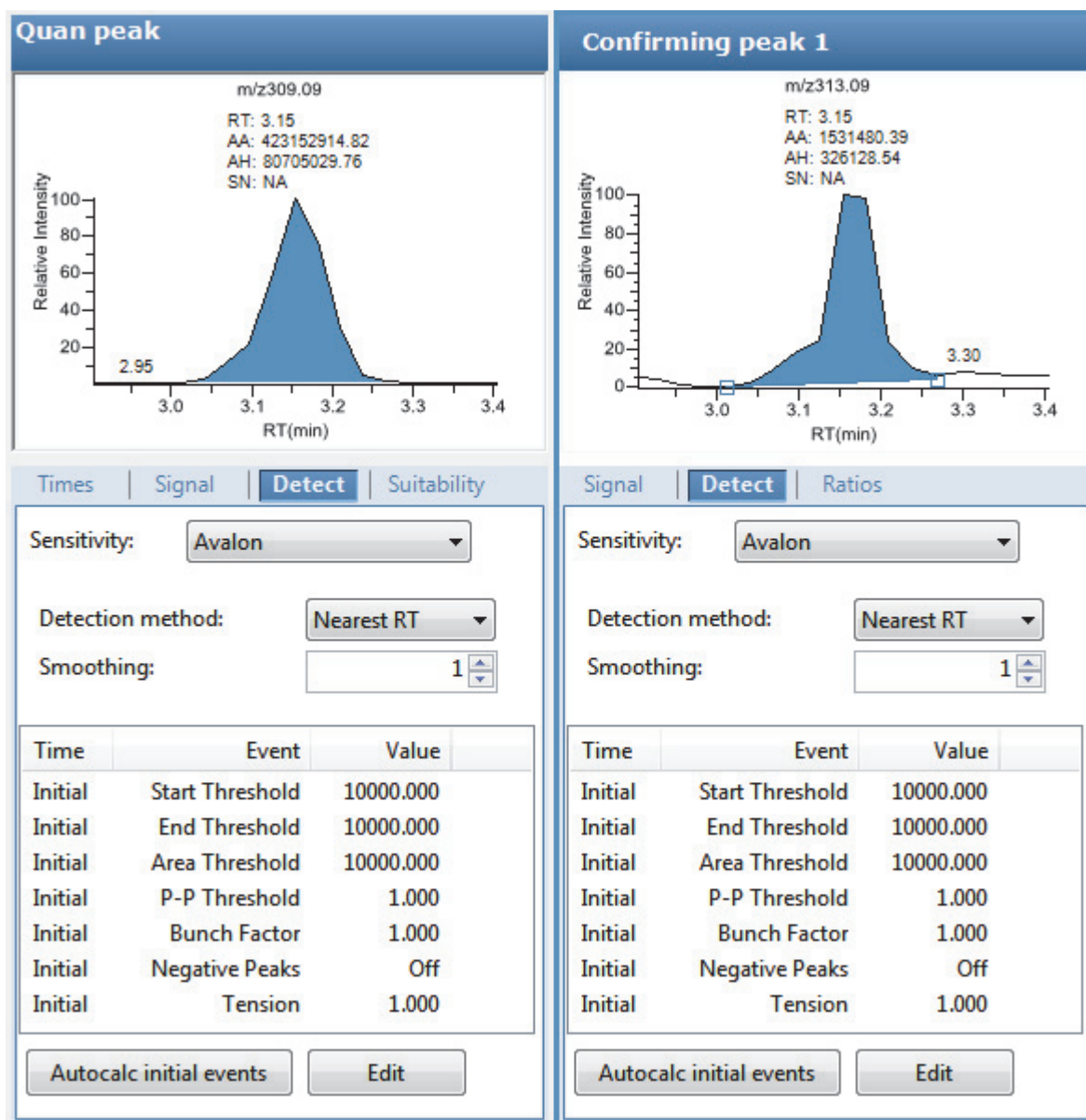| Parameter	Description
Noise Method	The options are INCOS or Repetitive. INCOS: Uses a single pass algorithm to determine the noise level. Repetitive: Uses a multiple pass algorithm to determine the noise level. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but the analysis takes longer.
Min Peak Width	The minimum number of scans required in a peak. Default: 3 Range: 0 to 100 scans
Multiplet Resolution	The minimum separation in scans between the apexes of two potential peaks. This is a filter to determine if two peaks are resolved. Default: 10 Range: 1 to 500 scans
Area Tail Extension	The number of scans past the peak endpoint to use in averaging the intensity. Default: 5 Range: 0 to 100 scans
Area Scan Window	The number of allowable scans on each side of the peak apex. A zero value defines all scans (peak-start to peak-end) to be included in the area integration. Default: 0 Range: 0 to 100 scans
RMS	Specifies that the TraceFinder application calculate noise as RMS. By default, the application uses Peak To Peak for the noise calculation. RMS is automatically selected if you manually determine the noise region.
Shortcut menu	
Apply to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks in Method	Updates all compounds in the method with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks with Like Sensitivity Setting	Uses the current settings on the Detect page to update all compounds in the method that use the ICIS sensitivity mode. These updates apply to both quantitative and confirming ion peaks that use the ICIS sensitivity mode.

Figure 40. Detect page for Avalon

Table 25. Detect page parameters for Avalon (Sheet 1 of 2)

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

Table 25. Detect page parameters for Avalon (Sheet 2 of 2)

Parameter	Description
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Default: 1 Range: Any odd integer from 1 through 15 points
Autocalc Initial Events	Automatically calculates the events in the Event list.
Edit	Opens the Avalon Event List dialog box. See "Avalon Event List" on page 58.
Shortcut menu	
Apply to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks in Method	Updates all compounds in the method with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.
Apply to All Peaks with Like Sensitivity Setting	Uses the current settings on the Detect page to update all compounds in the method that use the Avalon sensitivity mode. These updates apply to both quantitative and confirming ion peaks that use the Avalon sensitivity mode.

Suitability

Use the Suitability page to determine if the column is degrading and to identify suspicious peaks eluting at the same time as the target compound. Suspicious peaks caused by highly retained compounds from a previous injection tend to have a broader than expected peak profile. Tailing peaks frequently indicate a degrading column.

The Suitability page displays the parameter values to check the suitability of chromatographic peaks during processing. You can edit these parameters in the System Suitability dialog box.

Detect	**Suitability**	Spectrum	◄ ►

Edit...

Symmetry parameters

Peak height (%):	**50**
Symmetry threshold (%):	**90**

Peak classification parameters

Detect peak width

Peak height (%):	**50**
Min peak width (sec):	**1.80**
Max peak width (sec):	**3.60**

Detect tailing

Peak height (%):	**10**
Failure threshold:	**2.0**

Detect column overload

Peak height (%):	**50**
Failure threshold:	**1.5**

Detect baseline clipping

Number of peak widths for noise detection:	**1.0**

❖ **To set system suitability parameters**

1. Click **Edit**.

   The System Suitability dialog box opens. See System Suitability dialog box.

2. To perform symmetry testing, do the following:

   a. Select the Symmetry Parameters check box.

   b. Type a peak height for symmetry testing in the Peak Height box.

   c. Type a threshold for symmetry testing in the Symmetry Threshold box.

3. To carry out classification tests, do the following:

   a. Select the Peak Classification Parameters check box.

   b. To adjust Xcalibur peak width testing thresholds, type parameters in the Detect Peak Width area.

      - To enter a peak height for the test, type a value in the Peak Height box.

      - To enter a minimum peak width threshold, type a value in the Min Peak Width box.

   c. To adjust the Xcalibur peak tailing test, type parameters in the Detect Tailing area.

      - To enter a peak height for the test, type a value in the Peak Height box.

      - To enter a threshold limit for peak tailing, type a value in the Failure Threshold box.

   d. To adjust the Xcalibur column overload test, type parameters in the Detect Column Overload area.

      - To enter a peak height for the test, type a value in the Peak Height box.

      - To enter a threshold limit for peak tailing, type a value in the Failure Threshold box.

   e. To adjust the Xcalibur baseline clipping test, type parameters in the Detect Baseline Clipping area.

      To define the test window, type a value in the Number of Peak Widths for Noise Detection box.

4. To save your settings, click **OK**.

Figure 41. System Suitability dialog box
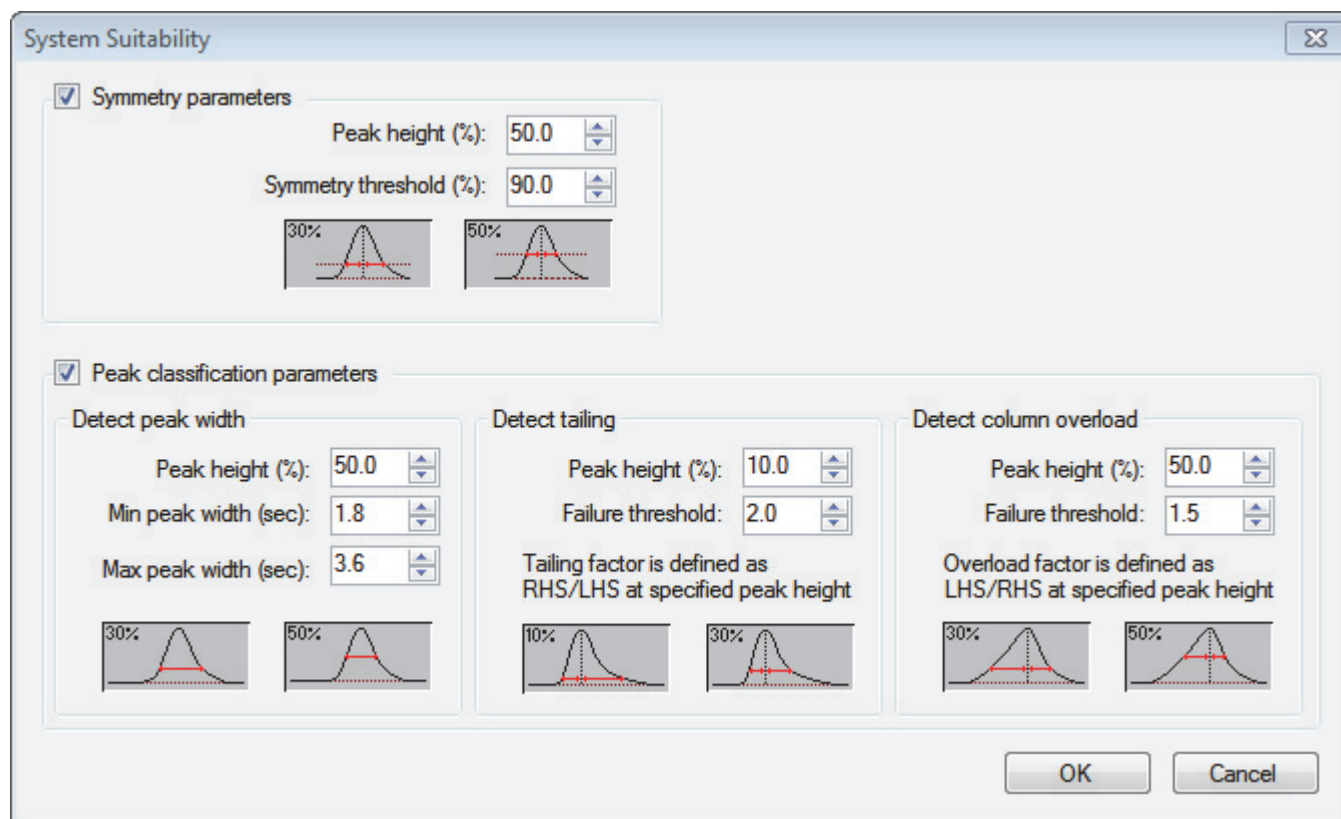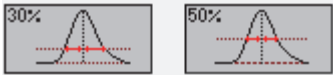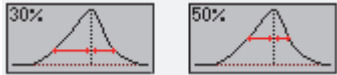
Table 26. System Suitability dialog box parameters (Sheet 1 of 2)

Parameter	Description
Symmetry Parameters	Determines the symmetry of the left and right sides of the detected peak.
Peak Height	The percentage of the peak height at which to compare the symmetry of the left and right peak widths. —— Left and right widths measured at 30% and 50% of the peak height
Symmetry Threshold	The minimum percentage difference to be considered symmetrical and pass the suitability test.
Peak Classification Parameters	
Detect Peak Width	Determines the minimum width of each side of the peak measured at the specified percentage of the peak height.
Peak Height	The percentage of the peak height at which to measure the full peak width. —— Full width measured at 30% and 50% of the peak height

Table 26. System Suitability dialog box parameters (Sheet 2 of 2)

Parameter	Description
Min Peak Width	Minimum peak width (measured at the specified percentage of the peak height) required to pass the suitability test.
Max Peak Width	Maximum allowed peak width (measured at the specified percentage of the peak height) to pass the suitability test.
Detect Tailing	The width of the right side of the peak divided by the width of the left side of the peak at the specified percentage of the peak height.
Peak Height	The percentage of the peak height at which to measure the left and right sides of the peak. Left and right widths measured at 10% and 30% of the peak height
Failure Threshold	Minimum Detect Tailing value (RHS/LHS) required to pass the suitability test.
Detect Column Overload	The width of the left side of the peak divided by the width of the right side of the peak at the specified percentage of the peak height.
Peak Height	The percentage of the peak height at which to measure the left and right sides of the peak. Left and right widths measured at 30% and 50% of the peak height
Failure Threshold	Minimum Detect Column Overload value (LHS/RHS) required to pass the suitability test.

Spectrum

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

For detailed descriptions of all the shortcut menu commands on the Spectrum page, see "Spectrum Page" on page 170.

Follow these procedures:

- To create a reference spectrum

- To update confirming ion ratios

- To change the quantitation mass used for a quantitative peak

- To add ions together to get an accumulated signal

- To add a quantitative peak to an existing compound

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

- To zoom in on the chromatogram or spectrum displays

❖ **To create a reference spectrum**

1. Click a peak in the quantitative peak chromatogram pane.

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

2. Right-click the Spectrum pane and choose **Apply Background Subtraction to Peak and Set as Reference Spectrum** from the shortcut menu.

   The application uses the background-subtracted reference spectrum during quantitative processing and reports the background-subtracted reference spectrum (indicated with BS in the scan heading) as the last scan for each compound on the Quantitation Report - 2 report.

   Note This command is available only when you select a background subtraction method on the General page in the master method. See "Editing the General Page" on page 113.

❖ **To update confirming ion ratios**

1. Click a peak in the quantitative peak chromatogram pane.

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

2. Right-click the Spectrum pane and choose **Update Confirming Ion Ratios with This Spectrum** from the shortcut menu.

❖ **To change the quantitation mass used for a quantitative peak**

1. Click a peak in the chromatogram pane.

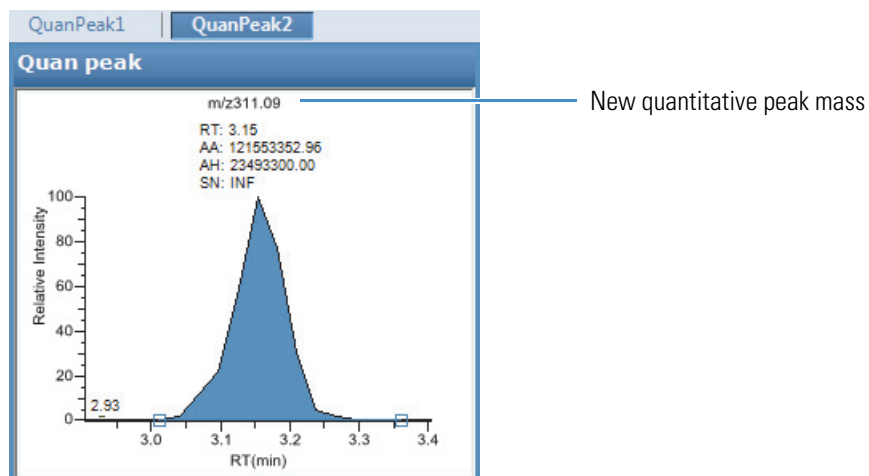   The mass spectrum for the peak is displayed in the Spectrum pane.

2. In the Spectrum pane, hold the cursor over the mass-to-charge value for an ion.

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

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

   • Set This Mass as Quan Mass > Don't Update Ion Ratios

   • Set This Mass as Quan Mass > Update Ion Ratios Using This Reference Spectrum

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

Figure 42. Original quantitative peak mass example
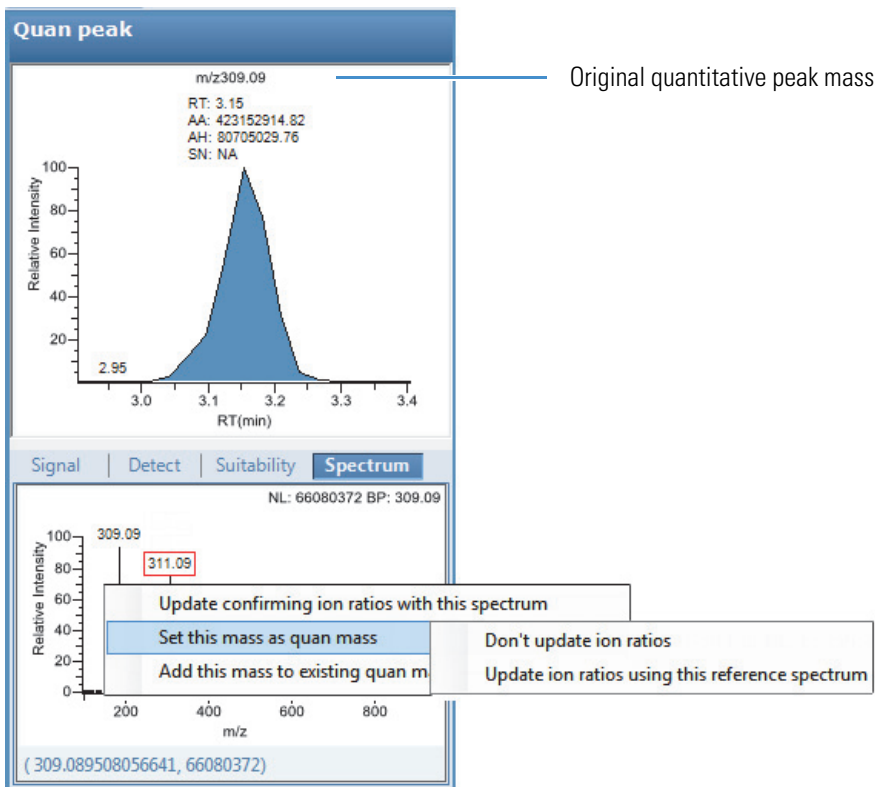
The TraceFinder application replaces the original quantitation mass with the selected mass.

Figure 43. Updated quantitative peak mass example

New quantitative peak mass
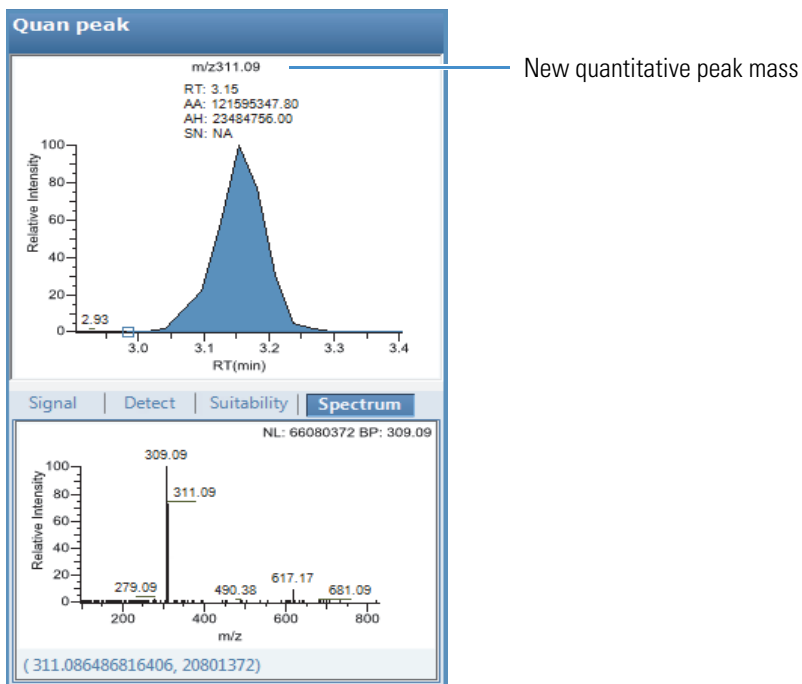
❖ **To add ions together to get an accumulated signal**

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

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

2. Right-click and choose **Add This Mass to Existing Quan Mass Range** from the shortcut menu.

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

❖ **To add a quantitative peak to an existing compound**

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

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

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

   A red box around the ion's *m/z* value indicates that the ion is selected.
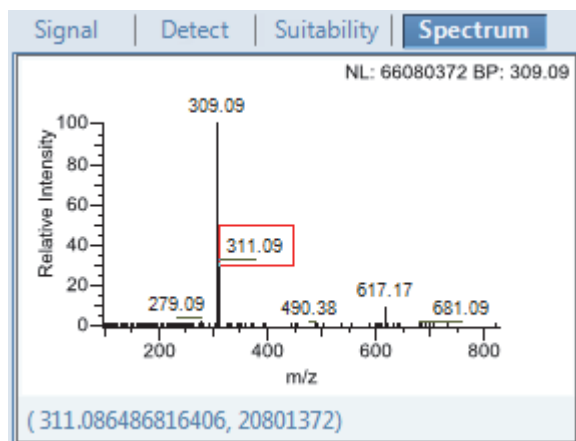
3. Right-click and choose **Set This Mass as New Quan Peak** from the shortcut menu.

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

New quantitative peak mass

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

1. Click the quantitative peak in the chromatogram pane.

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

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

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

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

   The TraceFinder application adds the selected mass as a confirming peak for this quantitative peak.
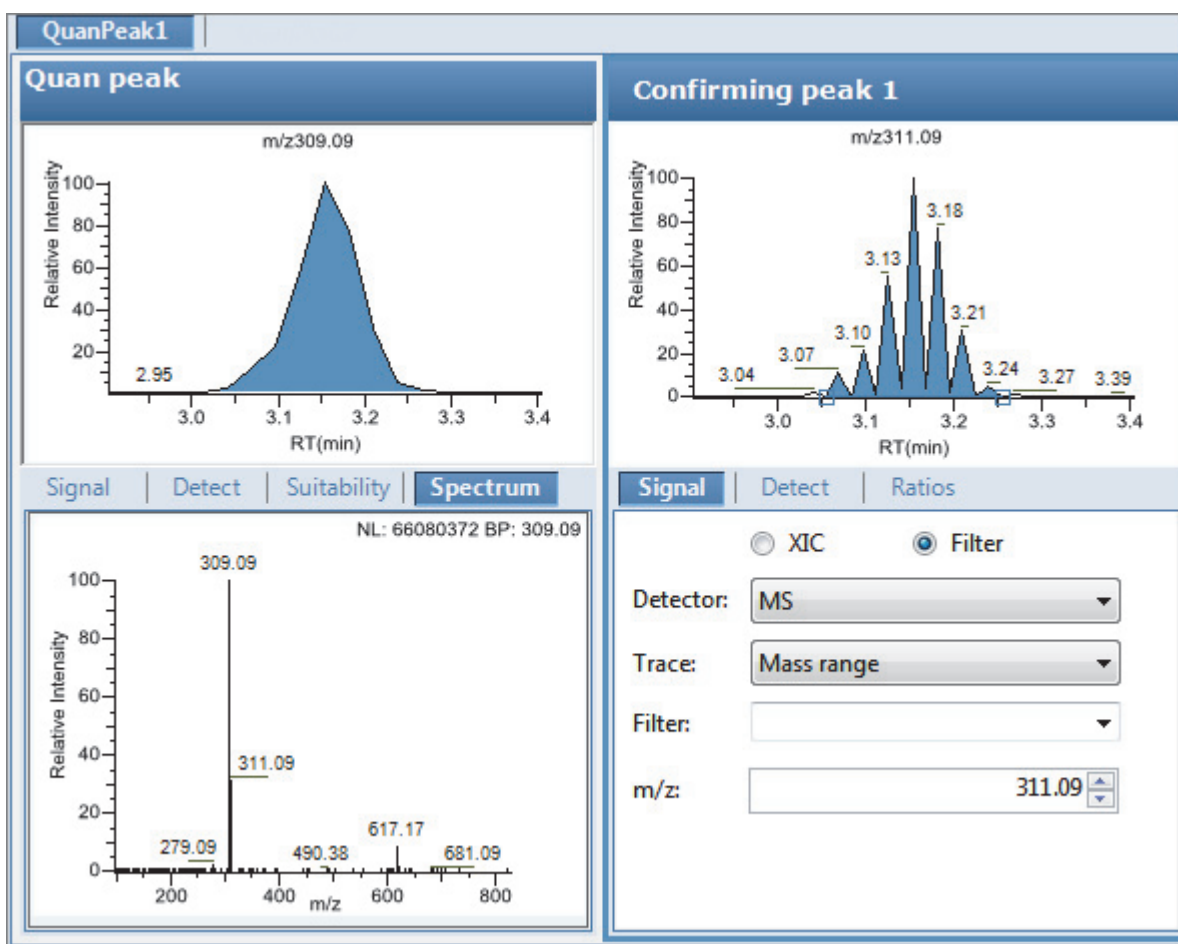
❖ **To zoom in on the chromatogram or spectrum displays**

1. Drag the cursor to delineate a rectangle.

   The display zooms in on the specified rectangle.

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

Spectrum Page

Use the shortcut menu commands on the Spectrum page to store a reference mass spectrum for a quantitative peak or compound.

Figure 44. Spectrum page
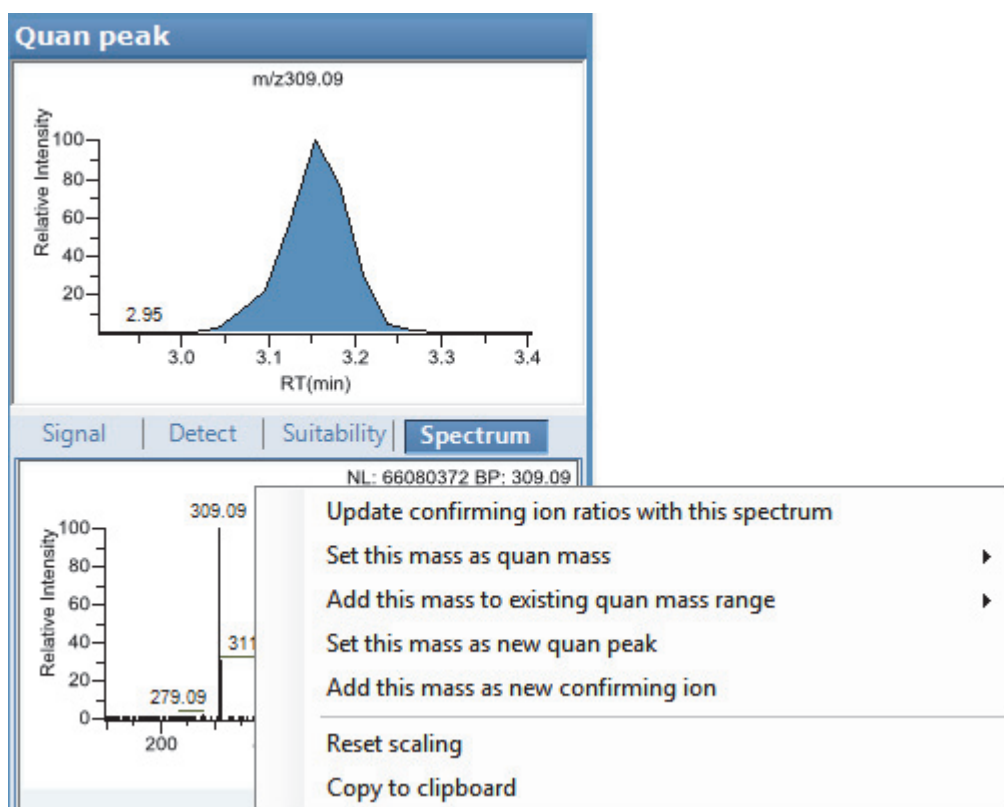
Table 27. Spectrum page shortcut menu commands

Command	Description
Update Confirming Ion Ratios With This Spectrum	Updates the confirming ion ratios using the selected peak.
Set This Mass as Quan Mass	Adds the quantitation mass of the selected ion to the quantitation mass used for the quantitative peak. You can choose to update the ion ratios or not update the ion ratios using this reference spectrum.
Add This Mass to Existing Quan Mass Range	Adds the selected mass to your existing quantitation mass range. You can choose to update the ion ratios to adjust the confirming ion comparisons to the new summed quantitative peak signal.
Set This Mass as New Quan Peak	Adds a new quantitative peak to an existing compound.
Add This Mass as New Confirming Ion	Adds one or more confirming ion peaks to an existing compound.
Reset Scaling	Returns the chromatogram or spectrum display to its original size.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Library

Use the Library page to define the criteria for library matching. For detailed descriptions of all the features on the Library page, see Library page.

❖ **To activate library matching**

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

2. From the Library Search Type list, select the type of library to use for matching.

   • **NIST**: Uses the NIST library that you installed with the TraceFinder application. See "Installing the NIST and QED Libraries" on page 15.

   > **Note** Because the NIST library is large, using this library can slow sample processing.

   • **Library Manager**: Uses the library that you specified in the Configuration console. See "Screening Libraries" on page 68.

   The application searches the library, matches the fragment ion spectrum in the library to the compound's ion spectrum, and returns the highest score (best match).

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

   To match a compound, the resulting score percentage from a library search match must be higher than your entered threshold value.

4. (Optional) Select the **Use Reverse Library Searching Only** check box.

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

Figure 45. Library page
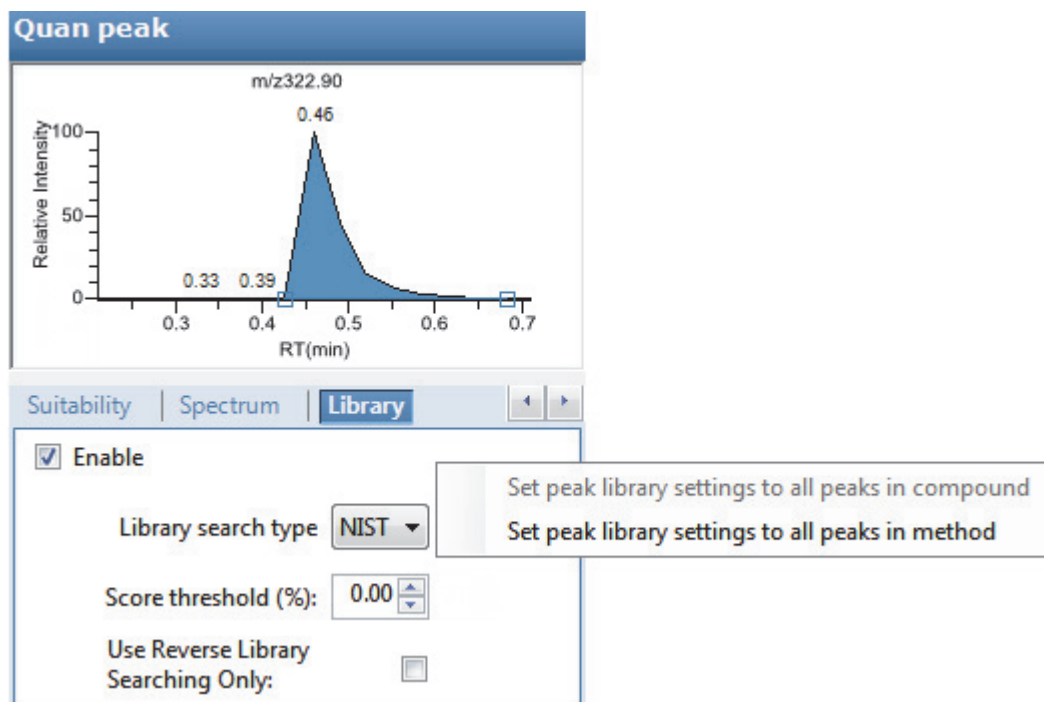
Table 28. Library page shortcut menu commands

Command	Description
Library Search Type	Specifies the type of library to use for target screening. • **NIST**: Uses the NIST library that you installed with the TraceFinder application. See "Installing the NIST and QED Libraries" on page 15. • **Library Manager**: Uses the library that you specified in the Configuration console. See "Screening Libraries" on page 68.
Score Threshold	The resulting score percentage from a library search match must be higher than your specified threshold value to identify or confirm the presence of a compound. Default: 0%
Use Reverse Library Searching Only	Compares a library entry to an unknown compound (a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
Shortcut menu commands	
Set Peak Library Settings to All Peaks in Compound	Updates all peaks in the current compound with the current settings on the Library page. These updates apply to both quantitative and confirming ion peaks. The application reprocesses all peaks in the compound and performs a new library search.
Set Peak Library Settings to All Peaks in Method	Updates all compounds in the method with the current settings on the Library page. These updates apply to both quantitative and confirming ion peaks. When you use this command in the local method for a processed batch, the application prompts you to reprocess the batch to update the library settings.

Ratios

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

For detailed descriptions of all the features on the Ratios page, see Ratios page.

❖ **To specify ion ratio criteria**

1. Select the **Enable** check box to activate the confirming ion.

2. In the Target Ratio box, select the theoretical ratio of the confirming ion's response to the quantification ion's response.

3. In the Window Type list, select **Absolute** or **Relative** as the calculation approach for determining the acceptable ion ratio range.

4. In the Window (+/-%) box, select the acceptable ion ratio range.

5. In the Ion Coelution box, select the maximum difference in retention time between a confirming ion peak and the quantification ion peak.

   In the following example, the target ratio is expected to be 61.02% and the window is Absolute 20%, so the acceptable window for this confirming ion peak is 41.02–81.02%.

   However, if the window type is Relative, the plus or minus value is 20% of 61.02% (or 12.20%), so the acceptable window for this confirming ion peak is 48.82–73.22%.

Figure 46. Ratios page
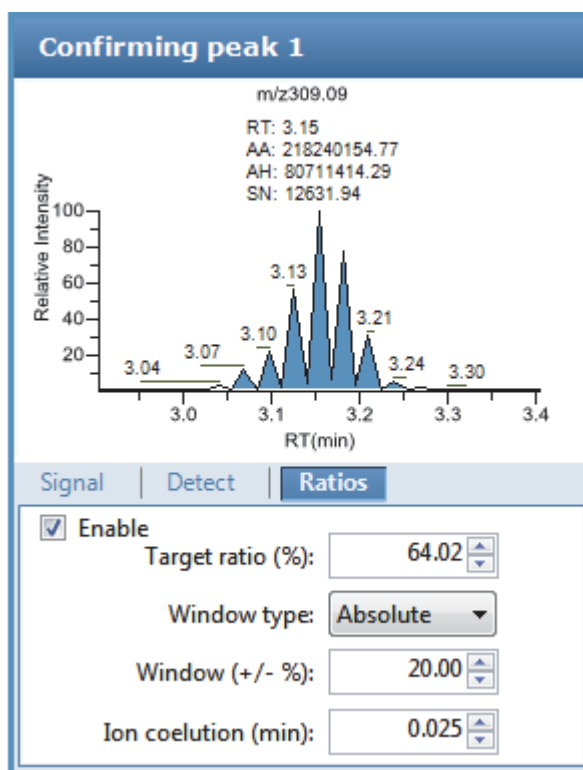
Table 29. Ratios page parameters

Parameter	Description
Enable	Makes the ion ratio criteria available.
Target Ratio (%)	The theoretical ratio of the confirming ion's response to the quantification ion's response.
Window Type	The absolute or relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	The acceptable ion ratio range.
Ion Coelution (min)	The maximum difference in retention time between a confirming ion peak and the quantification ion peak.
Shortcut menu commands	
Set Ion Ratio to All Confirming Peaks in Compound	Copies the Window Type, Window, and Ion Coelution values to all confirming ion peaks for the compound and updates the compound. Available only when a compound has multiple confirming ion peaks.
Set Ion Ratio to All Confirming Peaks in Method	Copies the Window Type, Window, and Ion Coelution values to all quantitative peaks for the method and updates the method.

Calibration

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

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

Typically, general quantitation uses a measured response (area or height) to determine the amount of a compound contained in a sample. The application compares the response of an unknown, target compound to the response of a calibration sample that contains a known amount of the compound by building a calibration curve to interpolate the amount in the target compound.

To use a semi-quantitative process, you specify the compound's standard type as Estimated and then identify another compound as the linked compound. Instead of using the target compound to create a calibration curve, the application uses a calibration curve from the linked compound to calculate the amount in the target compound.

To use a real sample for the calibration procedure, you specify the compound's standard type as Std Addition. The autosampler divides the sample into multiple portions (one unspiked portion and at least two spiked portions). To maintain consistent conditions across all samples, the autosampler adds selected amounts of standard into the vials and adds a volume of a solvent calculated to maintain constancy in the total volume of liquid in each vial.

For detailed descriptions of all the features on the Calibration page, see "Calibration Page" on page 177.

Follow these procedures:

- To specify an internal standard type for a compound
- To specify an estimated standard type for a compound
- To specify a standard addition standard type for a compound

❖ **To specify an internal standard type for a compound**

1. On the Identification page, specify at least one compound in the method as an internal standard compound type. See "Identification" on page 123.

2. On the Calibration page, do the following:

   a. In the Standard Type column, select **Internal**.

   b. In the ISTD column, select the compound that you want to use as the internal standard for this compound.

   The application lists only compounds specified as internal standards on the Identification page.

To view the internal standard peak in the Analysis mode, see "Compound Details" on page 506.

❖ **To specify an estimated standard type for a compound**

1. In the Standard Type column, select **Estimated**.

2. In the Linked Compound column, select any other compound in the method that you want to link to this compound.

The Estimation Method value defaults to Ext Curve and is read-only.

The Compound Results in Data Review display the Calculated Amt value as N/F (not found) highlighted in green.
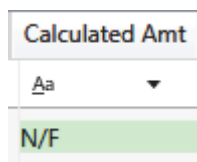
❖ **To specify a standard addition standard type for a compound**

In the Standard Type column, select **Std Addition**.

- The Curve Type column value defaults to Linear and is read-only.

- The Origin column value defaults to Ignore and is read-only.

- The Weighting column value defaults to Equal and is read-only.

When you process this sample, the application divides the sample into multiple portions: one portion is not spiked and at least two portions are spiked. The application calculates the analyte concentration as *intercept/slope*, where *intercept* is the *y*-intercept of the regression line and *slope* is the slope of the regression line.

When you use the Std Addition calibration, the *y*-intercept on the calibration curve might not be at 0, as shown in the following figure:
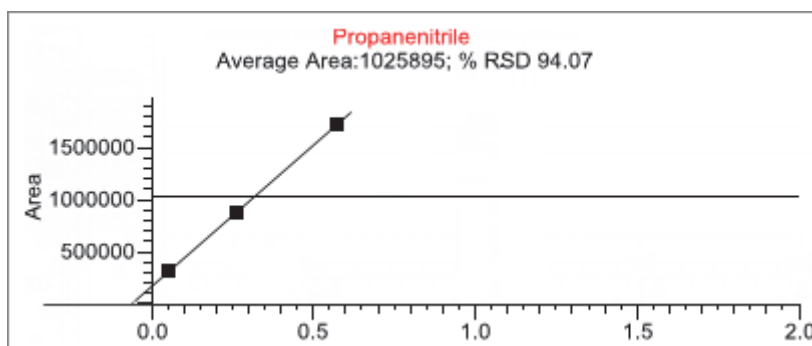
The Compound Results in Data Review display the following:

- The Calculated Amt value is the spiked amount from the calibration curve.

- The Theoretical Amt value is the level defined in the method.

- The Sample Amt value is the actual amount in the standard spike plus the spiked amount in each standard.

Calibration Page

Use the features on the Calibration page to define the mathematical model used for preparing the initial calibration evaluation for one or more calibration standards.

Figure 47. Calibration page

Table 30. Calibration page parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Compound Type	Displays the compound type as a Target Compound or Internal Standard.
Standard Type	Specifies Internal, External, Estimated, or Std Addition standards.
Response Via	The use of area or height. When you set the standard type to Estimated, this column is inactive.
Curve Type	Specifies Linear, Quadratic, or AverageRF curve types. When you set the standard type to Estimated, this column is inactive. When you set the standard type to Std Addition, this column value defaults to Linear and is read-only.
Origin	The origin treatment is Ignore, Include, or Force. The Origin and Weighting columns are available only when you use Linear or Quadratic curve types. When you set the standard type to Estimated, this column is inactive. When you set the standard type to Std Addition, this column value defaults to Ignore and is read-only.
Weighting	Specifies the weighting as Equal, 1/X, 1/X^2, 1/Y, or 1/Y^2. When you set the standard type to Estimated, this column is inactive. When you set the standard type to Std Addition, this column value defaults to Equal and is read-only.
Units	The units to be displayed with the calculated values.
ISTD	The internal standard (ISTD) for a target compound or surrogate. The list displays all compounds with the compound type of Internal Standard. This column is available only when you set the standard type to Internal.
Amount	The amount of the internal standard for ISTD compounds. When you set the standard type to Estimated, this column is inactive.

Table 30. Calibration page parameters (Sheet 2 of 2)

Parameter	Description
Linked Compound	This column is available only when the standard type is set to Estimated. The list of available compounds to be linked does not include any compounds whose standard type is set to Estimated.
Estimation Method	This column is unavailable for editing when the standard type is set to Estimated. • When the compound type for the associated linked compound is Target Compound, the estimation method is automatically set to Ext Curve. • When the compound type for the associated linked compound is Internal Standard, the estimation method is automatically set to Ratio.
Shortcut menu	The Calibration page uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 188.

Calibration Levels

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

For detailed descriptions of all the features on the Calibration Levels page, see Calibration Levels page.

You can use the copy-and-paste functions on the shortcut menu to copy calibration levels from one column to another or from one master method to another. For detailed instructions, see "Copying and Pasting Column Values" on page 183.

❖ **To specify calibration levels and concentrations**

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

	RT	Compound			
▶ 1	3.15	Pyrazinamide			
2	3.67	1,3-Dioxolane, 2-heptyl-			

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

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

   Manage Calibration levels

	Level
1	Cal1
🖉 2	Cal2
✳ 3	

3. Continue adding calibration levels.

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

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

   a. Select the first calibration level table cell.

   b. Click the cell again to make it editable.

   c. Type a concentration value.

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

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

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

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

Figure 48. Calibration Levels page

		RT	Compound	Cal1	Cal2	Cal3
	1	3.14	Propanenitrile	5.000	10.000	15.000
	2	3.15	Pyrazinamide			
▶	3	3.67	1,3-Dioxolane, 2-heptyl-			
	4	4.70	Pyrazinamide *2*			

Manage Calibration levels

		Level
	1	Cal1
	2	Cal2
	3	Cal3

Table 31. Calibration Levels page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
CalLevel_1–CalLevel_n	User-defined calibration levels for the compound. The names you enter here become the column headers for the calibration levels.
Manage Calibration Levels	Defines values for each of the calibration level values for the selected compound.
Shortcut menu	The Calibration Levels page uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 188.

QC Check Levels

Use the QC Check Levels page for a master method to define the standards for QC Check levels. You can edit QC Check levels for master methods only. The contents of this page are read-only when you are editing a local method. For detailed descriptions of all the features on the QC Check Levels page, see QC Check Levels page.

You can use the copy-and-paste functions on the shortcut menu to copy QC Check levels from one column to another or from one master method to another. For detailed instructions, see "Copying and Pasting Column Values" on page 183.

❖ **To specify QC Check levels and concentrations**

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

	RT	Compound			
1	3.15	Pyrazinamide			
2	3.67	1,3-Dioxolane, 2-heptyl-			
3	4.70	Pyrazinamide *2*			

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

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

3. Type a value for the % Test.

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

Manage QC Check levels

	Level	% Test
1	Level1	5.00
✱ 2		NA

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

Manage QC Check levels

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

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

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

   a. Select the first QC Check level table cell.

    b.   Click the cell again to make it editable.

    c.   Type a concentration value.

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

		RT	Compound	Level1	Level2	Level3
	1	3.14	Propanenitrile	5.000	10.000	15.000
	2	3.15	Pyrazinamide			

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

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

Figure 49. QC Check Levels page

		RT	Compound	Level1	Level2	Level3
▶	1	3.14	Propanenitrile	5.000	10.000	15.000
	2	3.15	Pyrazinamide	5.000	10.000	15.000
	3	3.67	1,3-Dioxolane, 2-heptyl-	5.000	10.000	15.000

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

Manage QC Check levels

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

Table 32. QC Check Levels page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Level_1–Level_n	User-defined quality control levels for the compound.
Manage QC Check Levels	
Level	User-defined quality control level names. The names you enter here become the column headers for the QC Check levels.
% Test	A value for the acceptable difference (as a percentage) between the known amount and calculated (measured) amount of each QC Check level.
Shortcut menu	The QC Check Levels page uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 188.

Copying and Pasting Column Values

You can use the copy-and-paste functions on the shortcut menu to copy column values within a master method or from one master method to another. You can use these copy-and-paste techniques on any pages with grids of data in the Compounds and QAQC views.

After you copy grid values to the Clipboard, you can paste them into a text application such as Notepad, an e-mail, a spreadsheet, other grid cells in the same master method, or into another master method.

> **Tip** When copying data into an application other than a TraceFinder master method grid, use the Copy with Headers command instead of the Copy command on the shortcut menu to preserve the column headers.

Following these procedures:

- To copy a value from one cell to another cell

- To copy all values in a column to another column

- To copy multiple columns

- To copy an entire grid to another master method

❖ **To copy a value from one cell to another cell**

1. Select a cell value to copy to the Clipboard.

   You can select either an entire table cell or just a cell value.

   | 10.000 | —— Cell is selected.

   | 10.000 | —— Cell value is selected.
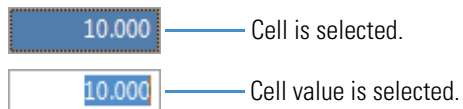
2. Right-click and choose **Copy** from the shortcut menu.

   The application copies either the selected cell value or the selected cell to the Clipboard.

3. In this or another master method, select the cell value or table cell that you want to overwrite.

   - If you copied a cell value, you can select the cell value or simply click in the cell.

   - If you copied an entire cell, you must select a table cell to overwrite.

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

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

❖ **To copy all values in a column to another column**

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

Cal_1
5.000
5.000
5.000
5.000

2. Right-click and choose **Copy** from the shortcut menu.

3. In this or another master method, use the SHIFT key to select the column to overwrite.

Cal_3
10.000
10.000

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

   The application overwrites the selected cells with the cells that you copied to the Clipboard.

Cal_3
5.000
5.000
5.000
5.000

❖ **To copy multiple columns**

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

Cal_1	Cal_2
5.000	10.000
5.000	10.000
5.000	10.000
5.000	10.000

2. Right-click and choose **Copy** from the shortcut menu.

3. In this or another master method, use the SHIFT key to select the columns to overwrite.

Cal_A	Cal_B

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

The application overwrites the selected cells with the cells that you copied to the Clipboard.

Cal_A	Cal_B
5.000	10.000
5.000	10.000
5.000	10.000
5.000	10.000

❖ **To copy an entire grid to another master method**

1. Use the SHIFT key to select all the columns in the grid.

LOD (Detection limit)	LOQ (Quantitation limit)	LOR	ULOL (Linearity limit)	Carryover limit
10.000	20.000	30.000	0e0	0e0
10.000	20.000	30.000	0e0	0e0

2. Right-click and choose **Copy** from the shortcut menu.

3. In another master method, use the SHIFT key to select the columns to overwrite.

LOD (Detection limit)	LOQ (Quantitation limit)	LOR	ULOL (Linearity limit)	Carryover limit
0.000	0.000	0.000	0e0	0e0
0.000	0.000	0.000	0e0	0e0

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

The application overwrites the selected cells with the cells that you copied to the Clipboard.

> **Note** When the Clipboard contains more cells of data than there are selected target cells for the paste operation, the application overwrites the selected cells and reports that the Clipboard contents were truncated to fit the grid.

Real Time Viewer

Use the Real Time Viewer page to specify which traces display in the Real Time Status pane when you perform acquisition in the Acquisition mode or when you acquire a development batch in the Method Development mode. See "Real Time Status Pane" on page 368.

Figure 50. Real Time Viewer page
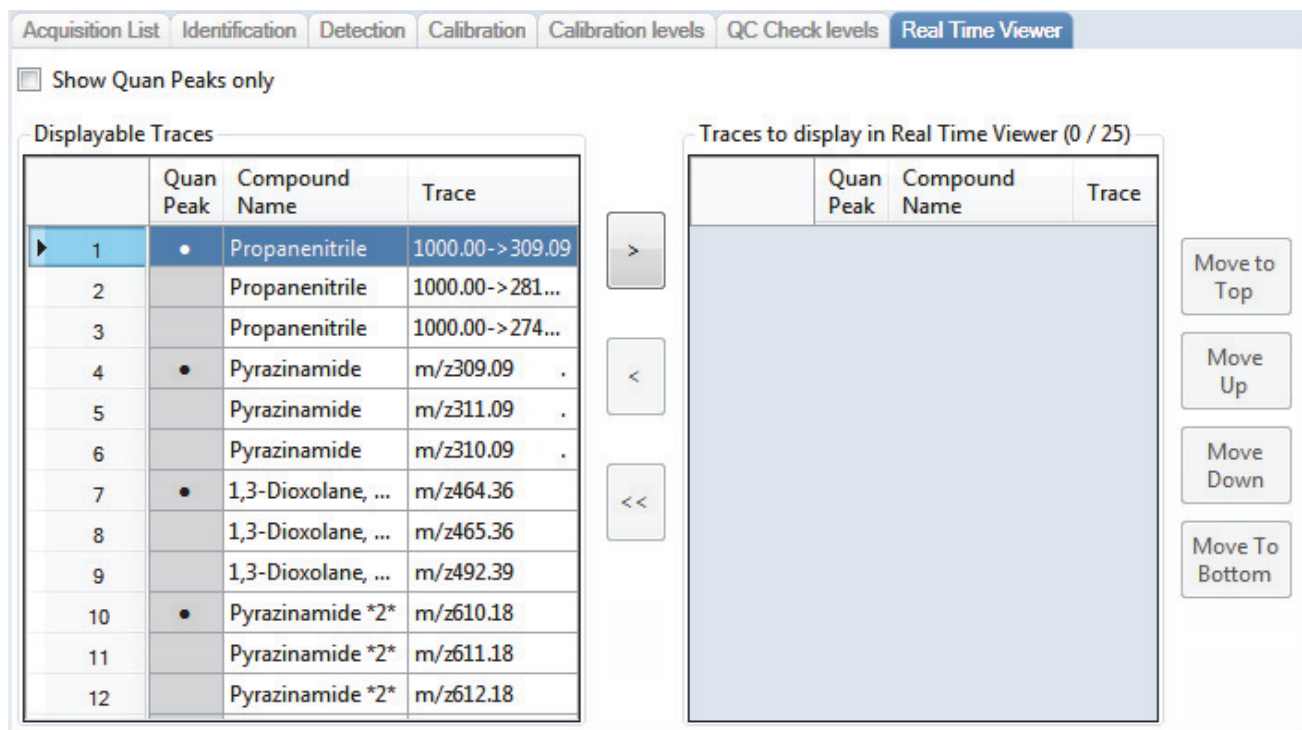
Table 33. Real Time Viewer page parameters (Sheet 1 of 2)

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

Table 33. Real Time Viewer page parameters (Sheet 2 of 2)

Parameter	Description
Trace	Lists the simple mass or precursor mass for all traces—both quantitative peak and confirming ion peak—for each compound.
$>$	Moves the selected trace to the Traces to Display in Real Time Viewer pane.
$<$	Moves the selected trace to the Displayable Traces pane.
$<<$	Moves all traces to the Displayable Traces pane. To move multiple traces to the Traces to Display... pane, hold down the SHIFT key, select multiple traces, and then click $>$.
Traces to Display in Real Time Viewer (*n*/25)	List the traces to be displayed and the display order used in the real-time display in the Acquisition mode. See "Real-Time Trace Display" on page 382. Maximum number of traces is 25.
Move to Top	Moves the selected trace to the top of the Traces to Display... list and the second position in the real-time display. The TIC is always the first position in the real-time display in the Acquisition mode.
Move Up	Moves the selected trace up one position in the list.
Move Down	Moves the selected trace down one position in the list.
Move to Bottom	Moves the selected trace to the bottom of the list.

Using the Shortcut Menu Commands

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

Table 34. Compounds page shortcut menu commands (Sheet 1 of 2)

Command	Description
Copy Down	Copies the value in the selected row to all rows below it. This command is available only when you have selected a value that can be copied down. See Appendix C, "Using Copy Down and Fill Down."
Display Retention Time Column	Displays or hides the RT column in the compound list.
Delete Compound From Method	Removes the selected compound from the current master method.
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy compound information to another application, such as an Excel spreadsheet. You cannot paste this data back into the method development compound list.
Copy With Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information to another application, such as an Excel spreadsheet. You cannot paste this data back into the method development compound list.
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column. The pasted data must be valid data for the selected column.

Table 34. Compounds page shortcut menu commands (Sheet 2 of 2)

Command	Description
Undo Last Paste	Removes the last pasted item in the method development compound list.
Export to CSV File	Opens the Save As dialog box where you can save the current compound list to a CSV file.
Sort by Compound Name	Sorts the compounds alphabetically from A to Z.
Sort by Retention Time	Sorts the compounds from shortest retention time to longest retention time.
Add This Compound to CDB	Adds the selected compound to the compound database. When the compound already exists in the compound database, the TraceFinder application updates the compound database with the current compound information.
Add All Compounds to CDB	Adds all compounds in the current method to the compound database. When any of these compounds already exist in the compound database, the TraceFinder application updates the compound database with the current compound information.

Editing the QAQC Page

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

On most QAQC pages, you can use the copy-and-paste functions on the shortcut menu to copy grid values from one column to another or from one master method to another. For detailed instructions, see "Copying and Pasting Column Values" on page 183.

❖ **To open the QAQC page**

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

Available only when you activate
Intelligent Sequencing in
the Configuration console

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

- Limits

- Calibration

- QC Check

- Negative

- ISTD

- Solvent Blank

- Threshold

- Hydrolysis

Limits

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

Figure 51. Limits page

Table 35. Limits page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
LOD (Detection Limit)	Limit of detection. The lowest amount that can be detected. Usually derived from a method detection limit (mdl) study.
LOQ (Quantitation Limit)	Limit of quantitation. The lowest amount that can be confidently and accurately quantitated. This is usually the lowest calibration amount.
Cutoff	Also called limit of reporting (LOR) in some industries. This is the lowest amount that can be reported, as determined by each laboratory's standard operating practices.
ULOL (Linearity Limit)	Upper limit of linearity. This is usually the highest calibrator amount.
Carryover Limit	The highest amount of a substance that does not leave a residual amount in the instrument. If a substance has a carryover limit of 5, amounts higher than 5 usually dirty the instrument and leave residue behind, tainting the following sample. A carryover limit of less than 5 does not leave any residual amounts of the substance.

Calibration

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

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

Figure 52. Calibration page

	RT	Compound	R^2 threshold	Max RSD (%)	Min RF	Max Amt Diff (%)	CV Test (%)
1	3.14	Propanenitrile	0.9900	20.00	0.000	20.00	0.000

Tabs: Limits | Calibration | QC Check | Negative | ISTD | Solvent Blank | Threshold | Hydrolysis

Table 36. Calibration page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
R^2 Threshold	The minimum correlation coefficient (r^2) for an acceptable calibration (when in linear or quadratic mode).
Max RSD (%)	The maximum relative standard deviation (RSD) for an acceptable calibration (when in average RF mode). **Note** This RSD value is not the same value used in Data Review or the Compound Calibration Report. The application uses this RSD value when you select AverageRF as the curve type for the method. See "Calibration Page" on page 177.
Min RF	The minimum average response factor (RF) for an acceptable calibration (when in average RF mode).
Max Amt Diff (%)	The maximum deviation between the calculated and theoretical concentrations of the calibration curve data points (when in linear or quadratic mode).
CV Test (%)	Coefficient of Variance test. The coefficient of variance percentage is the standard deviation of the multiple samples of one level, multiplied by 100, and then divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.

QC Check

Use the QC Check page to review the calibration on an ongoing basis. The TraceFinder application compares the quality check standard results for each compound in the sample to the initial calibration using values defined on this page.

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

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

Figure 53. QC Check page

Table 37. QC Check page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Max RF Diff (%)	The maximum deviation between the response factor (RF) of the QC sample and the average response factor from the calibration (when in average RF mode).
Min RF	The minimum response factor for the QC sample (when in average RF mode).
CV Test (%)	Coefficient of Variance test. The coefficient of variance percentage is the standard deviation of the multiple samples of one level, multiplied by 100, and then divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.

Negative

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

For detailed descriptions of all the features on the Negative page, see Negative page parameters.

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

❖ **To specify the maximum concentration as a percentage**

1. From the Method column list, select one of the following methods:
   - % of LOD
   - % of LOQ
   - % of LOR

2. In the Percentage column, type a percentage value.

❖ **To specify the maximum concentration**

1. From the Method column list, select **Concentration**.

2. In the Max Conc column, type an absolute value.

Figure 54. Negative page

Table 38. Negative page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Method	The evaluation process used for comparing the calculated concentration. You can specify no maximum, a specific concentration, or a percentage of the LOR, LOD, or LOQ.
Percentage	The percentage of the LOR, LOD, or LOQ if you are using the percentage approach.
Max Conc	The maximum concentration if you are using an absolute value.

ISTD

Use the ISTD page to review the response and retention time of internal standards (when available). The TraceFinder application compares the area and retention time results for each internal standard compound in the sample to a specified range.

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

Figure 55. ISTD page

Table 39. ISTD page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Min Recovery (%) Max Recovery (%)	The minimum and maximum percent recoveries for the internal standards to define an acceptable range. For check standards, the TraceFinder application compares the response of each internal standard in each sample to a range around the average of the responses of that compound in all of the calibration standards. For all other samples, the application calculates the comparison range around the check standard responses if a check standard is available in the batch. If no check standard is available, the application tests against the initial calibration.
Min RT (–min) Max RT (+min)	The minimum and maximum drift (in minutes) for the internal standards to define an acceptable range. For check standards, the TraceFinder application compares the retention time of each internal standard in each sample to a range around the average of the retention times of that compound in all of the calibration standards. For all other samples, the application calculates the comparison range around the check standard retention times if a check standard is available in the batch. If no check standard is available, the application tests against the initial calibration.
CV Test (%)	Coefficient of Variance test. The coefficient of variance percentage is the standard deviation of the multiple samples of one level, multiplied by 100, and then divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.

Solvent Blank

Use the Solvent Blank page to view or edit QC values for solvent reporting. The application compares the calculated response for each compound in the sample to the maximum response defined on this page.

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

Figure 56. Solvent Blank page

Table 40. Solvent Blank page parameters

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

Threshold

Use the Threshold page (see "Threshold page" on page 198) to specify how to create a
threshold guide to overlay on compounds in the Comparative View in the Data Review mode.
For each compound, you can specify an absolute value or you can specify a percentage of the
peak height. The application uses the selected threshold method and the specified amount to
create a threshold guide in the Comparative View chromatograms. See "Comparative View"
on page 474.

When you create a batch, you can group samples and then specify a sample in the group as the
threshold sample to use in the Comparative View. For instructions about specifying a
threshold sample, see "Threshold Samples Page" on page 434.

In the following figures, the threshold for the dibutyl phthalate compound is 50% of the peak
height in the threshold sample, the samples Benzo26473, Benzo25557, and Benzo26154 are
members of groupB, and the threshold sample for the group is Benzo26473. In the
Comparative Data view, you can easily see that the peak height of dibutyl phthalate in the
other samples in the group is less than 50% of the peak height in the threshold sample.

Figure 57. QAQC page in Method View

Threshold method

Threshold at 50% of the
peak height in the threshold
sample

Figure 58. Samples page in Batch View

Samples belong to the same group

Figure 59. Threshold Samples page in Batch View

	Group	Sample
▶	groupb	Benzo26473

Benzo26473 selected as the
threshold sample for groupb.

Figure 60. Comparative View in Data Review
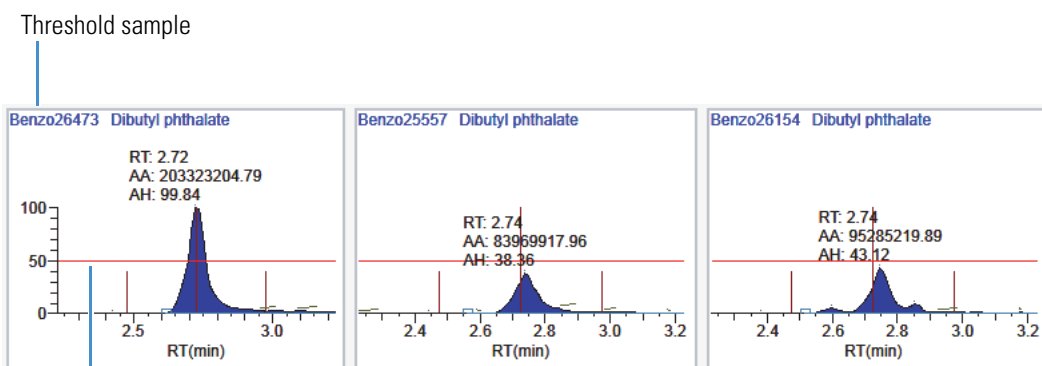
Threshold sample

Threshold percentage - 50%

Figure 61. Threshold page

	RT	Compound	Method		Threshold	Percentage
▶	3.14	Propanenitrile	Threshold	▼	1.000	
	3.15	Pyrazinamide	Threshold	▼	1.000	
	3.67	1,3-Dioxolane, 2-heptyl-	% of Threshold Sample	▼		0.1
	4.70	Pyrazinamide *2*	% of Threshold Sample	▼		0.1

Table 41. Threshold page parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Method	Species the threshold method as a specific peak height value or as a percentage of the peak height in the threshold sample.

Table 41. Threshold page parameters (Sheet 2 of 2)

Parameter	Description
Threshold	Specifies the absolute peak height value to use when you select the Threshold method. This value represents the default threshold value to use when you do not specify a Threshold Sample for a group of samples. Default: 1.000
Percentage	Specifies the percentage of the peak height value to use when you select the % of Threshold Sample method. This value represents a percentage of the actual peak height in the Threshold Sample you select for a group of samples. For instructions about specifying a Threshold Sample, see "Threshold Samples Page" on page 434. Default: 0.1 Range: 0.1 to 100.1

Hydrolysis

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

Figure 62. Hydrolysis page

Table 42. Hydrolysis page parameters

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

Editing the Groups Page

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

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

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

❖ **To open the Groups page**

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

Available only when you activate Intelligent Sequencing in the Configuration console
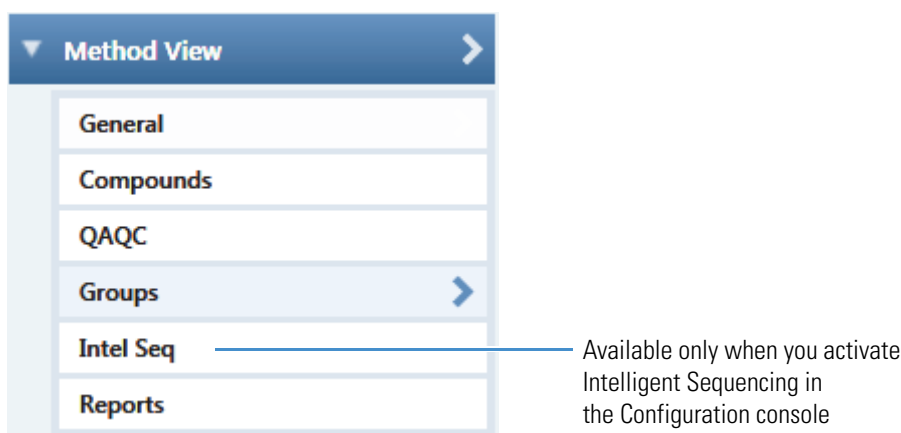
❖ **To create a group**

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

   The Add a New Group dialog box opens.

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

   The new group appears in the Groups area.

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

4. To remove all the compounds from a group, rename the group, or delete it, right-click the group name and choose from the shortcut menu.
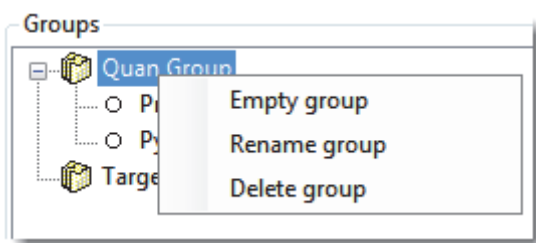
5. To remove a single compound, right-click the compound name in the group and choose **Remove from Group** from the shortcut menu.
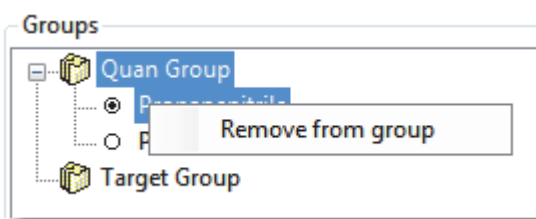
Groups Page

Use the features on the Groups page to organize compounds into functional or logical groups.

Figure 63. Groups page
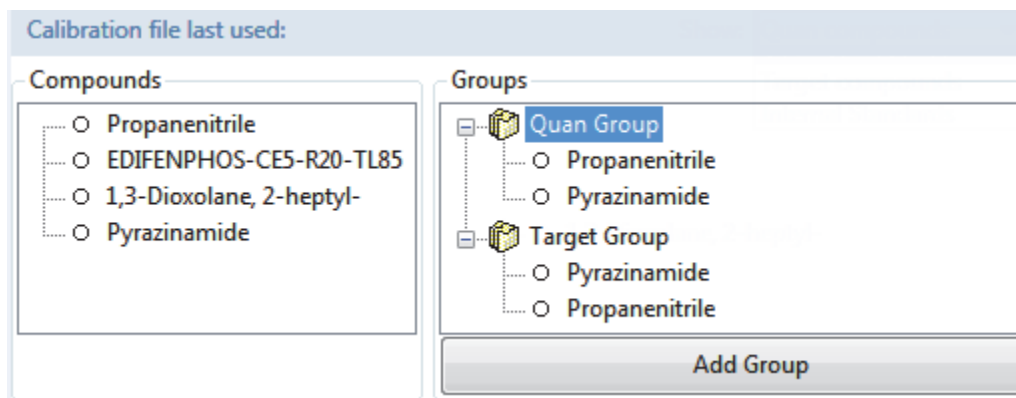
Table 43. Groups page parameters (Sheet 1 of 2)

Parameter	Description
Compounds	Lists all available compounds.
Groups	Lists all available groups.
Add Group	Opens the Add a New Group dialog box where you can create a new group.

Table 43. Groups page parameters (Sheet 2 of 2)

Parameter	Description
Shortcut menu	
Empty Group	Removes all compounds from the selected group.
Rename Group	Changes the name of the selected group.
Delete Group	Removes the selected group and all the compounds in it.
Remove From Group	Removes the selected compound from its group.

Editing the Intelligent Sequencing Page

Use the Intelligent Sequencing page to specify the actions you want the application to take when there are acquisition failures with each sample type. The Intelligent Sequencing page is available only when you activate Intelligent Sequencing in the Configuration console. See "Intelligent Sequencing" on page 71.

❖ **To open the Intelligent Sequencing page**

Click **Intel Seq** in the Method View navigation pane.

The Intelligent Sequencing page opens.

❖ **To specify actions for sample acquisition failures**

1. In the Sample Types list, select a sample type.

   Each sample type has a specific set of failure flags. See "Sample-Specific Failure Flags" on page 207.

2. For each failure flag, select a failure action.

   The failure action choices are the same for each failure flag except flags for Solvent or Negative sample types. The Solvent and Negative sample types do not have Auto Sample or Auto Sample and Reinject failure actions.

Each Failure Action requires one or more of the following values:

- Sample Type

- Priority

- Max Action Count

- Failure Continuation

For a detailed description of each of these parameters, see "Actions" on page 206.

3. Select a sample type to use for the failure action.

This value is available only for Auto Sample and Auto Sample and Reinject failure actions. When you create your samples list on the Auto Samples page, you must include at least one sample with this sample type for the autosampler to use when it encounters this error condition. See "Auto Samples Page" on page 431.

4. In the Priority column, type a priority value for this action.

The priority value can be any positive or negative integer.

- The application performs the failure action for the highest priority failure it encounters and ignores all others.

- When you assign the same priority to two or more failures, the application performs the failure action for the first failure it encounters and ignores all others.

5. In the Max Action Count column, type a value for the maximum number of times the application should repeat a sample.

6. In the Failure Continuation column, do one of the following:

- Select the check box to skip this sample and continue to the next sample when this sample exceeds the Max Action Count value.

- Clear the check box to stop the batch when this sample exceeds the Max Action Count value.

Actions

Use the Actions pane to specify what action the application takes when it encounters a submission failure for the type of failure flag associated with each sample type.

Table 44. Actions parameters (Sheet 1 of 2)

Parameter	Description
Flag	Flag (error) types specific to each sample type. See Sample-Specific Failure Flags. Each flag type has a set of user-specified actions that the application follows when it encounters this error.
Failure Action	In the event of a failed sample, the application does one of the following: • **Continue**: Continues to the next sample in the batch. • **Stop**: Stops the batch. • **Auto Sample**: Injects the sample type specified for the Auto Sample Type parameter and continues to the next sample. • **Reinject**: Reinjects the current sample by inserting a "reinject" sample in the batch. • **Auto Sample and Reinject**: Injects the sample type specified for the Auto Sample Type parameter and then reinjects the failed sample.
Sample Type	Specifies either a Solvent or Negative sample type to use for the auto sample injection. Default: Solvent
Priority	The priority value can be any positive or negative integer. When two or more failures have the same priority, the application performs the failure action for the first failure it encounters and ignores all others. The application performs the failure action for the highest priority failure and ignores all others.

Table 44. Actions parameters (Sheet 2 of 2)

Parameter	Description
Max Action Count	Specifies the maximum number of times the application should repeat a sample before it continues to the next sample or stops the sequence, as determined by the value in the Failure Continuation parameter. Default: 1
Failure Continuation	When this check box is selected, samples that exceed the value specified for the Max Action Count parameter cause the application to skip the sample and continue to the next sample. Default: Selected When this check box is cleared, samples that exceed the value specified for the Max Action Count parameter cause the application to stop the batch.

Sample-Specific Failure Flags

Each sample type has a specific set of failure flags.

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

Editing the Reports Page

Use the Reports page to specify how you want to save or print your reports. For detailed descriptions of the features on the Reports page, see Reports Page.

For the quantitation report types, you can modify quantitation limits flags, user interface options, and quantitation flag options on the Quan Report Settings page.

For ToxID report types, you can modify default report options, semi-quantitative results options, ion ratio calculation methods, the exact mass window, and Exactive™ options on the Target Screening Export Settings page.

This section includes instructions for the following tasks:

- Specifying Report Formats

- Specifying Quan Report Settings

- Specifying Target Screening Export Settings (for ToxID Reports)

Specifying Report Formats

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

- For each Custom report type, you can create a hardcopy printout or an Excel Macro-Enabled Workbook (.xlsm) file.

- For each ToxID report type, you can create a hardcopy printout or a PDF file.

❖ **To open the Reports page**

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

Available only when you activate
Intelligent Sequencing in
the Configuration console

The Reports page opens with a list of all configured reports.

To configure which reports are available when you create a master method or which reports create a batch-level report, see "Specifying the Reports" on page 40.

❖ **To specify report types and output formats**

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

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

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

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

All check boxes in the column below the selected cell duplicate the selected or cleared state of the selected cell. This action applies only to reports where this output format is available. By default, all report types are cleared.

Reports Page

Use the features on the Reports page to specify how you want to save or print your reports.

Figure 64. Reports page

Table 45. Reports page parameters (Sheet 1 of 2)

Parameter	Description
Example	Opens a PDF file that displays an example of the report type.
Report Name	The name of a report.
Report Title	The user-defined description to be used on a report.
Report Type	The type of report: Standard, Custom, or ToxID.
Print	Sends reports to the printer. Available for all report types.
Create PDF	Saves reports as PDF files. Available only for Standard and ToxID report types.
Create XML	Exports reports in XML format. Available only for Standard report types.

Table 45. Reports page parameters (Sheet 2 of 2)

Parameter	Description
Create XLSM	Exports reports in Excel Macro-Enabled Workbook (.xlsm) format. Available only for Custom report types.
Batch Level	Rather than creating separate reports for each sample, the application uses a composite of the data from all the appropriate samples to create a single report for the entire batch. Batch-level reports are prepended with a **B** to differentiate them. You cannot select this option from the Reports page. You must select the Batch Level option for the report in the report configuration. See "Specifying the Reports" on page 40.
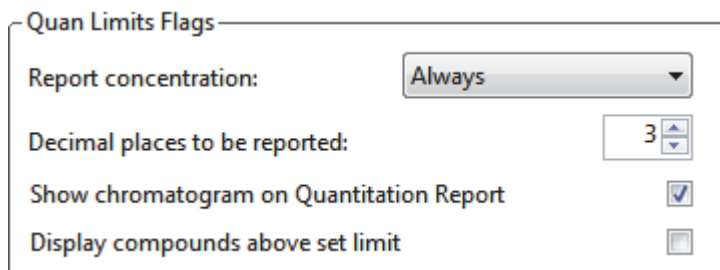
Specifying Quan Report Settings

Use the options on the Quan Report Settings page to choose parameters for flagging values and displaying information in standard report types. See "Quan Report Settings Page" on page 213.

Follow these procedures:

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

❖ **To specify quantitation limits**

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

    For a description of concentration limits, see "Editing the QAQC Page" on page 190.

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

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

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

❖ **To specify user interface options**

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

2. To separate the ion overlay pane from the confirming ion plots, select the **Separate Ion Overlay Display** check box.

3. To use an alternate format for the Calibration Report designed to print more concisely and limit the report to a maximum of seven calibration standards, select the **Use Alternate Calibration Report Format** check box.

4. To display flags and a legend on high density reports, select the **Display Quan Flags and Legend** check box.

❖ **To specify quantitation flag options**

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

Values are above or below the limits defined on the Quan page.
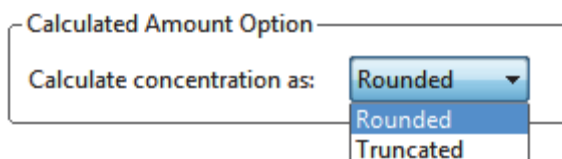
These flags appear on a variety of reports and are defined in "Quan Report Settings page parameters" on page 214.

Quan Report Settings Page

Use the features on the Quan Report Settings page to specify parameters for flagging values and displaying information in standard report types.
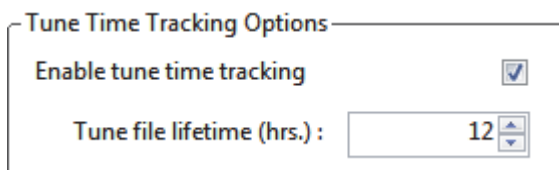
❖ **To specify the concentration calculation method**

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

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

- **Truncated**: Truncates the calculated amount at the number of decimal places specified in the Quan Limits Flags area.

See "To specify quantitation limits" on page 211.

❖ **To track the use of the tune file**

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

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

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

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

Figure 65. Quan Report Settings page

Table 46. Quan Report Settings page parameters (Sheet 1 of 2)

Parameter	Description
Quan Limits Flags	
Report Concentration	Reports the concentration at all times or only when the quantified value exceeds either the limit of detection (LOD), the limit of quantitation (LOQ), or the limit of reporting (LOR). Report concentration: Always, >LOD, >LOQ, or >LOR.
Decimal Places to be Reported	Number of decimal places to be included in the report. Maximum value is 6.
Show Chromatogram on Quantitation Report	Displays a chromatogram (TIC trace) of the sample on the quantitation report.
Display Compounds Above Set Limit	Prints reports for only the compounds that are found in a sample. If a compound is above the specified Quan Flag Options limits, the TraceFinder application reports the compound. This prevents generating "empty" reports for the compounds that are not found.
User Interface Options	
Shade Row When Sample is Outside of Evaluation Criteria	Shades a compound row on any of the reports if a value fails one of the criteria used for evaluation.
Separate Ion Overlay Display	Separates the ion overlay pane from the confirming ion plots in an analysis.
Use Alternate Calibration Report Format	Uses an alternate format for the Calibration Report that is designed to print more concisely (this report is limited to a maximum of seven calibration standards).
Display Quan Flags and Legend	Displays manual flags, confirming manual flags, quantitation flags, and a legend on high-density reports.

Table 46. Quan Report Settings page parameters (Sheet 2 of 2)

Parameter	Description
Quan Flag Options	Values that are above or below limits defined on the Limits page. These flags appear on a variety of reports.
Flag Values Below LOD	Flags values below the limit of detection (LOD).
Flag Values Below LOQ	Flags values below the limit of quantitation (LOQ).
Flag Values Above LOR	Flags values above the limit of reporting (LOR).
Flag Values Above ULOL	Flags values above the upper limit of linearity (ULOL).
Flag Values Above Carryover	Flags values above the carryover limit.
Flag Values Between LOD and LOQ	Flags values between the limit of detection and the limit of quantitation known as the J flag.
Calculated Amount Option	
Calculate Concentration As	Specifies the Rounded or Truncated method for reporting concentration amounts.
Tune Time Tracking Options	
Enable Tune Time Tracking	Tracks the number of hours between the last instrument tune and each sample acquisition.
Tune File Lifetime	Specifies the maximum number of hours between the last instrument tune and a sample acquisition. Any sample acquired outside this maximum allowable time is flagged on the Batch report.

Specifying Target Screening Export Settings (for ToxID Reports)

Use the options on the Target Screening Export Settings page to set the parameters required to produce ToxID reports. For detailed descriptions of the features on the Target Screening Export Settings page, see "Target Screening Export Settings Page" on page 220.

The TraceFinder application uses these parameters to process a raw data file and create a report similar to a ToxID report.

> **Note** The Target Screening Export Settings page is available only when you activate the ToxID features. See "ToxID" on page 65.

Follow these procedures:

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

❖ **To specify the default parameters**

1. Click the Processing Configuration File browse button and select a configuration file (.csv).

2. From the Screening Method list, select one of these compound screening methods.
   - (Default) Auto Detect
   - Based on Full MS2 scans
   - Based on SRM and MS2 scans
   - Based on MS2 and MS3 scans

- Based on MS3 scans
- Based on accurate mass scans
- Based on SRM scans
- Based on Exactive screening method

3. Type the name of the company to print on the report.

4. Type the name of the laboratory to print on the report.

5. Click the Company Logo browse button and select a graphic file (.jpg, .gif, or .bmp) to print on the report.

6. In the *m/z* Window box, enter a value for the window above and below the *m/z* value for the compounds.

7. In the RT Window box, enter a value for the window above and below the retention time value for the compounds.

8. In the MS2 Search Library boxes, type the names of as many as three search libraries for searching MS/MS spectra.

9. In the MS3 Search Library boxes, type the names of as many as three search libraries for searching MS^3 spectra.

10. Select the **Use Full MS Scan to Confirm** check box if you want to confirm library search results with parent ion peak detection in the full scan.

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

❖ **To calculate and report semi-quantitative results**

1. In the Semi Quantitative area, do the following:

   a. Select the **Report Semi-Quantitative Result** check box.

   b. Type the measurement units.

      The measurement units are used only for labeling purposes.

2. Select either the **Scan Intensity** or the **Peak Area** option.

   - Scan Intensity: The application measures the intensity of the MS/MS peak without performing background subtraction.

   - Peak Area: The application measures the peak area of the reconstructed full-scan chromatogram peak of the parent ion. When you select Peak Area, the Use Full MS Scan to Confirm check box is automatically selected.

❖ **To specify the ion ratio calculation method**

> ┌─Ion Ratio Calculation Method (In SRM Experiment):─────────────────────┐
> │ ◉ Use Scan at Peak Apex   ○ Use Average Scan   Ion Ratio Window (%): 20 │
> └──┘

1. Select the **Use Scan at Peak Apex** or the **Use Average Scan** option.

   • Use Scan at Peak Apex: The application calculates the ion ratio based on the peak apex scan spectrum.

   • Use Average Scan: The application calculates the ion ratio based on the average scan spectrum over the range of the peak's half height. The relative intensity in the configuration file must use the selected scan method.

2. In the Ion Ratio Window (%) box, type the acceptable percentage of the intensity of the qualifier ion to the quantitation ion.

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

❖ **To specify the exact mass window**

> ┌─Accurate Mass Experiment:──────────────────────────────┐
> │   │
> │   Exact Mass Window (ppm):   40   │
> │   │
> └──┘

Type a total window width value in parts per million for the Exact Mass Window.

For example, when you expect a mass of 50 with a window of 2, the algorithm creates an XIC based on the responses of all masses from 49 to 51.

❖ **To specify the Exactive parameters**

> ┌─Exactive:───┐
> │ Adduct 1: H+   Adduct 2: NH4+   Adduct 3: Na+ │
> │ ☐ No Specified Retention Time   │
> │   Report Retention Time Based on: ○ First Peak   ◉ Highest Peak │
> │ ☑ Report All Compounds Listed in Configuration File   │
> └──┘

1. Type values for Adduct 1, Adduct 2, and Adduct 3.

   These values identify the adducts listed in and applied throughout the configuration file. Adducts are polarity sensitive. For negative ionization, enter negative adduct values. These values default to H+, NH4+, and Na+, respectively.

   To add or remove adducts from the default lists, see "Specifying Adducts" on page 61.

2. To search the entire raw data file for the specified peak, do the following:

    a. Select the **No Specified Retention Time** check box.

    b. Select either the **First Peak** or the **Highest Peak** option.

        When the search finds more than one *m/z* match in the raw data file, the application uses the specified peak for processing.

3. Select the **Report All Compounds Listed in Configuration File** check box to report all compounds in the configuration file whether or not matches are found for them.

    The default reports on only those compounds where matches are found in the raw data file. This option applies to the Exactive experiment only.

Target Screening Export Settings Page

Use the features on the Target Screening Export Settings page to specify the parameters required to produce ToxID reports.

Figure 66. Target Screening Export Settings page

Table 47. Target Screening Export Settings page parameters (Sheet 1 of 2)

Parameter	Description
Processing Configuration File	Specifies a configuration file (.csv).
Screening Method	Specifies one of the following screening methods: • (Default) Auto Detect • Based on Full MS2 scans • Based on SRM and MS2 scans • Based on MS2 and MS3 scans • Based on MS3 scans • Based on accurate mass scans • Based on SRM scans • Based on Exactive screening method **Note** Using the Auto Detect method, the ToxID application can identify the screening experiment implemented in the acquired data file.
Company Name	Specifies the name of the company to print on the report.
Laboratory Name	Specifies the name of the laboratory to print on the report.
Company Logo	Specifies a graphic file (.jpg, .gif, or .bmp) to print on the report.
m/z Window (mu)	Specifies a value for the window above and below the *m/z* value for the compounds.

Table 47. Target Screening Export Settings page parameters (Sheet 2 of 2)

Parameter	Description
RT Window (min)	Specifies a value for the window above and below the retention time value for the compounds.
MS2 Search Library	Specifies the names of as many as three search libraries for searching MS/MS spectra.
MS3 Search Library	Specifies the names of as many as three search libraries for searching MS^3 spectra.
Use Full MS Scan to Confirm	Specifies that the application confirms library search results with parent ion peak detection in the full scan. When the application does not detect a peak in the full scan, the compound is not reported as a hit.
Semi Quantitative	
Report Semi-Quantitative Result	Includes the semi-quantitative results in the target screening reports.
Measurement Unit	Units used for labeling purposes.
Calculation Based On	Specifies one of the following calculation methods: • Scan Intensity: Specifies that the application measures the intensity of the MS/MS peak without performing background subtraction. • Peak Area: Specifies that the application measures the peak area of the reconstructed full-scan chromatogram peak of the parent ion. When you select Peak Area, the Use Full MS Scan to Confirm check box is automatically selected.
Ion Ratio Calculation Method (In SRM Experiment)	
Use Scan at Peak Apex	Specifies that the application calculates the ion ratio based on the peak apex scan spectrum.
Use Average Scan	Specifies that the application calculates the ion ratio based on the average scan spectrum over the range of the peak's half height. The relative intensity in the configuration file must use the selected scan method.
Ion Ratio Window(%)	Specifies the acceptable ion ratio range.
Accurate Mass Experiment	
Exact Mass Window	Specifies a value in parts per million for the accurate mass experiment.
Exactive	
Adduct 1–n	Specifies the adducts listed in and applied throughout the configuration file. Adducts represent a gain or loss to the neutral mass. For negative ionization, enter negative adduct values. Defaults: Adduct 1: H+, Adduct 2: NH4+, and Adduct 3: Na+
No Specified Retention Time	Specifies either First Peak or Highest Peak to use for processing when the search finds more than one *m/z* match in the raw data file.
Report All Compounds Listed in Configuration File	Specifies that in an Exactive experiment, the application reports all compounds in the configuration file whether or not matches are found for them. Default: Reports only those compounds where matches are found in the raw data file.

Editing a Target Screening Master Method

You can open a target screening master method to specify method instructions, reporting options, peak filter settings, screening databases, identification and confirmation settings, and peak detection parameters.

This section includes instructions for the following tasks:

- Opening a Target Screening Master Method

- Editing the General Page

- Editing the Reports Page

- Editing the Screening Page

- Editing the Peak Detection Page

Opening a Target Screening Master Method

For target screening methods, you select the databases that you want to use in the Compound Databases area of the Target Screening Settings pane. The application lists the compound databases that are stored in the following folder:

…\Thermo\TraceFinder\3.1\Forensic\Databases*filename*.cdb

The target screening method uses only the target list of compounds in the selected compound databases to identify the compounds in the samples.

❖ **To open a saved master method**

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

2. Choose **File > Open > Master Method** from the main menu.
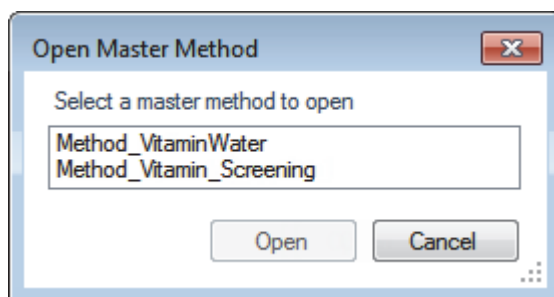
The Open Master Method dialog box opens, displaying all available methods.

Figure 67. Open Master Method dialog box
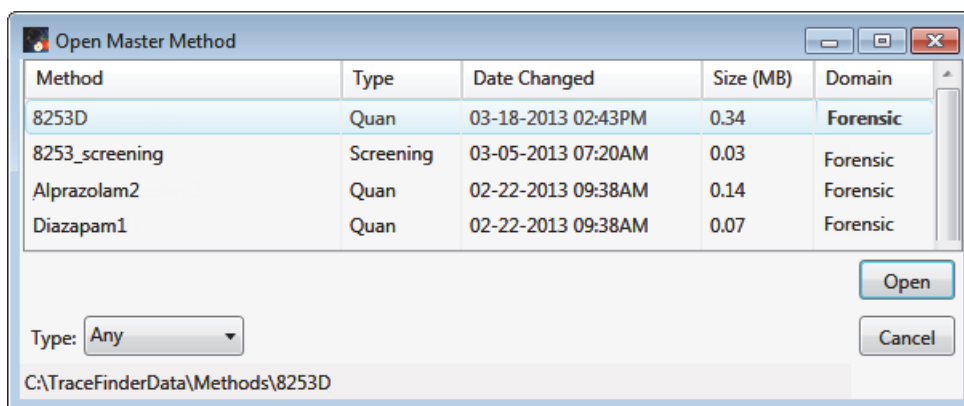
Table 48. Open Master Method dialog box parameters (Sheet 1 of 2)

Parameter	Description
Method	Name of the methods for the selected type.
Type	Type of method: Quan or Screening.

Table 48. Open Master Method dialog box parameters (Sheet 2 of 2)

Parameter	Description
Date Changed	Date the method was last updated.
Size	Size in megabytes.
Domain	TraceFinder domain for which the method was created: General, EFS, Clinical, or Forensic.
Type	Type of method to display: Quan, Screening, or Any.
Path	Path to the selected method in the TraceFinderData\Methods folder.

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

3. Select **Screening** in the Type list.
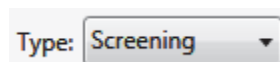
Type: Screening

The method list displays only target screening methods.

4. Select a target screening master method and click **Open**.

The General page for the selected method opens. For detailed descriptions of all the features on the General page, see "General page parameters" on page 228.

The Method View for a target screening method includes General, Reports, Screening, and Peak Detection pages.

Editing the General Page

Use the General page to define basic information about the master method.

❖ **To edit the parameters on the General page**

1. Click **General** in the Method View navigation pane.

   The General page for the screening method opens. See "General Page for a Screening Method" on page 228.

2. In the Lab Name box, type the name to be displayed on the top of each printed, saved, or exported report.

   The default name is Default Laboratory.

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

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

   Range: 0.1 to 2000 µL

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

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

5. From the Mass Precision box, select the number of decimal places to be used in reports and in peak and spectrum displays.

   Valid values: Integers from 2 to 6, inclusive

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

   Instrument method: [AS Method 1 ▼]   [Edit]   [Update]

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

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

Figure 68. Thermo Xcalibur Instrument Setup window
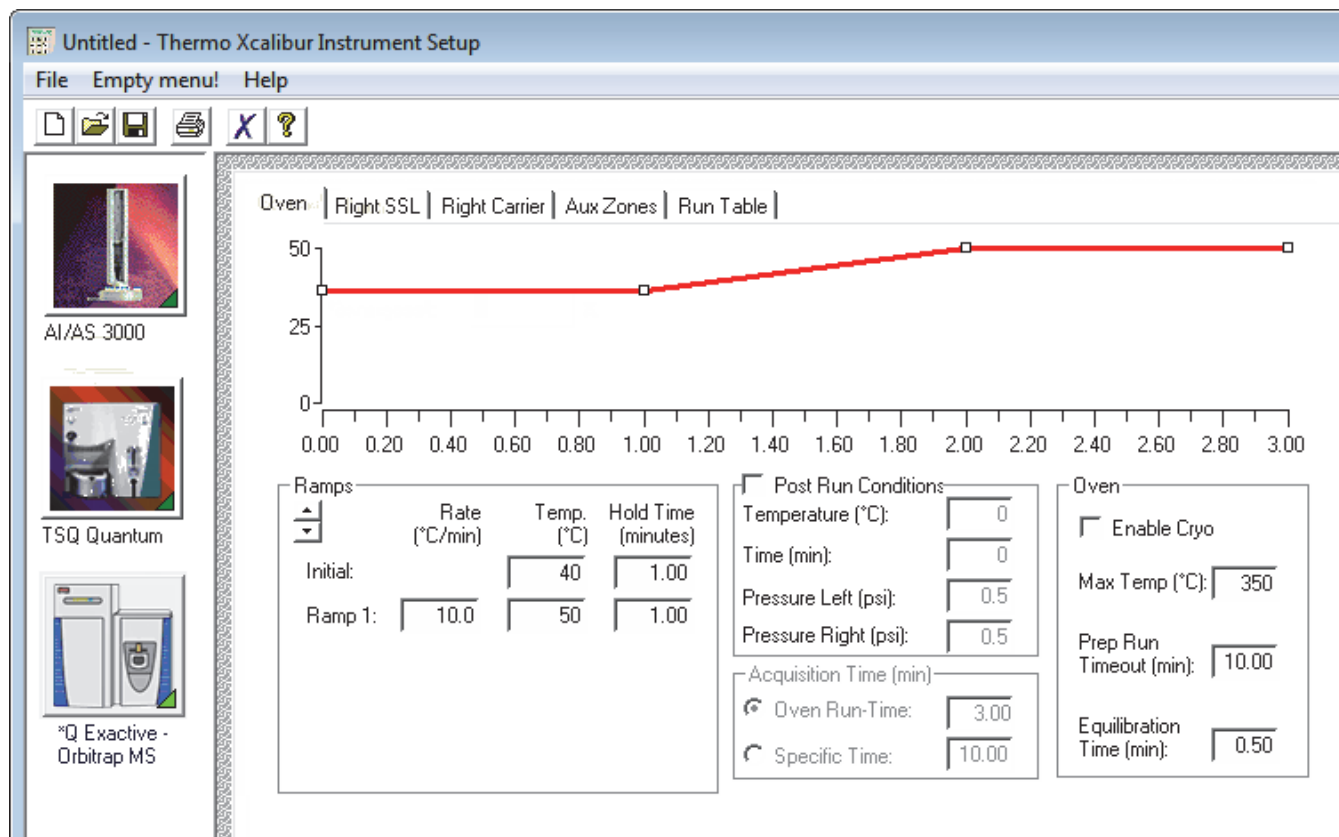
8. Edit the values on the instrument page for your instrument.

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

   The TraceFinder application returns you to the General page of the Method View.

10. Select the units of measure that you want to use.

    • (Default) MMU (millimass units): A static calculation to the extracted mass.

    • PPM (parts per million): A variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.

11. From the Mass Tolerance box, select the number of millimass units or parts per million to use as the *m/z* ± tolerance value.

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

    The application applies this mass tolerance to the extracted chromatograms.

12. From the Library Search Type list, select the type of library to use for target screening.

   - **NIST**: Uses the NIST library that you specified in the Configuration console. See "Screening Libraries" on page 68.

     > **Note** Because the NIST library is large, using this library can slow sample processing.

   - **Library Manager**: Uses the library that you specified in the Configuration console. See "Screening Libraries" on page 68.

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

13. To display all compounds specified in the method, including those that are not found in the sample, select the **Show All Compounds** check box.

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

   You can add a note to explain what makes this method unique.

General Page for a Screening Method

Use the features on the General page to define basic information about the target screening master method.

Figure 69. General page for a screening method

Table 49. General page parameters (Sheet 1 of 2)

Parameter	Description
Lab Name	The laboratory name to be displayed on the top of each printed, saved, or exported report. Default: Default Laboratory To specify this default laboratory name, see "Specifying Application Defaults" on page 45.
Assay Type	The name for the analysis type to be targeted by the method. The assay type associates the method with the analysis of a compound or specific class of compounds (for example, you might use an assay type of PAH for the analysis of Polynuclear Aromatic Hydrocarbons).
Injection Volume	The system uses the injection volume (in µL) for sample injection. For a more detailed explanation, refer to the documentation for the autosampler. The injection volume in the master method overrides the injection volume in the instrument method. The injection volume in the batch overrides the injection volume in the master method. Range: 0.1 to 2000 µL

Table 49. General page parameters (Sheet 2 of 2)

Parameter	Description
Mass Precision	Number of decimal places used in reports and in peak and spectrum displays. Valid values: Integers from 2 to 6, inclusive.
Instrument Method	Instrument method used for acquiring samples.
Edit	Opens the Thermo Xcalibur Instrument Setup dialog box where you can edit the instrument method.
Update	Choose one of the following: **Send to Xcalibur Method**: Overwrites the Xcalibur method with the current instrument method. **Get From Xcalibur Method**: Overwrites the current instrument method with the Xcalibur method.
Mass Tolerance	Upper limit of MMU or PPM. Default: 500 Range: 0.1 through 50 000 • (Default) MMU (millimass units): A static calculation to the extracted mass. • PPM (parts per million): A variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.
Library Search Type	Specifies the type of library to use for target screening. • **NIST**: Uses the NIST library that you installed with the TraceFinder application. See "Installing the NIST and QED Libraries" on page 15. • **Library Manager**: Uses the library that you specified in the Configuration console. See "Screening Libraries" on page 68.
Show All Compounds	Display all compounds specified in the method, including those that are not found in the sample.
Notes	Optional notes about the method.

Editing the Reports Page

Use the Reports page to specify the reports and report output formats that you want to create for the method. See Reports Page for a Target Screening Method.

Follow these procedures:

- To open the Reports page
- To specify report types and output formats

❖ **To open the Reports page**

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

The Reports page for the screening method opens. See "Reports page for a target screening method" on page 231. The reports list displays only the Target Screening report types.

For information about configuring the Target Screening Summary Report or Target Screening High Density Sample Report when you create a target screening method, see "Specifying the Reports" on page 40.

❖ **To specify report types and output formats**

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

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

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

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

All check boxes in the column below the selected cell duplicate the selected or cleared state of the selected cell. This action applies only to reports where this output format is available.

By default, all report types are cleared.

Reports Page for a Target Screening Method

Use the features on the Reports page to specify the reports and report output formats that you want to create for the method.

Figure 70. Reports page for a target screening method

	Example	Report Name	Report Title	Report Type	Print	Create PDF	Create XML	Create XLSM	Batch Level
1	🔎	Batch Report	TS Summary	Target Screening	☐	☐	☐	☐	☑
2	🔎	Batch Report Rev 1	TS Summary	Target Screening	☐	☐	☐	☐	☑
3	🔎	Target Screening Summary Report	TS Summary	Target Screening	☐	☐	☐	☐	☐
4	🔎	Target Screening High Density Sar...	TS Summary	Target Screening	☐	☐	☐	☐	☐

Table 50. Reports page parameters

Parameter	Description
Report list columns	
Example	This option is not available for target screening reports.
Report Name	The name of a report.
Report Title	The user-defined description to be used on a report.
Report Type	In a target screening method, all reports are the Target Screening report type.
Print	Sends reports to the printer.
Create PDF	Saves reports as PDF files.
Create XML	Exports reports as XML files.
Create XLSM	This option is not available for target screening reports.
Batch Level	This option is not available for target screening reports.

Editing the Screening Page

Use the Screening page to specify peak filter settings, screening databases, and identification and confirmation settings for a screening method.

❖ **To open the screening page**

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

The Screening page for the screening method opens. See "Screening Page" on page 245.

This section includes instructions for the following tasks:

- Specifying Peak Filter Settings

- Specifying Compound Databases

- Specifying Identification and Confirmation Settings

Specifying Peak Filter Settings

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

Peak Filter Settings			
Use RT Limits ☐	Search from	0.00	minutes
	to	999.00	minutes
Use Matrix Blank ☐	Amplifier	1.00	
Chromatogram View Width		0.75	minutes
Use Source CID Scans ☐			

❖ **To specify peak filter settings**

1. To set a retention time range that excludes searching for peaks outside the range, do the following:

   a. Select the **Use RT Limits** check box.

   The application activates the Search From and To options.

   b. In the Search From box, enter the lower limit; in the To box, enter the upper limit.

2. To use one or more negative samples for subtraction to filter the resulting peaks, do the following:

   a. Select the **Use Matrix Blank** check box.

   The application activates the Amplifier option.

During automatic processing, the TraceFinder application subtracts the areas of the peaks in the negative samples from the matching areas in the specimen samples.

To determine the pair of peaks to subtract from each other, the application selects the two peaks with the mass and the retention time that are closest to each other (as defined in the compound database), within the mass tolerance specified in the method.

When the same compound peak (same mass and retention time within the predefined tolerance windows) is in multiple selected negative samples, the application subtracts only the one with the highest area.

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

When no negative sample exists in the sequence, or if one or more negative samples exist but you do not select the Use Matrix Blank check box, then subtraction does not occur. If subtraction occurs and the subtracted area is less than 0, the application sets the subtracted area to 0.

b. In the Amplifier box, type an amplifier value.

Use the up/down arrows to change the value in increments/decrements of 1 unit, or use the keyboard to enter non-integer values.

The TraceFinder application multiplies a negative area by this value before performing subtraction. The larger the amplifier value, the more peaks the application filters from the final results.

In the Batch View for sequences created with this method, you can select which negative samples to use for subtraction. See "Blank Subtraction in Target Screening Batches" on page 397.

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

4. To use source CID scans for target screening confirmation (fragment ion or library search), select the **Use Source CID Scans** check box.

When you select this check box, the TraceFinder application uses the source CID scans when they are available in the data file. If they are not available, then the application uses AIF or MS/MS scans when available.

Specifying Compound Databases

The Target Screening Settings pane displays the compound databases stored in the following folder:

…\Thermo\TraceFinder\3.1\Forensic\Databases

❖ **To specify compound databases**

1. Select the **Enabled** check box for at least one compound database.

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

   a. Edit the database.

      See "Editing Compounds in the Database" on page 285.

   b. When you finish editing the database, click **Screening** in the Method View navigation pane to return to the Screening page.

Specifying Identification and Confirmation Settings

By default, the TraceFinder application uses the mass-to-charge ratio (*m/z*) for filtering compound peaks. In the Identification and Confirmation Settings area, you can select additional criteria to help increase confidence using either of the following:

- Compound identification for identifying a sample compound as a minimum requirement for a match to be displayed in the results.

  To identify a compound, the application searches within the specified RT window (or the RT window override if specified in the method) and compares the measured *m/z* of the sample peak against the expected *m/z* of the target compound. When the sample peak's *m/z* is within the default ±5 ppm tolerance of the target compound's *m/z*, the application considers that this target compound is identified.

- Compound confirmation for confirming a sample compound and to increase confidence in the match results.

  To confirm a compound, the application searches the entire raw data file and compares the measured *m/z* of the sample peak against the expected *m/z* of the target compound. When the sample peak's *m/z* is within the tolerance of the target compound's *m/z*, the application considers that this target compound is confirmed.

❖ **To specify identification and confirmation settings**

1. To set a target threshold override and include only peaks with areas above this designated threshold, do the following:

   a. Select the **Threshold Override** check box.

   b. In the associated box, type the threshold as an area value.

      This threshold overrides the Response Threshold value set in the compound database. The application ignores the peaks with areas below your specified threshold.

   c. To include only peaks with signal-to-noise ratios (S/Ns) that are above a specified value, in the S/N Ratio Threshold box, type the threshold as a ratio value.

      The application ignores the peaks with S/Ns that are below the specified threshold.

2. To specify the Retention Time option, do the following:

   a. Select either the **Identity** or **Confirm** check box.

   b. Select the **Window Override** check box and type the window value.

      This window overrides the RT Window value that was set in the compound database and includes only peaks within this designated window. The application identifies or confirms the presence of a compound only when its measured retention time matches the target compound's expected retention time within the specified Window Override retention time.

   For additional information about how the application identifies retention time, see "Retention Time" on page 240.

3. To specify the Fragment Ions option, do the following:

   a. Select either the **Identity** or **Confirm** check box.

   b. To ignore the Fragment Ions options when no fragment is defined in the compound database, select the **Ignore if Not Defined** check box.

      When the compound database does not define fragments for a compound, the application does not include the results of identification or confirmation for fragment ions in the target screening results.

   c. In the Min. # of Fragments box, type the minimum number of fragments required to identify or confirm the presence of a compound.

   d. In the Intensity Threshold box, type the intensity threshold value.

      The intensity of a fragment must be above this threshold to be identified or confirmed.

e. In the Mass Tolerance box, type a mass tolerance value and then select **ppm** or **mmu** for the mass tolerance units.

This mass tolerance value indicates the number of millimass units or parts per million to use as the *m/z* ± tolerance value for the fragment ions. It is separate from the mass tolerance value specified for the parent. See "Editing the General Page" on page 225.

> **Note** When using ion trap data, the application uses 300 mmu regardless of the value you enter here.

For additional information about how the application identifies fragment ions, see "Fragment Ions" on page 241.

4. To specify the Isotopic Pattern option, do the following:

a. Select either the **Identity** or **Confirm** check box.

b. In the Fit Threshold box, type the fit threshold percentage.

To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

c. In the Allowed Intensity Deviation box, type a value to specify the allowed intensity deviation of the mass spectrometer relative to the monoisotopic ion, as a percentage of the base peak height.

The TraceFinder isotopic pattern algorithm considers an isotope peak as not found if its intensity, relative to the monoisotopic ion's intensity, is more than the deviation percentage from the theoretical relative intensity of the isotope ion. For best results, set this value to a number that causes up to 98% of all intensity deviations to be smaller than the allowed intensity deviation value.

d. To specify that isotopic pattern calculations use internal mass calibration instead of external mass calibration, select the **Use Internal Mass Calibration** check box.

When this check box is selected, the application applies a requirement that an isotope's *m/z* must be closer to its theoretical value to avoid a score penalty.

For additional information about how the application calculates isotopic pattern scores, see "Isotopic Pattern" on page 242.

5. To specify the Library Search option, do the following:

a. Select either the **Identity** or **Confirm** check box.

b. Type the threshold value in the Score Threshold box.

The resulting score percentage from a library search match must be higher than your entered threshold value to identify or confirm the presence of a compound.

For additional information about how the application performs library searches, see "Library Search" on page 243.

Understanding the Identification and Confirmation Process

The TraceFinder application processes identification and confirmation settings in a specific order. When a compound passes identification at each point in the order of processing, the application continues to the next automatic or selected identification or confirmation test.

> **Note** When you select the Ignore if Not Defined option and the related data is not defined in the compound databases, the application skips that criteria test.

When a compound fails identification at a point in the processing, the application skips the testing of all remaining criteria, even when they are selected, and the flags for those criteria are blank.

The TraceFinder application processes identification and confirmation settings in the following order:

1. *m/z* and Retention Time

   The application automatically identifies the mass to charge ratio for all compounds. When you select the Retention Time settings, the compound must pass this criteria first. When a compound fails the *m/z* or the Retention Time identification test, the application does not perform identification or confirmation testing for any other selected criteria lower in the processing order.

   For additional information about the *m/z* and Retention Time parameters, see "Mass to Charge (m/z)" on page 239 and "Retention Time" on page 240.

2. Threshold

   The application automatically identifies the default area threshold (5000) for the compound after the compound passes the *m/z* and Retention Time criteria. When you specify a Threshold Override, the application uses the specified threshold value instead.

   When a compound fails the Threshold identification test, the application does not perform the selected Fragment Ions or Library Search testing for identification or confirmation.

   For additional information about the Threshold parameter, see "Threshold" on page 239.

3. Isotopic Pattern

   For additional information about the Isotopic Pattern parameter, see "Isotopic Pattern" on page 242.

4. Fragment Ions

   For additional information about the Fragment Ions parameter, see "Fragment Ions" on page 241.

5. Library Search

   For additional information about the Library Search parameter, see "Library Search" on page 243.

Mass to Charge (*m/z*)

The application automatically uses the *m/z* and mass tolerance values to identify each compound, using the mass tolerance value you specified on the General page. See "Editing the General Page" on page 225.

The application compares the measured *m/z* of the sample peak against the expected *m/z* of the target compound. When the measured *m/z* is within the mass tolerance of the expected *m/z*, the application considers that this target compound is found and the *m/z* criteria passes.

On the Target Screening page in Data Review, the MZ column in the Compounds table indicates whether this criteria passes or fails. The Flag column indicates whether the target compound is identified, fully confirmed, or both. For details, see "Compounds Pane" on page 465.

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

Threshold

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

In the Identification and Confirmation Settings pane, you can specify a threshold override to use instead of the area threshold defined in the compound database.

The application compares the area of the sample peak against the defined area thresholds. When the sample peak's area is greater than or equal to the corresponding area threshold from the compound database or the override area threshold, the target compound is identified.

On the Target Screening page in Data Review, the Flag column in the Compounds table indicates whether this criteria passes or fails. The Flag column indicates whether the target compound is identified, fully confirmed, or both. For details, see "Compounds Pane" on page 465.

The Compounds table also displays Measured Area column displays the area value in green to indicate that the peak's area is greater than or equal to the area threshold; otherwise, this column displays the area value in red.

Retention Time

The application uses the expected retention time and retention time window values defined in the selected compound database to identify or confirm each sample compound.

In the Identification and Confirmation Settings pane, you can set an override retention time window value to use instead of the retention time window specified in the compound database.

When the compound database defines an expected retention time for a compound, it uses the following process to identify or confirm the compound.

- Identify: the application searches within the specified retention time window (or the retention time window override) and compares the measured *m/z* of the sample peak against the expected *m/z* of the target compound. When the measured *m/z* is within the mass tolerance of the expected *m/z*, this target compound is identified.

- Confirm: the application searches the entire raw data file and compares the measured *m/z* of the sample peak against the expected *m/z* of the target compound. When the measured *m/z* is within the specified mass tolerance of the expected *m/z*, the target compound is confirmed.

When the compound database does not define an expected retention time for a compound, the application cannot identify or confirm the compound. If you select the Ignore if Not Defined option, the application does not perform testing for the retention time and the RT flag is blank on the Target Screening page in Data Review.

On the Target Screening page in Data Review, the RT column in the Compounds table indicates whether this criteria passes or fails. The RT column indicates whether the target compound is identified, fully confirmed, or both. For details, see "Compounds Pane" on page 465. The Compounds table also displays the RT Expected, RT Measured, and RT Delta values for each compound.

Fragment Ions

To use fragment ions for identification or confirmation, the application requires the following conditions:

- The selected compound databases contain the charged mass for each defined fragment ion of interest for the compounds in the target list.

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

When no fragment is defined in a compound database for a target compound, the following apply:

- When the Ignore if Not Defined option is selected in the method, the application does not perform filtering for the Fragment Ions. In the Data Review view, the FI column is blank.

- When the Ignore if Not Defined option is not selected in the method, the application considers that this target compound is not identified. The Fragment Ions filter fails.

- When the Ignore if Not Defined option is selected in the method, the application does not perform filtering for the Fragment Ions and, in the Data Review view, the FI column is blank.

The application uses the number of fragment masses defined in the compound database when it processes a sample for fragment ions. The value you specify for Min. # of Fragments cannot be greater than the number of fragments defined in the compound database.

For example, if a compound has three fragment ion masses defined in a compound database, any of the following scenarios can occur:

- You enter "2" in the Min. # of Fragments box of the screening method, and the application finds at least two out of the three defined fragment ions. The Fragment Ions filter passes.

- You enter "4" in the Min. # of Fragments box of the screening method, and the application finds only the three defined fragment ions. The Fragment Ions filter fails.

- You enter "2" in the Min. # of Fragments box of the screening method, but the application finds only one of the three defined fragment ions. The Fragment Ions filter fails.

The application repeats the following process for each of the fragment ions:

1. When the mass of the parent (plus or minus half of the isolation window value from the acquired raw data file) is not within the mass range of the extracted ion chromatogram shown in the Chromatogram pane of the Data Review view, the application considers the fragment ion as not found and the application fails the Fragment Ions filter; otherwise, the application continues.

2. The application inspects the processed fragment ion scan closest to the target compound's expected retention time and locates the MS/MS spectrum closest to the compound's apex.

Within this spectrum, the application finds the intensity for the tallest fragment whose mass is within the mass tolerance of an entered fragment ion mass. When this intensity is not found or when it is less than the intensity threshold defined in the screening method, the application determines that the entered fragment ion is not found; otherwise, it determines that the fragment ion is found.

Isotopic Pattern

You can choose to either identify or confirm the isotopic patterns for all compounds in a batch. The TraceFinder application calculates an isotopic pattern score (as a percentage value), using the target compound's formula.

For the isotopic pattern filter, enter the isotopic pattern parameters, including a fit threshold value, in the processing method. To identify or confirm the presence of a compound, the resulting score from isotopic pattern matching must be higher than the fit threshold.

To identify or confirm an isotopic pattern, the application must detect the compound for at least one of its defined adduct ions. The application identifies the elemental composition to match using the formula that is associated with the most intense adduct peak. The application then generates an isotopic pattern score (as a percentage value) for the match between the measured and expected isotopic patterns of the calculated elemental composition.

- For profile data, the application calculates the measured isotopic pattern using the average of all scans (within the allowed intensity deviation of the spectrum closest to the compound's apex retention time). In the Data Review view, the application displays both the expected and measured spectra in the profile mode.

- For centroid data, the application calculates the measured isotopic pattern using the apex scan. In the Data Review view, the application displays the expected spectra in the centroid mode.

A high isotopic pattern score (approaching 100 percent) occurs when the measured isotope patterns, the expected isotope patterns, and the intensities are almost identical using the scoring parameters specified in the processing method. When the patterns are not similar, the score is closer to 0 percent. When the score is greater than or equal to your entered fit threshold and the number of isotopes matched is not 1 out of 1, this filter passes.

When you view results in the Data Review view, the IP column displays a green or red flag to indicate whether the compound passed or failed based on the criteria specified in the method.

Library Search

For a target screening analysis, you can select the Library Search criterion for either identification or confirmation in the processing method. The TraceFinder application identifies or confirms the sample compound by searching the selected library and returning the library entry with the highest score (as a percentage value) for the fragment ion spectrum in that library that matches the compound's ion spectrum.

- For this criterion, you enter a score threshold value in the processing method. The resulting score from a library search match must be higher than your entered threshold value, and the library entry must match a compound's name, a compound's formula, or both to identify or confirm the presence of the compound.

The application uses the following logic to determine when a match is successful:

- When a formula is available in the library entry and the formula matches the target compound formula:

  - The criteria passes when the library score is higher than or equal to the score threshold.

  - The criteria fails when the library score is lower than the score threshold.

- When a formula is available in the library entry and the name in the library entry matches the target compound name but the formula does not match the target compound formula (or it is not available):

  - The criteria passes when the library score is higher than or equal to the score threshold.

  - The criteria fails when the library score is lower than the score threshold.

- When neither the formula nor the library entry name match the target compound, the criteria fails and the Lib Match Name, Library Score, and Library Match Rank columns display N/A in black text.

  > **Note** When the compound is identified, but no MS/MS scan has been performed, the Lib Match Name, Library Score, and Library Match Rank columns display N/A in red text.

- When an MS/MS scan has been performed and both the library entry and the formula match the target compound:

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

  - The criteria fails when the library score is lower than the score threshold. The Lib Match Name, Library Score, and Library Match Rank columns display their values in red text.

To use a library search for identification or confirmation, the TraceFinder application requires that the data meet these conditions:

- The raw data file contains HCD (higher energy collision-induced dissociation), source CID (source collision-induced dissociation), or AIF (all ions fragmentation) ion spectra.

- The spectra exist at a time point within the compound's elution time range.

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

When a parent-selected MS/MS spectrum does not exist, the application performs a reverse library search because the compound scan contains a mixture of fragments from all co-eluting parents. A forward search with such a mixture biases the results toward the strongest parent because its fragments would be dominant, and a forward search also takes more time because the application must search every spectrum in the library.

When a parent-selected MS/MS spectrum exists, the application performs a forward library search because the scan usually contains fragments of only one or two parents, so matching this spectrum against the library is faster and more accurate. When you select the Use Reverse Library Searching Only check box in the processing method, the application performs only a reverse library search.

When you use profile data, the application uses the averaged spectrum of the unknown peak as the input spectrum for the library search. This averaged spectrum is based on the average of all scans within 10 percent of the spectrum closest to the peak's apex retention time. When you use centroid data, the application uses the apex scan as the input spectrum for the library search.

When the application locates a match, it generates a score percentage for the matching library entry. This library search can result in multiple matches with different scores.

After searching based on the *m/z* in the input spectrum, the application performs another search for only the matches from the first library search, but this time based on the name, and then the formula, of the target compound. If at least one match is found, the application displays the highest scoring match from the second search for data review. If no match is found from the second search, the application displays the highest scoring match from the first search.

Screening Page

Use the features on the screening page to specify peak filter settings, screening databases, and identification and confirmation settings for a screening method.

Figure 71. Screening page for a target screening method

Table 51. Screening page parameters (Sheet 1 of 4)

Parameter	Description
Peak Filter Settings	
Use RT Limits	Specifies a lower and upper limit for searches. Ranges: 0.00 to 999.99 minutes Default: 0.00 minutes for lower limit; 999.00 minutes for upper limit
Use Matrix Blank	Specifies that during automatic processing, the TraceFinder application subtracts the areas of the peaks in the selected negative samples from the matching areas in the specimen samples.
Amplifier	The application multiplies a negative area by this value before performing subtraction. The larger the amplifier value, the more peaks the application filters from the final results. Range: .01 to 1000.00 Default: 1.00
Chromatogram View Width	Specifies a a window width to define the chromatogram viewing range in the Data Review view. Range: 0.10 to 999.00 minutes Default: 0.75 minutes
Use Source CID Scans	Specifies that the application use the source CID scans when they are available in the data file. If they are not available, then the application uses AIF or MS/MS scans when available.
Compound Databases	
Enabled	Specifies databases to use for target screening processing.
Database Name	Lists available databases in the Databases folder.
Identification and Confirmation Settings	
Peaks	Specifies that the application use the mass-to-charge ratio (*m/z*) for filtering compound peaks.
Threshold Override	This threshold overrides the Response Threshold value set in the compound database. The application ignores the peaks with areas below this specified threshold. Range: 1000 to 1 000 000 000 Default: 5000
S/N Ratio Threshold	Includes only peaks with signal-to-noise ratios (S/Ns) above the specified value. Range: 1.0 to 100 000 Default: 5.0

Table 51. Screening page parameters (Sheet 2 of 4)

Parameter	Description
Retention Time	Specifies either the Identify or Confirm option for a retention time search. To identify a compound, the application searches the specified RT window for a match. To confirm a compound, the application searches the entire raw data file.
Ignore if Not Defined	Ignores the values you specify for Retention Time options when no retention time is defined in the compound database, and does not include the results of identification or confirmation for retention time in the Data Review target screening results.
Window Override	Specifies the number of seconds to override the RT Window value set in the compound database and include only peaks within this designated window. The application identifies or confirms the presence of a compound only when its measured retention time matches the target compound's expected retention time within the specified Window Override retention time. Range: 0 to 999 seconds Default: 30 seconds
Fragment Ions	Specifies either the Identify or Confirm option for a fragment ion match. To identify a fragment, the application searches the specified RT window for a match. To confirm a fragment, the application searches the entire raw data file.
Ignore if Not Defined	Ignores the values you specify for Fragment Ions options when no fragment is defined in the compound database, and does not include the results of identification or confirmation for fragment ions in the Data Review target screening results.
Min. # of Fragments	Specifies the minimum number of fragments required to identify or confirm the presence of a compound. Range: 1 to 5 Default: 1
Intensity Threshold	Specifies the minimum height of a fragment ion peak. The peak of a fragment ion must be above this intensity threshold to be identified or confirmed. Range: 1 to 1e9 Default: 10 000

Table 51. Screening page parameters (Sheet 3 of 4)

Parameter	Description
Mass Tolerance	Specifies the number of millimass units or parts per million to use as the *m/z* ± tolerance value for the fragment ions and is separate from the mass tolerance specified for the parent (see "Editing the General Page" on page 225). Range: 0 to 500 Default: 5 Unit: mmu or ppm **Note** When using ion trap data, the application uses 300 mmu regardless of the value you enter here.
Isotopic Pattern	Specifies either the Identify or Confirm option for an isotopic pattern match. To identify a compound, the application searches the specified RT window for a match. To confirm a compound, the application searches the entire raw data file.
Fit Threshold	To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage. Default: 90%
Allowed Mass Deviation	Specifies the allowed mass deviation in the spectrum data. The TraceFinder isotopic pattern algorithm considers an isotope peak as found if its measured *m/z* is less than this amount away from its expected *m/z*. For best results, set this value to a number that causes up to 98 percent of all mass deviations to be smaller than the allowed mass deviation value. Range: 3 to 100 ppm Default: 3 ppm
Allowed Intensity Deviation	Specifies the allowed intensity deviation of the mass spectrometer, relative to the monoisotopic ion, as a percentage of the base peak height. The TraceFinder isotopic pattern algorithm considers an isotope peak as not found if its intensity relative to the monoisotopic ion's intensity is more than this deviation percentage from the theoretical relative intensity of the isotope ion. For best results, set this value to a number that causes up to 98% of all intensity deviations to be smaller than the allowed intensity deviation value. Default: 10%
Use Internal Mass Calibration	Specifies that the application require an isotope's *m/z* to be closer to its theoretical value to avoid a score penalty.

Table 51. Screening page parameters (Sheet 4 of 4)

Parameter	Description
Library Search	Specifies either the Identify or Confirm option for a library search. To identify a compound, the application searches the specified RT window for a match. To confirm a compound, the application searches the entire raw data file.
Score Threshold	The resulting score percentage from a library search match must be higher than your specified threshold value to identify or confirm the presence of a compound. Default: 80%
Use Reverse Library Searching Only	Compares a library entry to an unknown compound (a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry). This option is available for both NIST and Library Manager searches.

Editing the Peak Detection Page

The TraceFinder application can use any of the following peak detection algorithms: Genesis, ICIS, or Avalon.

❖ **To specify peak detection parameters**

1. Click **Peak Detection** in the Method View navigation pane.

   The Peak Detection page for the screening method opens.

2. Select a detection algorithm: Genesis, ICIS, or Avalon.

   • The Genesis peak detection algorithm is provided for backward compatibility with Xcalibur 1.0 studies.

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

   • The Avalon peak detection algorithm is designed for integrating UV/Vis and analog chromatograms.

3. Specify the peak detection parameters for your method.

   Figure 72. Parameters on the Genesis peak detection page for a target screening method

   Genesis peak detection parameters for screening methods are the same as for quantitation methods. See "Detect page parameters for Genesis" on page 153.

Figure 73. Parameters on the ICIS peak detection page for a target screening method

ICIS peak detection parameters for screening methods are the same as for quantitation methods. See "Detect page parameters for ICIS" on page 157.

Figure 74. Parameters on the Avalon peak detection page for a target screening method

Avalon peak detection parameters for screening methods are the same as for quantitation methods. See "Detect page parameters for Avalon" on page 159.

Saving a Master Method to a New Name

You can save any quantitation or target screening method to a new name, or you can use the current method data to overwrite an existing method. The new method contains all the data of the saved method.

❖ **To save a method to a new name**

1. From the main menu, choose **File > Save As.**

   The Save Master Method As dialog box opens, displaying all quantitative and target screening methods.

Method	Type	Date Changed	Size (MB)	Domain
8253B_screening	Screening	03-18-2013 06:33AM	0.03	General
8253_quan	Quan	03-18-2013 06:25AM	0.13	General
8253_screening	Screening	03-05-2013 07:20AM	0.03	EFS

   New Method 8253B_screening

   C:\TraceFinderData\Methods\8253B_screening
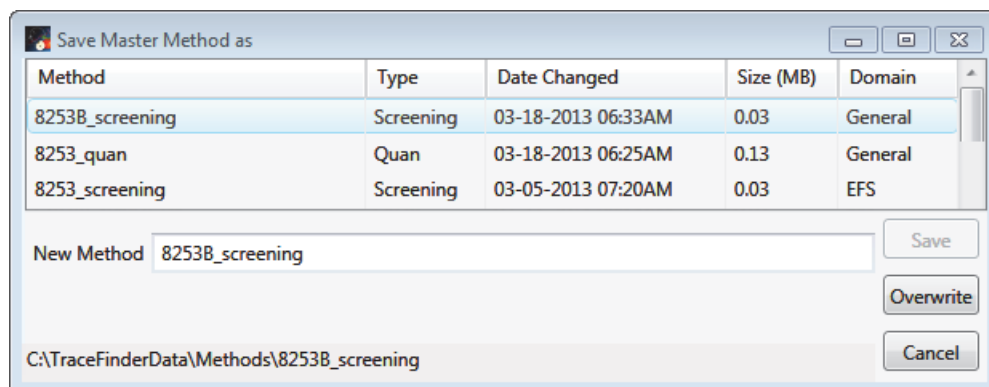
Table 52. Save Master Method As dialog box parameters

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

2. Do one of the following:

   • In the New Method box, type a name for the new method.

     The application enables the Save button.

   • In the Method column, select a method to overwrite.

     The application enables the Overwrite button.

3. Click **Save** or **Overwrite**.

   The application saves all the method data to the specified name and opens the General page of the new method.

Creating a Method Template

In the TraceFinder application, you can create a processing method using a method template that contains common settings. You can create a method template that specifies peak detection criteria, screening libraries, confirming ion criteria, compound calibration, and qualitative peak processing. For a complete description of the features on the Method Template Editor, see "Method Template Editor" on page 261.

The application uses the settings in the method template to identify the data to display in the Qualitative View. See "Qualitative View" on page 483.

Only quantitation methods use method templates. Target screening methods do not use method templates.

Follow these procedures:

- To open the Method Template Editor

- To specify peak criteria

- To identify the peaks

- To specify confirming ions

- To calibrate the compounds

- To enter a note for the method

- To save the method template

❖ **To open the Method Template Editor**

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

   Method Development

   The Method Development navigation pane opens.

2. Click **Method View**.

   ▼ Method View   ❯

3. From the main menu, choose **File > New > Method Template**.

   The Method Template Editor opens. See "Method Template Editor" on page 261.

❖ **To specify peak criteria**

* These parameters may also be used for qualitative peak processing.

1. In the Find the Peaks area, select a sensitivity level.

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

   • The Genesis peak detection algorithm is provided for backward compatibility with Xcalibur 1.0 studies.

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

   • The Avalon peak detection algorithm is designed for integrating UV/Vis and analog chromatograms.

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

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

   To consider a peak for a processing method, the TraceFinder application uses the Enable Peak Threshold filter to determine which peaks meet the specified percentage of the height or area of the largest peak.

4. To display a specific number of the largest peaks by height or area, select the **Only Select Top Peaks** check box and enter the number of peaks to display.

❖ **To identify the peaks**

Identify the peaks*

Use these libraries

☑ NISTDEMO
☑ QED NIST Library

Limit library hits: 3

Best match method: Reverse Search Index

* These parameters may also be used for qualitative peak processing.

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

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

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

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

❖ **To specify confirming ions**

Handle confirming ions

☑ Include confirming ions
   Number of confirming ions: 2

☑ Specify default ion ratio ranges
   Ion coelution (min): 0.025
   Window type: Absolute
   Window(+/- %): 20.00

☑ Include compound peak spectrum as reference spectrum

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

   This value is the number of other ions in the spectrum whose ratio is compared to the quantitation ion. Using this ratio, you can then determine if it is the target compound or something else. You can set this value to integers from 1 to 10, inclusive. This value defaults to **2** because you typically perform a 3-ion experiment with one quantitation mass and two confirming ions.

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

2. To define the criteria for evaluating confirming or qualifying ions, select the **Specify Default Ion Ratio Ranges** check box and set the following values:

   a. To specify the maximum difference in retention time between a confirming ion peak and the quantification ion peak, set a value in the Ion Coelution (min) box.

   b. To specify an absolute or relative calculation approach for determining the acceptable ion ratio range, select **Absolute** or **Relative** from the Window Type list.

   c. To specify the acceptable ion ratio range, set a value in the Window (+/– %) box.

3. To include the peak spectrum in the processing method, select the **Include Compound Peak Spectrum as Reference Spectrum** check box.

❖ **To calibrate the compounds**

1. From the Calibration Method list, select **Internal** or **External**.

2. From the Curve Type list, select one of the following:

   - **Linear**: All other settings are available with this exception: When you select Include in the Origin list, the Weighting parameter is unavailable.

   - **Quadratic**: All other settings are available with this exception: When you select Include in the Origin list, the Weighting parameter is unavailable.

   - **Average RF**: The Weighting and Origin parameters are unavailable.

3. From the Origin list, select one of the following:

   - **Ignore**: Specifies that the origin is not included as a valid point in the calibration curve when the curve is generated. When you select Ignore, the calibration curve might or might not pass through the origin.

   - **Force**: Specifies that the calibration curve passes through the origin of the data point plot when the calibration curve is generated.

   - **Include**: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select Include, the calibration curve might or might not pass through the origin.

4. From the Weighting list, select one of the following:

- **Equal**: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select Equal, the calibration curve might or might not pass through the origin.

- **1/X**: Specifies a weighting of 1/X for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their quantity.

- **1/X^2**: Specifies a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity.

- **1/Y**: Specifies a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio).

- **1/Y^2**: Specifies a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).

5. From the Response Via list, select **Area** or **Height**.

- **Area**: Specifies that the TraceFinder application use this area value in response calculations.

- **Height**: Specifies that the application use this height value in response calculations.

❖ **To specify qualitative peak processing**

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

The application uses the Genesis algorithm to match internal standards in a range plus/minus the value that you specify. For additional information about the Genesis algorithm, see "Genesis Detection Method" on page 51.

This parameter is available only when you set the Sensitivity parameter in the Find the Peaks area to **ICIS** or **Avalon**. When you select the Use Genesis Algorithm for Qual Processing check box, the application ignore the Sensitivity parameter in the Find the Peaks area.

2. Select or clear the **Exclude Matching Quan Peaks** check box and specify a value for the exclusion window.

   The application excludes quantitative peaks in a range plus or minus the value that you specify.

3. To process samples that include data-dependent scans, select the **Use Data Dependent Scans** check box.

   When you process a sample using this feature, the application uses the TIC trace to find all data-dependent full scans, lists them, and performs a library search against the data-dependent MS/MS or MS^n scan.

   This option constrains the Data Review to only data-dependent scan spectra. See "Working in the Report View" on page 555.

   In addition to the peak information, the TIC Report and TIC Summary Report display information about the data-dependent filtered data. See Appendix A, "Reports."

4. To indicate whether to select peaks above a minimum percentage of the nearest internal standard peak that results in compound selection, select the **Enable ISTD Threshold** check box and specify a minimum percentage.

   To consider a peak for a processing method, the TraceFinder application uses the Enable ISTD Threshold filter to determine which peaks meet the specified percentage of the height of the nearest internal standard peak.

   When you select the Enable ISTD Threshold parameter, the method ignores values set for the Enable Peak Threshold and Only Select Top Peaks parameters. See "To specify peak criteria" on page 255.

   > **Note** When you create a method with the Method Forge, the application ignores the parameters in the Qualitative Peak Processing area.

❖ **To enter a note for the method**

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

You can add a note to your method template to explain what makes this template unique.

❖ **To save the method template**

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

   The Save Method Template dialog box opens.

2. Do one of the following:

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

   –or–

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

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

   …\TraceFinderData\Templates\Methods\Forensic

   Saved method templates are available when you create a method using Method Forge. See .

Method Template Editor

Use the features on the Method Template Editor to specify peak detection criteria, screening libraries, confirming ion criteria, compound calibration, and qualitative peak processing.

Figure 75. Method Template Editor dialog box

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

Parameter	Description
Find the peaks	
Sensitivity	Defines how extensively the peak detector algorithm searches for low-level peaks.
Limit the Retention Time Range	Min RT specifies the beginning of the range. Max RT specifies the end of the range.
Enable Peak Threshold	Specifies whether to select peaks by relative height or area and the percentage of the highest peak that results in compound selection.
Only Select Top Peaks	Displays a specific number of the largest peaks by height or area.
Identify the peaks	
Use These Libraries	Lists the libraries that you can search.
Limit Library Hits	Specifies the number of hits returned when the system searches a spectrum against the selected libraries.
Best Match Method	Specifies how to sort the library searches. Valid values: Search Index, Reverse Search Index, Match Probability
Handle confirming ions	
Include Confirming Ions/ Number of Confirming Ions	Specifies the number of confirming ions, which are other ions in the spectrum whose ratio is compared to the quantitation ion to identify the compound. This value defaults to 2 because you typically perform a 3-ion experiment with one quantitation mass and two confirming ions. Range: Integers from 1 to 10, inclusive.
Specify Default Ion Ratio Ranges	Enables the ion ratio range features. Ion Coelution specifies the maximum difference in retention time between a confirming ion peak and the quantification ion peak. Window Type specifies an Absolute or Relative calculation approach for determining the acceptable ion ratio range. Window (+/-%) specifies the acceptable ion ratio range.
Include Compound Peak Spectrum as Reference Spectrum	Includes the peak spectrum in the processing method. Use this setting to perform a spectra comparison in Data Review.
Calibrate the compounds	
Calibration Method	Specifies an internal or external calibration method.
Curve Type	Specifies a linear, quadratic, or average RF curve type.

Table 53. Method Template Editor dialog box parameters (Sheet 2 of 3)

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

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

Parameter	Description
Use Data Dependent Scans	Constrains the Data Review to only data-dependent scan spectra. See "Working in the Report View" on page 555. In addition to the peak information, the TIC Report and TIC Summary Report display information about the data-dependent filtered data.
Enable ISTD Threshold	Specifies that, when identifying a peak, qualitative peak processing use the minimum threshold specified as a percentage of the nearest internal standard peak, rather than the threshold specified in the Enable Peak Threshold and Only Select Top Peaks parameters. See Enable Peak Threshold or Only Select Top Peaks in this parameter table.
% of Internal Standard	Percentage of the nearest internal standard peak to use as the minimum threshold for identifying a peak.

Importing Published Master Methods

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

…\Thermo\TraceFinder\3.1\Forensic\Published Master Methods

❖ **To import a published master method**

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

   The Import Published Method dialog box opens.
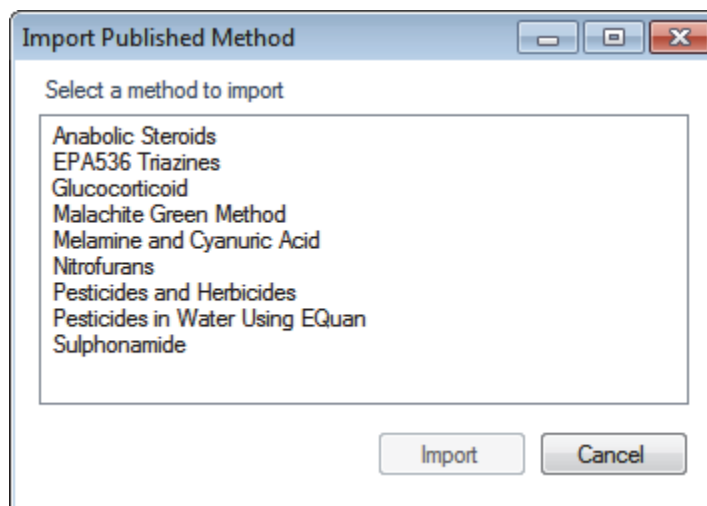
2. Select a method to import.

3. Click **Import**.

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

   …\TraceFinderData\Templates\Methods\Forensic

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

Exporting Mass Data

In the TraceFinder application, you can export the mass data list from a quantitation method to an XML file that can be read by TSQ, ISQ, Q Exactive, TSQ Endura, or TSQ Quantiva applications. You can export mass data only from quantitation methods.

This section includes examples of the following exported data formats:

- Triple Quadrupole Format

- Q Exactive Format

- TSQ Quantiva/Endura SIM Format

- TSQ Quantiva/Endura SRM Format

❖ **To export mass data list to an XML file**

1. Open the master method whose mass data list you want to export.

   If you make changes to the method, you must save it before you can export the mass data list.

2. To view a list of your mass data, click the **Acquisition List** tab on the Compounds page.
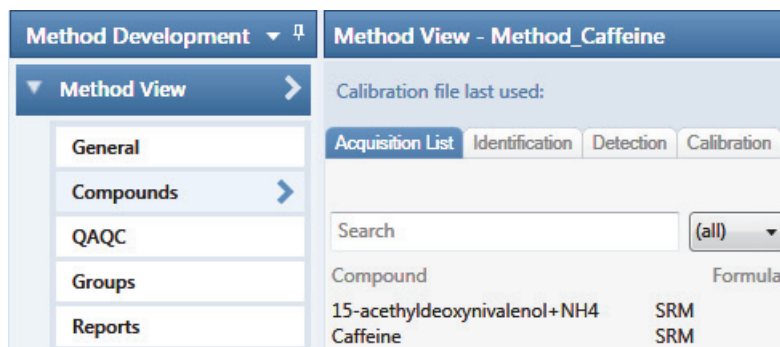
   You do not have to display the Acquisition List to export the data, but the compounds in the Acquisition List must contain at least one experiment type appropriate to the export file format. For information about displaying the Acquisition List, see "Acquisition List" on page 121. For information about editing the experiment type for a compound, see "Editing Compounds in the Database" on page 285.

3. Choose **Method View > Export Mass List** from the main menu.

   > **IMPORTANT** If you have neither a TSQ, an ISQ, a Q Exactive, a TSQ Endura, nor TSQ Quantiva instrument configured, a message asks which format you want to export: Triple Quadrupole, Q Exactive, TSQ Quantiva/Endura SIM, or TSQ Quantiva/Endura SRM.

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

   …\TraceFinderData\Methods*Methodname*

Triple Quadrupole Format

> **Note** You can export only SRM or SIM data types to the Triple Quadrupole format.

The TraceFinder application writes the mass data to the following file:

…\TraceFinderData\Methods*Methodname**.xml

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

Q Exactive Format

> **Note** You can export only XIC data types to the Q Exactive format.

The TraceFinder application writes the mass data to the following file:

…\TraceFinderData\Methods*Methodname**Methodname*.xml.include-masses

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

TSQ Quantiva/Endura SIM Format

> **Note** You can export only SIM data types to the TSQ Quantiva/Endura SIM format.

The TraceFinder application writes the mass data to the following file:

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

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

- Compound (as Name in the XML file)

- Product Mass (as Mass in the XML file)

- RT range (as StartTime and StopTime in the XML file)

- Polarity

- Lens (as TubeLens or S-Lens in the XML file)

TSQ Quantiva/Endura SRM Format

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

The TraceFinder application writes the mass data to the following file:

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

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

- Compound (as Name in the XML file)

- Precursor Mass

- Product Mass

- RT range (as StartTime and StopTime in the XML file)

- Polarity

- Lens (as TubeLens or S-Lens in the XML file)

- Collision Energy

Working with the Compound Database

When user security is activated, as a user with Method Development permission, you can manage compound definitions in the current database from either the Compound Detail Page or the Grid Page in the Compound Database view:

- The commands for opening, saving, and creating new databases are common to both display pages. See "Opening and Saving a Database" on page 270.

- The commands for importing or exporting compounds are common to both display pages. See "Exporting and Importing Compounds" on page 274.

- The parameters used in the Compound Detail and Grid pages are the same, although the names are slightly different. See "Compound Parameters" on page 297.

- The Experiment types used in the compound database are common to both display pages. See "Experiment Types" on page 302.

Opening and Saving a Database

You can load a compound database that was included with your TraceFinder installation, or you can create your own database. You can display the database parameters on the Compound Detail page or the Grid page.

When you save the edits for a compound, the application saves the changes to the compound database file.

- For instructions about editing compounds on the Compound Detail page, see "Editing Compounds in the Database" on page 285.

- For instructions about editing compounds on the Grid page, see "To edit values in the compound database grid" on page 294.

Follow these procedures:

- To open the Compound Database editor
- To load a compound database into the editor
- To create a new compound database
- To save changes to the database
- To save the database to a new name

❖ **To open the Compound Database editor**

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

The Compound Database view opens, displaying the Compound Detail page of the current database.

If there is no compound database displayed in the editor, follow the instructions .

> **Note** If you currently have a compound database open with unsaved changes, a message prompts you to save the changes. Click **Yes** to save the changes and continue opening another compound database.

You can add compounds to the database by importing a file of compounds into the new database, or you can manually add compounds one at a time. See .

❖ **To load a compound database into the editor**

1. Choose **File > Open Compound Database.**

   The Open Compound Database dialog box opens.
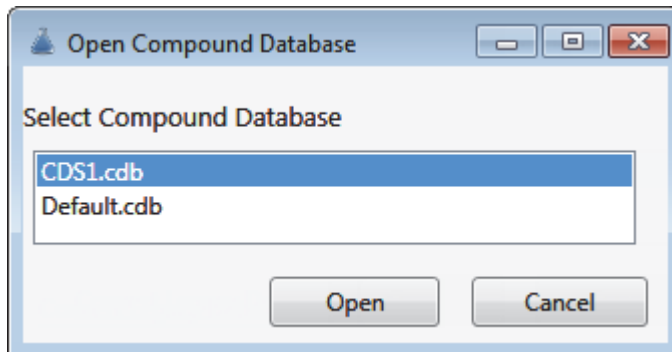
2. Double-click the name of the database that you want to open.

   The selected database opens in the Compound Detail page in the Compound Database view. See "Compound Detail Page" on page 279.

   > **Note** Or, you can choose **File > Recent Files >** *filename* from the main menu to load a previously opened database.

❖ **To create a new compound database**

1. Choose **File > New Compound Database** from the main menu.

   The New Compound Database dialog box opens.
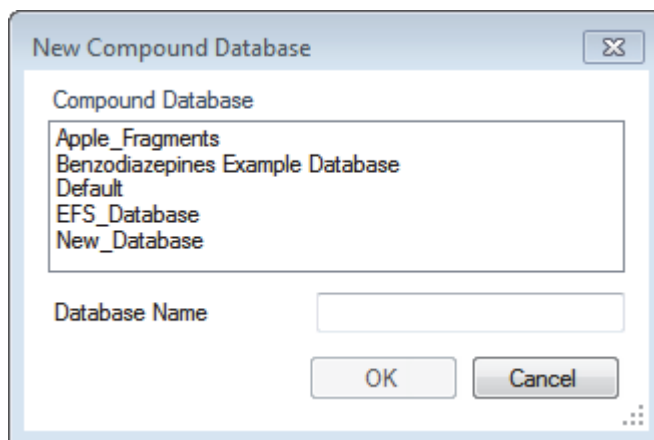
2. Type a file name for the new database and click **OK**.

   The application stores the database as

   …\Thermo\TraceFinder\3.1\Forensic\Databases*filename*.cdb

❖ **To save changes to the database**

> **Note** Databases with unsaved changes are indicated in the Compound Database page header with an asterisk after the database name.

Choose **File > Save Compound Database** from the main menu.

❖ **To save the database to a new name**

1. Choose **File > Save Compound Database As** from the main menu.

The Save Compound Database As dialog box opens.
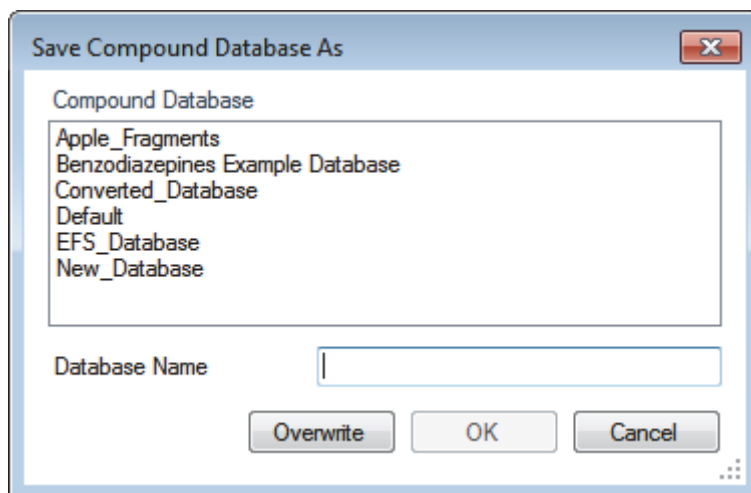
2. Do one of the following:

Type a file name for the new database and click **OK**.

–or–

Select the name of a database to overwrite, and click **Overwrite**.

If you attempt to overwrite the compound database that you currently have open, the application warns that you cannot overwrite the compound database because it is being used.

The application stores the database as

…\Thermo\TraceFinder\3.1\Forensic\Databases*filename*.cdb.

Exporting and Importing Compounds

From either the Compound Detail page or the Grid page in the Compound Database view, you can export compounds to a CSV file or mass list, or you can import compounds from an XML, a CSV, or a CDB file.

Follow these procedures:

- To export compounds to a CSV file

- To export compounds to a mass list

- To import compounds

In addition to procedures for importing and exporting compound data, this section also contains the following topics:

- Compound Database Names Mapped to CSV Column Names

- Data Columns with Default Values

❖ **To export compounds to a CSV file**

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

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

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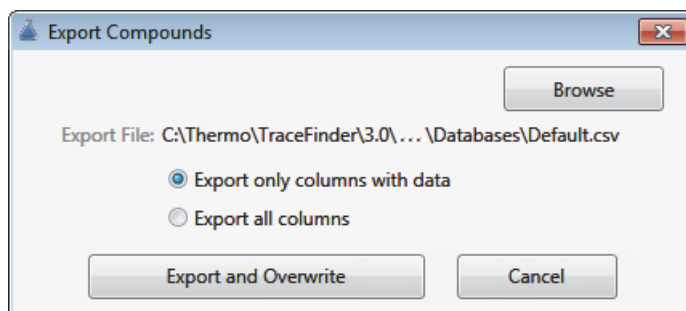
2. (Optional) Click **Browse** and locate a different folder or file name where you want to write the exported compound database.

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

3. Select one of these options:

   - **Export Only Columns with Data**: Writes only columns that contain nondefault data for at least one compound. This option does not export columns that contain only default data. See "Data Columns with Default Values" on page 308.

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

4. Click **Export and Overwrite**.

   The application stores the database as

   …\Thermo\TraceFinder\3.1\Forensic\Databases*databaseName*.csv

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

   Figure 76. Compound data in an Excel spreadsheet

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

Column names in an exported Excel spreadsheet do not always match the parameter names in the compound database editor. See "Compound Database Names Mapped to CSV Column Names" on page 305.

You can use the tools in the spreadsheet to edit the data in the compound database and then import the data in the CSV file back into the TraceFinder application. If you delete a column from the spreadsheet and then import the CSV file, the TraceFinder application replaces the data in that column with default values. For a list of default values, see "Data Columns with Default Values" on page 308.

❖ **To export compounds to a mass list**

1. Select the compounds that you want to export.

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

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

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

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

…\TraceFinderData\Methods*Methodname**.xml

> **Note** If you have neither a TSQ, an ISQ, a Q Exactive, a TSQ Endura, nor TSQ Quantiva instrument configured, a message asks which format you want to export: Triple Quadrupole, Q Exactive, TSQ Quantiva/Endura SIM, or TSQ Quantiva/Endura SRM.

For examples of exported mass lists, see the following:

- "Triple Quadrupole Format" on page 267

- "Q Exactive Format" on page 267

- "TSQ Quantiva/Endura SIM Format" on page 267

- "TSQ Quantiva/Endura SRM Format" on page 268

❖ **To import compounds**

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

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

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

You can import compounds from the following file types:

- ToxID Exactive CSV

- ToxID MS2 CSV

- TraceFinder CSV

- TraceFinder Mass List XML

- TraceFinder 3.0 Legacy CDB

- ExactFinder 2.0 CDB

> **IMPORTANT** Before you import data from a CSV file, verify that the following required columns have data for each compound. These columns have no default values and must have a value before you can import CSV data into the TraceFinder compound database:
> - CompoundName
> - ExperimentType
> - ProductMass (target peak)
> - Confirm Product (confirming peak)
> - Fragment
>
> If you delete one of these columns from the spreadsheet and attempt to import the CSV data into the TraceFinder application, the application warns that it is unable to parse the file and identifies the missing columns.

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

   The Import Compounds to CDB dialog box opens.
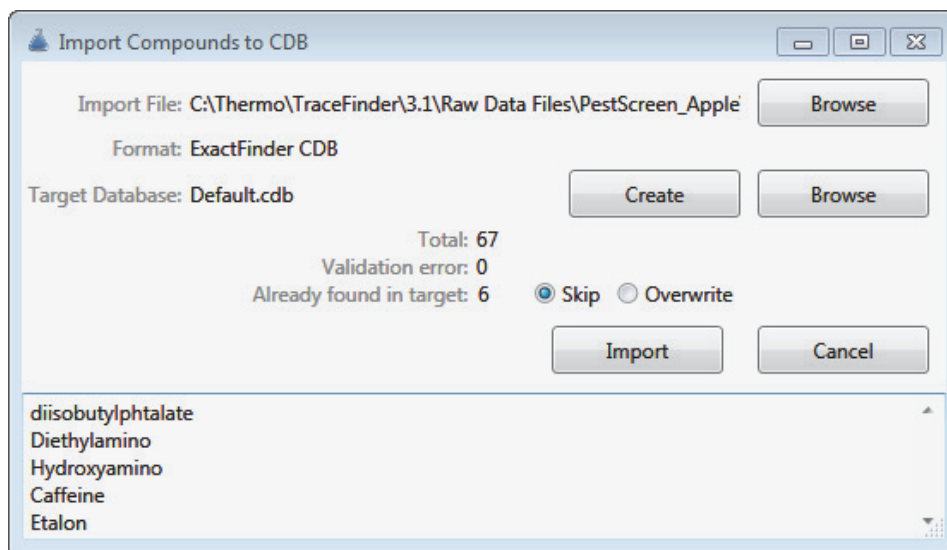
> **Note** If the import file is missing required compound information, the application warns that it is unable to parse the file and identifies the missing columns. For a list of required columns, see "Compound Detail Page" on page 279.

3. To select a different compound database, click **Browse,** locate an XML, a CSV, or a CDB compounds file, and click **Open**.

4. To select a different target database, do one of the following:

   a. Click **Browse.**

   b. Locate an XML, a CSV, or a CDB compounds file.

   c. Click **Open**.

–or–

    a. Click **Create**.

    b. Type a name for a new compound database.

    c. Click **OK**.

5. Confirm that the import file and the target database are correct.

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

6. (Optional) Select one of these options:

   - **Skip**: Imports only those compounds that do not already exist in the target database.

   - **Overwrite**: Replaces compounds that already exist in the target database with the imported compounds.

7. Click **Import**.

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

   The application reports the number of imported compounds.
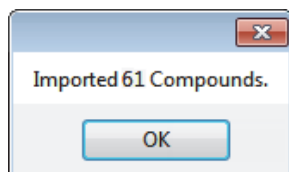
8. Click **OK**.

Compound Detail Page

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

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

- Compound Detail page for SRM experiments

- Compound Detail page for SIM experiments

- Compound Detail page for XIC experiments

This section includes the following topics:

- Sorting Compounds in the Database

- Editing Compounds in the Database

Figure 77. Compound Detail page for SRM experiments

Figure 78. Compound Detail page for SIM experiments

Figure 79. Compound Detail page for XIC experiments

Sorting Compounds in the Database

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

Follow these procedures:

- To search for compounds by name

- To display compounds by experiment type

- To display truncated compound names
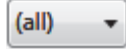
❖ **To search for compounds by name**

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

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

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

❖ **To display compounds by experiment type**

Select an experiment type from the (all) list.

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

- SRM: Selected Reaction Monitoring

- XIC: Extracted Ion Chromatogram

- SIM: Single Ion Monitoring

For detailed descriptions of each experiment type, see "Experiment Types" on page 302.

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

❖ **To display truncated compound names**

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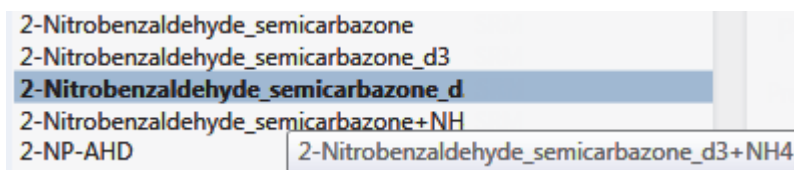
Editing Compounds in the Database

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

Follow these procedures:

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

❖ **To add a compound to the database**

1. Click the **Add Compound** icon, [＋].

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

2. Click the Compound box, and type the required Compound name.

3. Select the Experiment type: **SRM**, **SIM**, or **XIC**.

   The required parameters are different for each experiment type. See "Experiment Types" on page 302.

4. In the Target Peaks area, do the following:

   • For SRM experiments, enter values for Precursor Mass and Product Mass.

   • For SIM or XIC experiments, enter a value for Extracted Mass.

5. In the Confirming Peaks area, do the following:

   • For SRM experiments, enter values for Precursor and Product Mass.

   • For SIM or XIC experiments, enter a value for Precursor and Extracted Mass.

6. Enter or edit any of the other optional parameters described in the "Compound Parameters" on page 297.

7. When you have finished your changes, click the **Complete Edit** icon, [⬇].

   > **Tip** You cannot add another new compound or access the menu commands until you complete the edit, [⬇], or cancel the edit, [↩].

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

❖ **To remove compounds**

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

   The application supports the following methods to delete multiple compounds:

   - CTRL+A to select all compounds

   - CTRL+click to select noncontiguous compounds

   - SHIFT+click to select contiguous compounds
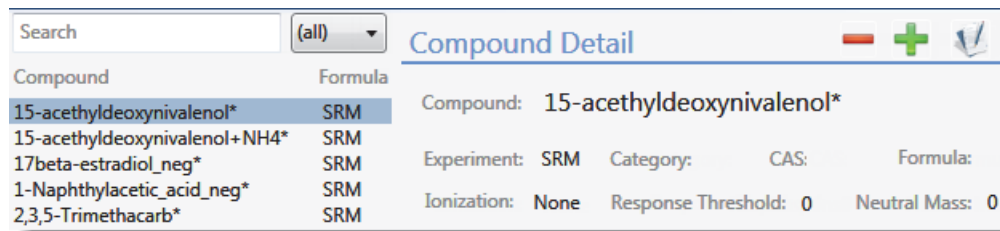
2. Click the **Delete Selected Compounds** icon, .

3. To confirm that you want to delete the selected compounds, at the prompt click **OK**.

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

❖ **To make a compound editable**

1. In the Compound list, select the compound that you want to edit.
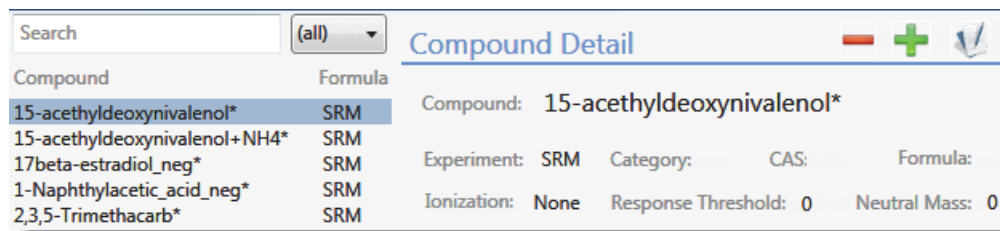
2. Click the **Edit Compound** icon, .

   The application makes the compound parameters editable and displays the

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

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

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

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

Add Target Peak icon

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

Delete Target Peak icon
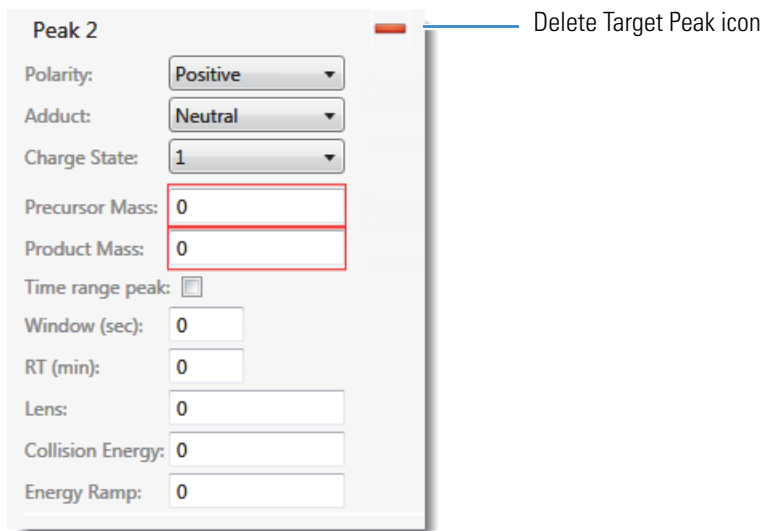
2. Enter all required parameters.

The required target peak values differ for each experiment type. See "Experiment Types" on page 302.

For a list of required and optional parameters, see the list of "Compound Parameters" on page 297.

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

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

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

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

Confirming Peaks — Add Confirming Peak icon

Precursor   Product Mass Collision Energy
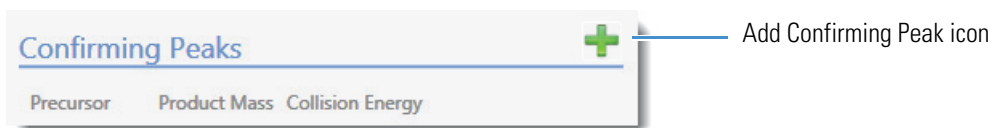
The application adds a new confirming peak to the target peak.

Confirming Peaks

Precursor   Product Mass Collision Energy

| 0 | 0 | 0 | — Delete Confirming Peak icon
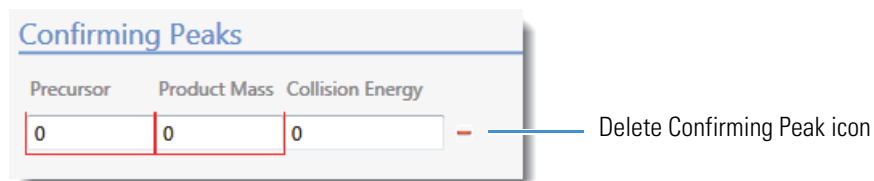
2. Type the required values for the confirming peak.

The required confirming peak values differ for each experiment type. See "Experiment Types" on page 302.

For a list of required and optional parameters, see "Compound Parameters" on page 297.

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

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

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

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

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

— Source compound

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

Target Peaks

Peak 1

Confirming Peaks (Quan Only)

Precursor Mass: 313   Precursor   Product Mass Collision Energy:
Product Mass: 285   313   241   40

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

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

— Source compound

IMPORTANT Be careful to keep the source compound selected.

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

Target Peaks
Peak 1

Add Peak 1 to 2 selected compounds

Set the Window for all peaks of 2 selected compounds to 54.00
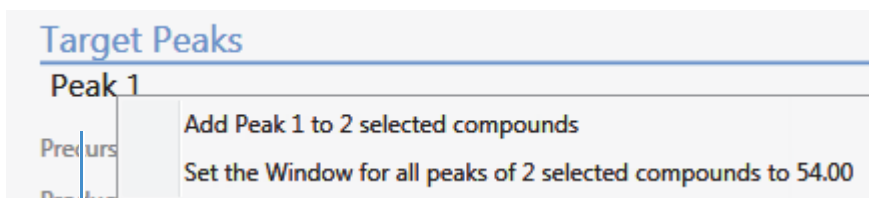
Right-click the target peak area.

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

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

5. Click **OK**.

❖ **To copy window values from one peak to another**

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

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

— Source compound

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

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

Source compound

IMPORTANT Be careful to keep the source compound selected.

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

Right-click the target peak area.

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

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

5. Click **OK**.

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

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

Add Fragment icon
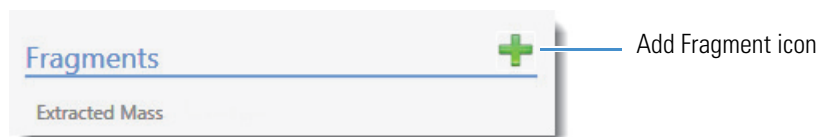
The application adds a new fragment to the target peak.

Delete Fragment icon
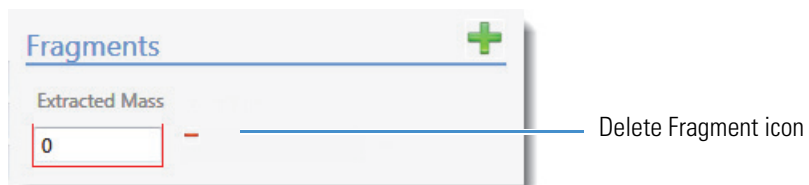
2. Click the Extracted Mass box, and type a value between **10** and **2999.999**.

3. Repeat these steps to add as many fragments as you want.

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

Grid Page

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

- There must be at least one compound in the compound database to view the Grid page.

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

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

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

❖ **To display the compound database on the Grid page**

Click **Grid** in the Compound Database navigation pane.
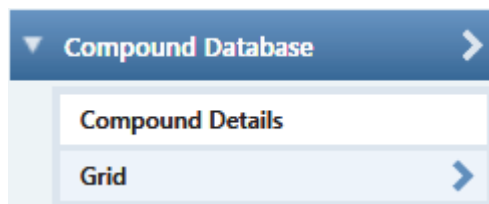
The current database opens on the Grid page.

The parameters displayed in the compound database depend on which experiment type the selected compound uses. For detailed descriptions of all parameters used in the compound database, see "Compound Parameters" on page 297.

Follow these procedures:

- To add a compound

- To remove a compound

- To edit values in the compound database grid

- To edit Experiment Type values in the compound database

- To sort the grid on column data

- To organize compounds by column data

❖ **To add a compound**

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

   There is always one blank row in the grid.
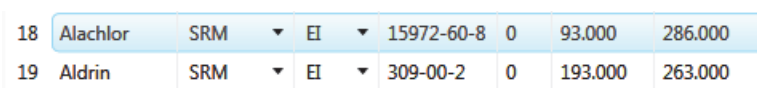
2. In the blank row, type or paste values into the columns.

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

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

❖ **To remove a compound**

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

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

2. Press the DELETE key.

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

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

   The application removes the compound from the database grid.

❖ **To edit values in the compound database grid**

Do either of the following:

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

–or–

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

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

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

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

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

❖ **To edit Experiment Type values in the compound database**

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

2. Double-click the new type in the cell, and press CTRL+C.

3. Select all Experiment Type cells in all the compounds in the database.

4. Press CTRL+V.

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

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

❖ **To sort the grid on column data**

1. Click the header of a column.

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

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

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

❖ **To organize compounds by column data**

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

Ionization

Aa ▾ ———— Down arrow

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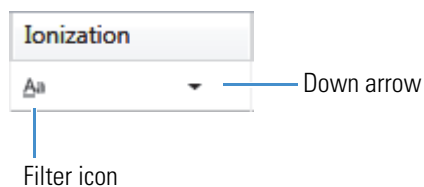
2. Select one of the filtering options, for example, **Starts With**.

Ionization	CAS
Aa ▾	Aa ▾

———— The down arrow changes to a list box.

▣ Contains
⬚ Does not contain
↦ Match (regular expression)
•⁻• Does not match (regular expression)
Aa Starts with
Ꭺa Does not start with
aA Ends with
aꞮ Does not end with
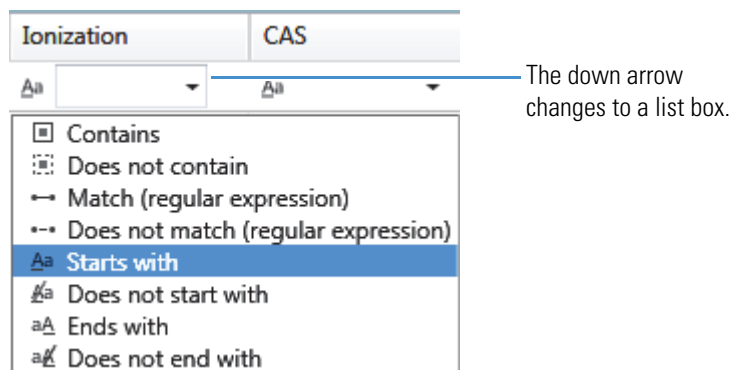
3. Click the down arrow and choose one of the column values in the list, for example, **EI**.

Ionization

Aa | ▾

(Custom)
(Blanks)
(NonBlanks)
EI
ESI
APCI
EI
CI
APPI
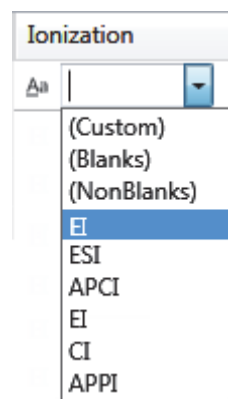
The grid displays only compounds that match the selected filter and data.

Ionization

Aa EI ▾ ▽ₓ

EI ▾
EI ▾
EI ▾
EI ▾
EI ▾
EI ▾

Compound Parameters
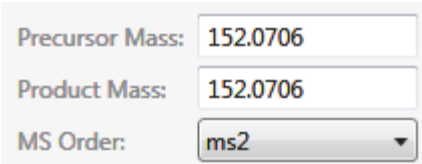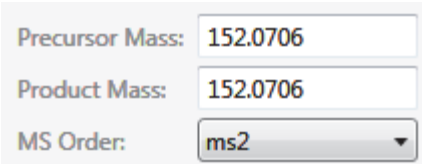
The parameters that are displayed in a compound database in either the Compound Detail page or the Grid page depend on which experiment type the selected compound uses. The Description column in the following table indicates if a parameter is used only for a specific experiment type.

The Compound Detail page and the Grid page occasionally use different names for the same parameter. The Parameter column in the following table indicates if the parameter uses different names in the Compound Detail page and the Grid page.

Table 54. Compound parameters (Sheet 1 of 5)

Parameter	Description
Compound Detail page: Compound Grid page: Compound Name	Alphanumeric name assigned to the compound.
Compound Detail page: Experiment Grid page: Experiment Type	Experiment type: SRM, XIC, or SIM. For details about the differences, see "Experiment Types" on page 302.
Category	(Optional) Alphanumeric identifier.
CAS	The Chemical Abstract Service (CAS) number that the TraceFinder application matched with the compound.
Compound Detail page: Formula Grid page: Chemical Formula	Chemical formula for the compound. Used to calculate the neutral mass for the compound.
Ionization	Alphanumeric identifier. Valid values: None, ESI, APCI, EI, CI, or APPI Default: None
Response Threshold	The application integrates only peaks with a response greater than this threshold. The response threshold is a minimum response that must be met to allow peak confirmation. Used only for target screening methods. Available only for XIC experiments. Default: 5000 Range: 1000 or greater
Neutral Mass	Mass calculated from the chemical formula. The neutral mass is the sum of all AMU elements in the compound. This parameter is informational only; it is not used for peak detection.

Table 54. Compound parameters (Sheet 2 of 5)

Parameter	Description
Target Peaks	
Compound Detail page: Precursor Mass Grid page: Peak *n* Precursor Mass	The mass-to-charge ratio (*m/z*) of a target peak. The location of the center of a target precursor ion peak in mass-to-charge ratio units. In confirming peaks, the precursor mass is the same as the target peak precursor mass. Default: 0.0 Range: 10.000 to 2999.999 Available for all SRM experiments and for XIC experiments with the MS Order set to MS2. Precursor Mass: 152.0706 Product Mass: 152.0706 MS Order: ms2 For mass values in XIC experiments when the MS Order is set to MS1, see Extracted Mass.
Compound Detail page: Product Mass Grid page: Peak *n*	The mass-to-charge ratio of the confirming peak. The location of the center of a target quan ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999 Available for all SRM experiments and for XIC experiments with the MS Order set to MS2. Precursor Mass: 152.0706 Product Mass: 152.0706 MS Order: ms2 For mass values in XIC experiments when the MS Order is set to MS1, see Extracted Mass.
Compound Detail page: Mass Grid page: Peak *n* Mass	The mass-to-charge ratio of the confirming peak. The location of the center of a target quan ion peak in mass-to-charge ratio (*m/z*) units. Available only for SIM experiments.

Table 54. Compound parameters (Sheet 3 of 5)

Parameter	Description
Compound Detail page: Extracted Mass Grid page: Peak *n* Extracted Mass	The mass-to-charge ratio of the target peak. The location of the center of a target quan ion peak in mass-to-charge ratio (*m/z*) units. You can enter a value for the Extracted Mass, but when you change the values for Formula, Adduct, Polarity, or Charge State, the application recalculates the Extracted Mass value, overwriting the value you entered. Default: 0.0 Range: 10.000 to 2999.999 Available only for XIC experiments with the MS Order set to MS1. Extracted Mass: 152.0706 MS Order: ms1 For mass values in XIC experiments when the MS Order is set to MS2, see Precursor Mass or Product Mass.
Compound Detail page: Polarity Grid page: Peak *n* Polarity	Positive or Negative
Compound Detail page: Adduct Grid page: Peak *n* Adduct	Lists the adducts specified in the configuration file. To add or remove adducts from the default lists, see "Specifying Adducts" on page 61. Adducts affect the calculated amount of the extracted mass by adding to or subtracting from the neutral mass. Adducts are polarity sensitive. Select the Polarity parameter before selecting the Adduct value. Default Positive valid values: Neutral, NH4, H, Na, K Default Negative valid values: Neutral, H, H3C2O2, HCO2 Default: Neutral
Compound Detail page: Charge State Grid page: Peak *n* Charge State	Specifies the charge state of the ion (the *z* value in *m/z*). For example, a charge state of 2 with a negative polarity means that the compound has 2 more electrons than protons. Valid values: 1 through 10 Default: 1
MS Order	Specifies whether the confirming peaks come from the same scan (MS1) or are fragments from an adjacent scan (MS2). Available only for XIC experiments.

Table 54. Compound parameters (Sheet 4 of 5)

Parameter	Description
Time Range Peak	Specifies whether the acquisition time is specified as a window around a specified RT value or as a retention time range in minutes.
	This parameter is visible only when you are editing a compound.
Window (sec)	The application uses RT and Window values to determine the start and stop time for the acquisition. Available only when the Time Range Peak option is not selected.
	Range: 0.00 to 499.50 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Compound Detail page: RT (min) Grid page: Peak *n* RT	Retention time. The application uses RT and Window values to determine the start and stop time for the acquisition. When the Time Range Peak option is selected, the RT value is specified as a range. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Compound Detail page: Lens Grid page: Peak *n* Lens	Range: –400 to 400
Compound Detail page: Collision Energy Grid page: Peak *n* Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00
Compound Detail page: Energy Ramp Grid page: Peak *n* Energy Ramp	Range: 0.00 to 200.00
Confirming Peaks	Confirming peak parameters are used only in quantitative methods.
Compound Detail page Precursor Grid page: Peak *n* Confirming *n* Precursor	The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor ion peak in mass-to-charge ratio (*m/z*) units. Available only for SRM experiments or XIC experiments with the MS Order set to MS2. Default: 0.0 Range: 10.000 to 2999.999

Table 54. Compound parameters (Sheet 5 of 5)

Parameter	Description
Compound Detail page: Product Mass Grid page: Peak *n* Confirming *n*	The mass-to-charge ratio of the quantitation ion. The location of the center of a target quan ion peak in mass-to-charge ratio (*m/z*) units. Available only for SRM experiments. Default: 0.0 Range: 10.000 to 2999.999
Compound Detail page: Mass Grid page: Peak *n* Confirming *n* Extracted Mass	The mass-to-charge ratio of the confirming peak. The location of the center of a target quan ion peak in mass-to-charge ratio (*m/z*) units. Available only for SIM experiments.
Compound Detail page: Extracted Mass Grid page: Peak *n* Confirming *n* Extracted Mass	The mass-to-charge ratio of the target peak. The location of the center of a target quan ion peak in mass-to-charge ratio (*m/z*) units. Available only for XIC experiments. Default: 0.0 Range: 10.000 to 2999.999
Compound Detail page: Collision Energy Grid page: Peak *n* Confirming *n* Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00
Compound Detail page: MS Order Grid page: Peak *n* Confirming *n* MS Order	Specifies whether the confirming peaks or fragments come from the same scan (MS1) or an adjacent scan (MS2). Available only for XIC experiments.
Fragments	Fragment parameters are used for XIC experiment types in target screening methods. The application uses fragments to define masses that are present in an adjacent scan (MS2).
Compound Detail page: Extracted Mass	The mass-to-charge ratio of the target peak. The location of the center of a target quan ion peak in mass-to-charge ratio (*m/z*) units. Available only for XIC experiments. Default: 0.0 Range: 10.000 to 2999.999

Experiment Types

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

Each of these experiment types uses a different structure for the mass filter. The target peak and confirming peak parameters for each experiment type are defined in the "Compound Parameters" on page 297.

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

SRM: Selected Reaction Monitoring

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

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

SIM: Single Ion Monitoring

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

Confirming peaks include an extracted mass value.

XIC: Extracted Ion Chromatogram

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

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

Compound Database Names Mapped to CSV Column Names

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

Table 55. CSV column names for compound parameters (Sheet 1 of 3)

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

Table 55. CSV column names for compound parameters (Sheet 2 of 3)

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

Table 55. CSV column names for compound parameters (Sheet 3 of 3)

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

Data Columns with Default Values

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

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

Table 56. Default values for compound parameters

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

Working with Instrument Methods

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

> **IMPORTANT** Do not open the Thermo Foundation Instrument Configuration window while the TraceFinder application is running.

Follow these procedures:

- To open the Instrument View

- To create a new instrument method

- To create a new multiplexing instrument method

- To open an instrument method

- To import an instrument method

❖ **To open the Instrument View**

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

   Method Development

   The Method Development navigation pane opens.

2. Click **Instrument View**.

   Instrument View ❯

   The Instrument View opens.

❖ **To create a new instrument method**

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

   The Thermo Xcalibur Instrument Setup window opens.

   Figure 80. Example instrument setup showing multiple configured instruments
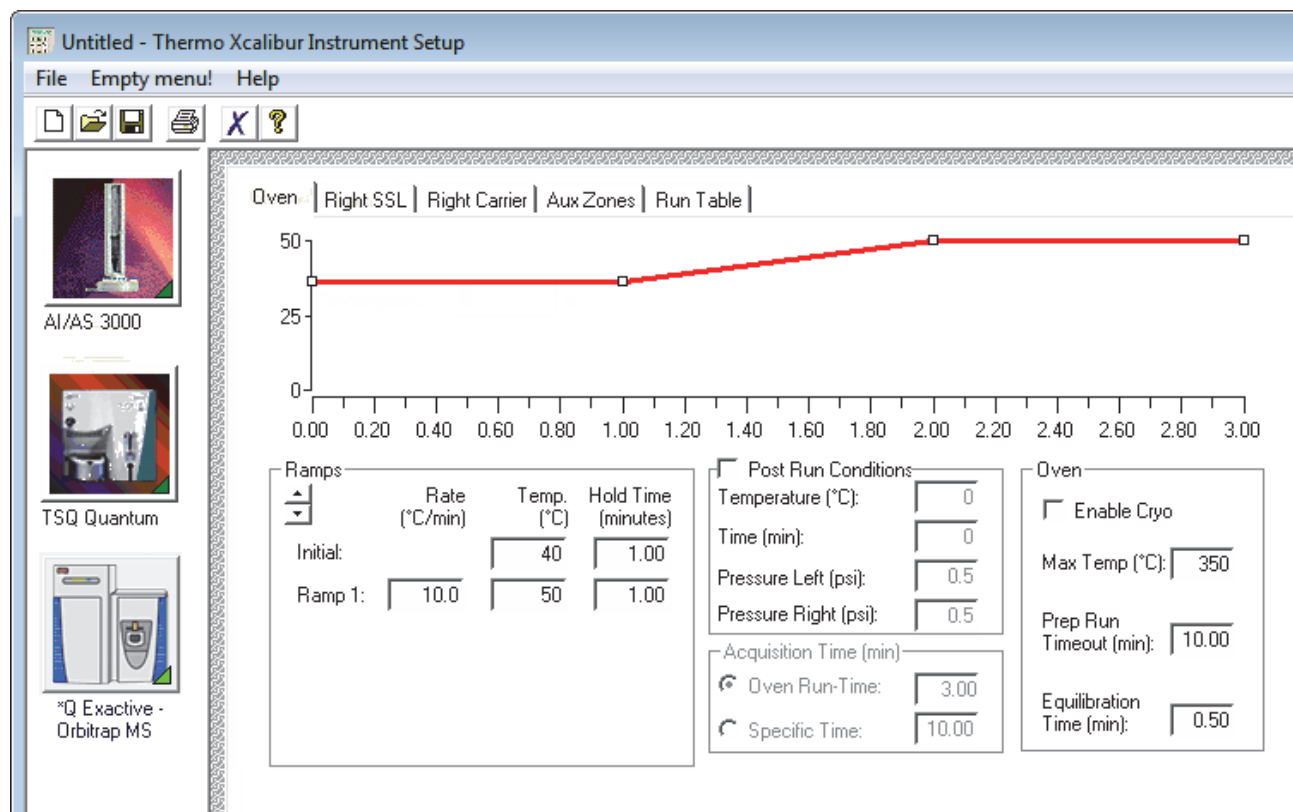
2. Click the icon for the instrument that you want to use for the method.

3. Edit the values on the instrument page.

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

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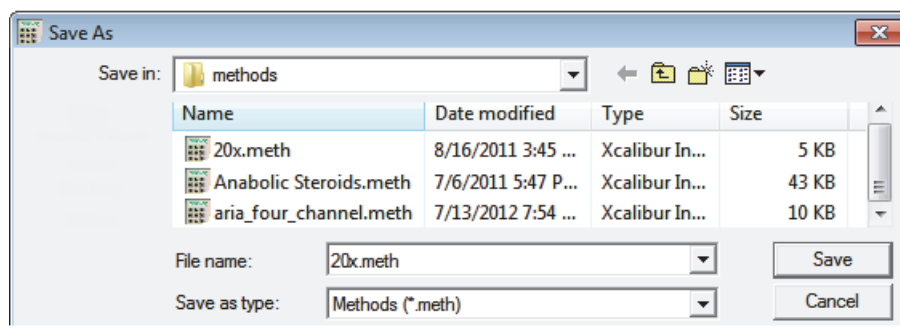
5. Select an instrument method name to overwrite, or type a new name for the instrument method, and click **Save**.

   The File Summary Information dialog box opens.
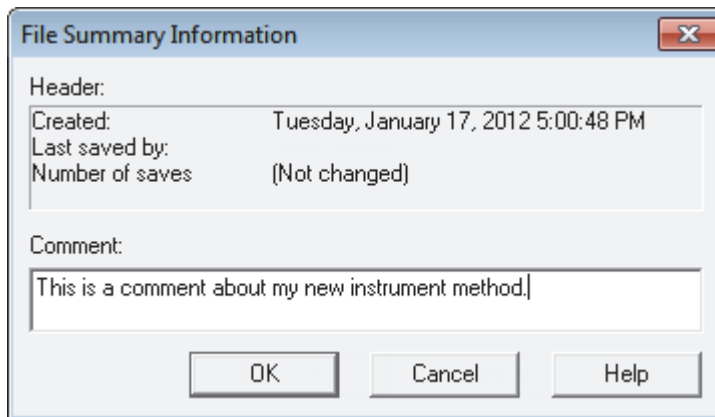
6. (Optional) Type a comment about the new instrument method.

7. Click **OK**.

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

   …\Xcalibur\methods

❖ **To create a new multiplexing instrument method**

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

   The Thermo Xcalibur Instrument Setup window opens.

   Figure 81. Example instrument setup showing a configured multiplexed instrument
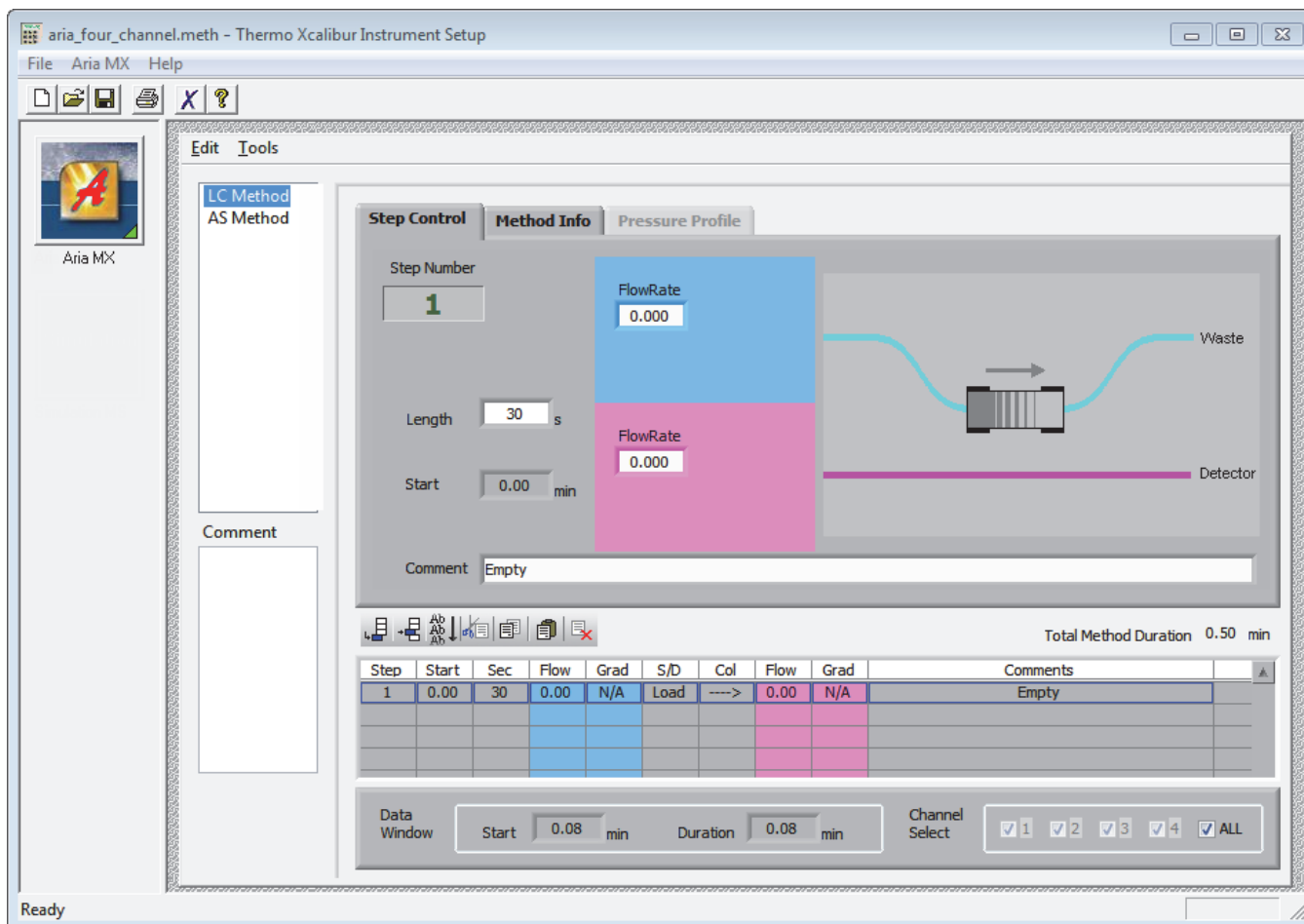
2. Click the icon for the instrument that you want to use for the method.

3. Edit the values for the instrument method.

   For information about specifying multiplexing values, refer to the documentation for your multiplexed instrument.

4. Specify the channels that you want to use for acquisition. For example:

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

   The Save As dialog box opens.

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

   The File Summary Information dialog box opens.
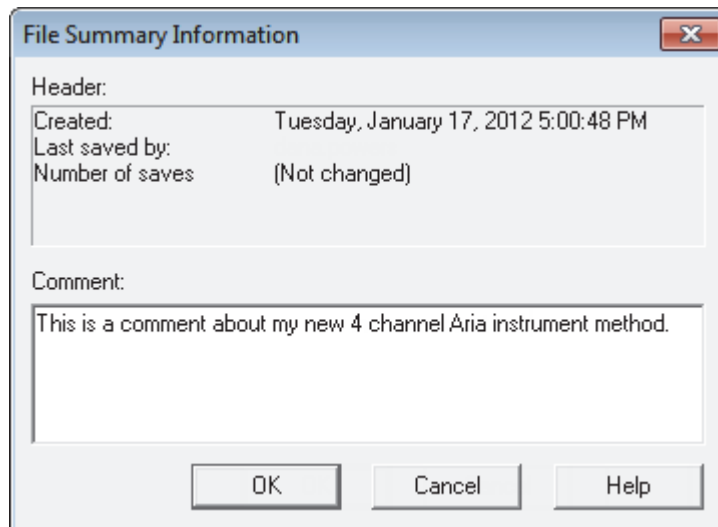
7. (Optional) Type a comment about the new instrument method.

8. Click **OK**.

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

   …\Xcalibur\methods

❖ **To open an instrument method**

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

   An instrument method browser opens.

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

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

   • Click **Xcalibur Instrument Method**, select a method from the list of recent methods, and click **Open**.

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

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

❖ **To import an instrument method**

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

   The Import Published Method dialog box opens. This dialog box lists the master methods in the Published Master Methods folder. You can import instrument methods that are associated with these published master methods.
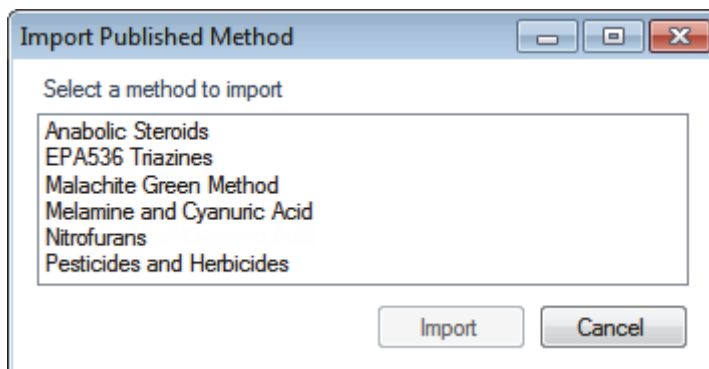
2. Select a method that includes the instrument method that you want to import.

   For instructions about importing the master methods, see "Importing Published Master Methods" on page 265.

3. Click **Import**.

   The Save Instrument Method dialog box opens.
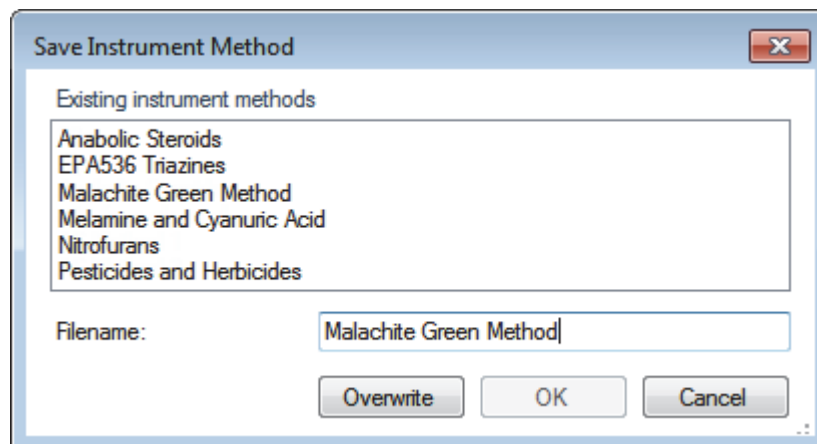
4. Do one of the following:

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

   –or–

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

   The application reports that the method successfully imported.

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

Working with Development Batches

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

This section includes instructions for the following tasks:

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

Creating a Development Batch

You create a development batch to test your instrument method and use it to acquire samples only once. You cannot save a development batch; you can save only the raw data files created when you acquire the samples in the batch.

Follow these procedures:

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

❖ **To open the Development Batch view**

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

   Method Development

   The Method Development navigation pane opens.

2. Click **Development Batch**.

   Development Batch ❯

   The Development Batch view opens a new, empty batch.

Development Batch - [C:\Thermo\TraceFinder\3.0\...\Temp]

	Filename	Sample ID	Sample name	Vial position	Injection volume	Instrument Method	Sample Volume	Dilution Factor	Sample Weight	Calculation Type	Final Units	Channel
▶ 1	Unknown1				1.0		1	1	1	Liquid ▼		Channel 1

Note The Channel column is available only when you have activated multiplexing in the Configuration console. See "Multiplexing" on page 70.

❖ **To specify a location for development batch data**

1. To specify a location for the files, choose **Development Batch > Select Batch Location** from the main menu.

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

   …\Thermo\TraceFinder\3.1\Forensic\Temp

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

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

   –or–

   Create a new folder:

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

   b. Click **Make New Folder**.

      The TraceFinder application creates a new folder in the selected folder.

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

   d. Type the name for the folder.

   e. Click **OK**.

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

❖ **To add samples to the development batch**

Do one of the following:

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

–or–

To add multiple sample rows, enter the number of rows and click the **Add Sample** icon.

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

❖ **To insert samples into the development batch**

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

2. Do one of the following:

   Right-click and choose **Insert Sample** from the shortcut menu.

   –or–

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

   The TraceFinder application inserts new, empty samples above the selected sample.

   Note You cannot insert samples into an empty batch. You must have at least one sample to select before you can use this icon.

❖ **To copy a sample**

1. Select the sample that you want to copy.

2. Right-click and choose **Insert Copy Sample** from the shortcut menu.

   The TraceFinder application adds a copy of the sample above the selected sample.

Editing Samples in a Development Batch

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

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

A development batch uses the same shortcut menu features as a batch in the Batch View in the Analysis mode. For detailed descriptions of the right-click shortcut menu, see "Batch View Shortcut Menu" on page 405.

For an example of a completed development batch, see "Completed Development Batch" on page 320.

Follow these procedures:

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

❖ **To enter column values**

1. Double-click the Filename column and type a file name for the raw data file.

2. (Optional) Enter values for the Sample Name or Sample ID columns.

3. Enter a vial position for each sample.

4. Enter an injection volume for each sample.

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

5. (Optional) To change the instrument method used for a sample, click the down arrow in the Instrument Method column and select a method from the list.

   This list contains all the available instrument methods. Instrument methods from external sources are prefixed with "Ext:".

   Note The instrument method parameter defaults to the instrument method specified in the master method.

6. To enter a channel for each sample, click the down arrow in the Channel column and select a channel from the list.

   You cannot specify the auto channel selection in a development batch.

   Note The Channel column is available only when you have activated multiplexing in the Configuration console. See "Multiplexing" on page 70.

❖ **To resize or reorganize the columns**

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

2. To move a column, drag the column header.

   You cannot move the Filename column.

❖ **To remove selected samples from the list**

1. Select the samples that you want to remove.

   Use the first column to ensure that the samples are selected.

Selected samples

2. Right-click and choose **Remove Selected Samples** from the shortcut menu.

❖ **To remove all samples from the list**

1. Choose **File > New Sample List** from the main menu.

   One of the following happens:

   - If the samples in the current batch have all been acquired, the list is cleared.

   - If the samples in the current list have not been acquired, a message confirms that you want to clear them and start a new list.

2. To create a new empty list, click **Yes**.

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

Completed Development Batch

After you complete all the parameters for a development batch, the batch table looks like this:

Figure 82. Completed development batch

	Filename	Sample ID	Sample name	Vial position	Injection volume	Instrument Method	Sample Volume	Dilution Factor	Sample Weight	Calculation Type	Final Units
▸ 1	Unknown1	A1		1	1.0	Ext: Glucocorticoid	1	1	1	Liquid ▾	
2	Unknown2	A2		2	1.0	Ext: Glucocorticoid	1	1	1	Liquid ▾	
3	Unknown3	A3		3	1.0	Ext: Glucocorticoid	1	1	1	Liquid ▾	
4	Unknown4	A4		4	1.0	Ext: Glucocorticoid	1	1	1	Liquid ▾	

Development Batch - [C:\Thermo\TraceFinder\3.1\...\Temp]

Acquiring Samples in a Development Batch

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

Follow these procedures:

- To acquire selected samples
- To acquire the batch

❖ **To acquire selected samples**

1. Select the samples that you want to acquire.

2. Right-click and choose **Submit Selected Samples** from the shortcut menu,

   or click the **Submit Selected Samples** icon, .

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

   C:\Thermo\TraceFinder\3.1\Forensic\Temp

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

   If you acquire a sample more than once, the application time-stamps the subsequent raw data files with the acquisition time.

❖ **To acquire the batch**

Right-click and choose **Submit Batch** from the shortcut menu,

or click the **Submit Batch** icon, .

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

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

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

Viewing Raw Data Files in the Qual Browser

You can view the chromatogram and spectra for completed samples in a development batch.

Follow these procedures:

- To open the Qual Browser

- To display the last completed raw data file in the Qual Browser

❖ **To open the Qual Browser**

From the main menu, choose **Go > Launch Qual Browser**.

The Thermo Xcalibur Qual Browser window opens.
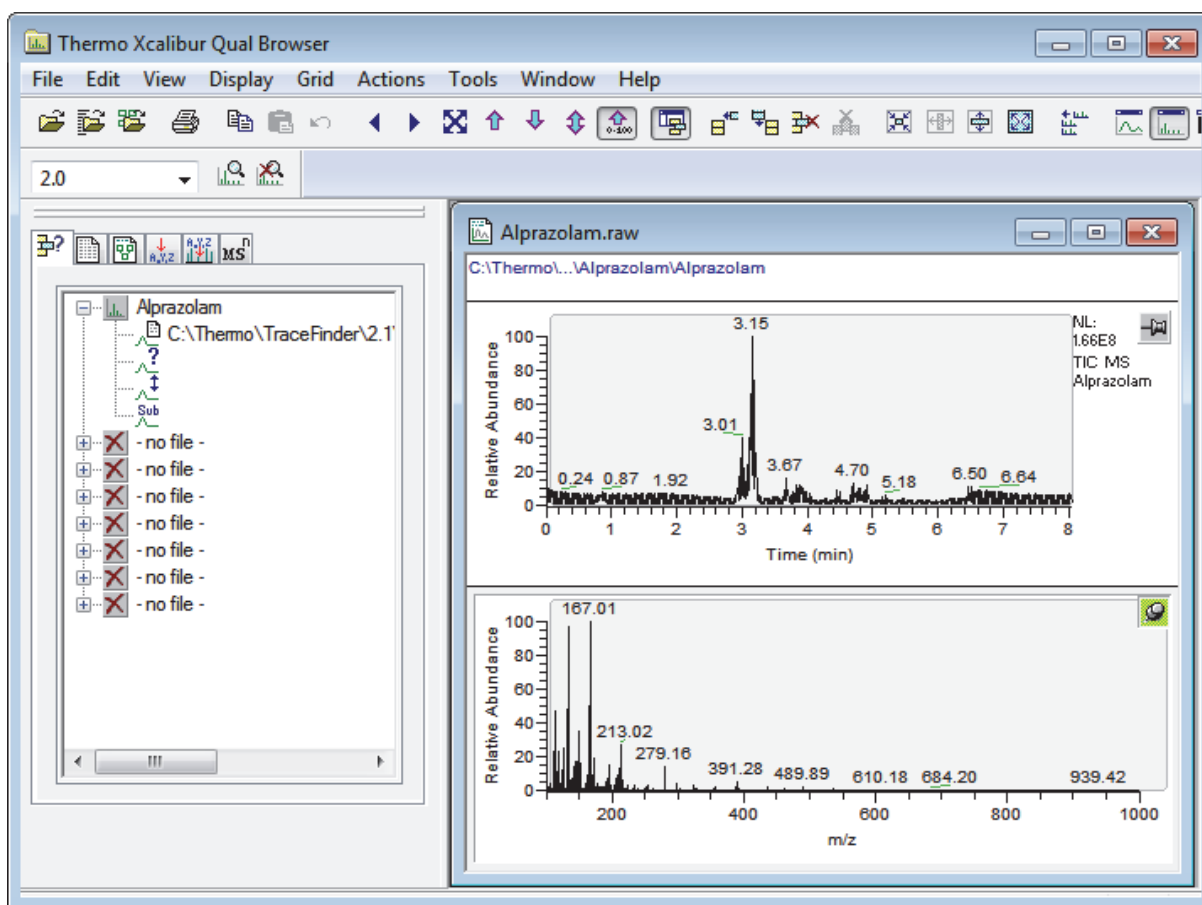
For detailed instructions about using the Qual Browser, refer to the Qual Browser Help.

❖ **To display the last completed raw data file in the Qual Browser**

On the Acquisition page of the real-time viewer, right-click and choose **View Last File in Qual Browser** from the shortcut menu.
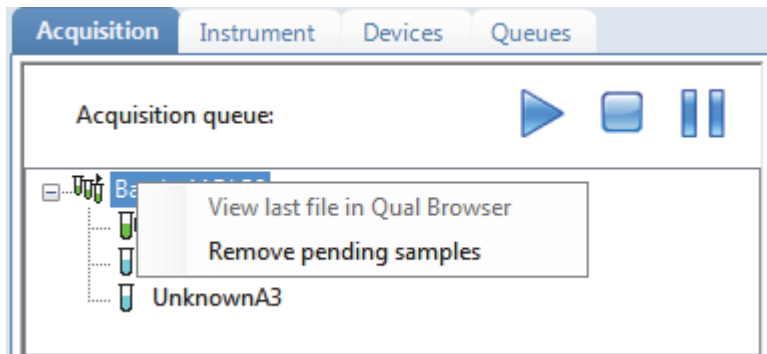
The last completed file opens in the Qual Browser.

When all samples are completed, you can view the last raw data file for the batch.

Using Quick Acquisition

Use the quick acquisition feature to quickly submit a single sample from any view of the Acquisition mode.

> **Note** The Quick Acquisition feature is available only when you activate it in the Configuration console. See "Quick Acquisition" on page 65.

❖ **To run a quick acquisition**

1. Choose **Go > Quick Acquire Sample** from the main menu or click the **Quick Acquire Sample** icon, 🔬.

   The Quick Acquisition dialog box opens.

2. Select an instrument method.

3. Type a name for the raw data file that you acquire.

   Do not enter the .raw file extension.

4. For the path, browse to a folder where you want to write the acquired raw data file.

5. Select either the manual injection or the autosampler option:

   • To perform manual injection, do the following:

   i.   Select the **Manual Injection** option.

   ii. Click **OK**.

   The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 369.

• To perform autosampler injection, do the following:

i.   Select the **Use Autosampler** option.

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

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

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

iv.   Click **OK**.

   The Quick Acquisition dialog box opens.

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

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

   This is usually the autosampler.

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

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

viii. (Optional) Select the **Priority** check box to place the sample immediately after
   any currently acquiring sample.

ix.   (Optional) Select a value for the Post-run System State: **Unknown**, **On** (default),
   Off, or **Standby**.

   The application sets the system to this state after it acquires the last sample.

x.   Click **OK**.

The application submits the sample to the Acquisition queue. See "Acquisition Page"
on page 369.

Using the Acquisition Mode

This chapter describes the tasks associated with the Acquisition mode.

This mode is available only when you select the Acquisition Batch Wizard style in the Configuration console. See "Batch Wizard Style" on page 66.

Contents

- Working with Batches

- Using Quick Acquisition

- Real Time Status Pane

- Sample Types

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

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

> **Note** When user security is activated, only a user assigned to a role with Acquisition Wizard, Template Editing permission can create a batch template.

Using a master method, you can create a batch and run the samples. A batch represents one or more samples that are to be acquired, processed, reviewed, and reported as a set. After you create a batch of samples, you can submit the batch and review the results in the Analysis mode or you can go directly to viewing and printing reports.

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

You can also use the Quick Acquisition feature to quickly submit a single sample from any page in the Acquisition mode. See "Using Quick Acquisition" on page 366.

Working with Batches

This section includes instructions for the following tasks:

- Opening and Navigating the Acquisition Mode

- Creating and Submitting Batches

Opening and Navigating the Acquisition Mode

❖ **To access the Acquisition mode**

Click **Acquisition** in the navigation pane.

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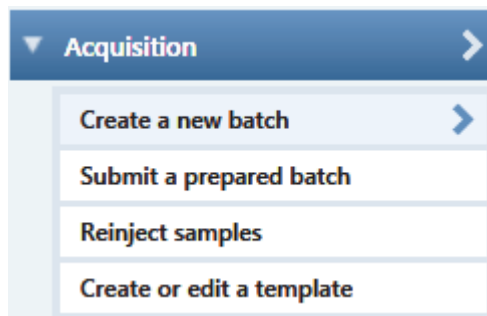
As you progress through the Acquisition mode using any of these methods for creating a batch, the task pane at the top of the view tracks your progress. As you complete each stage, you can hold your cursor over the view name in the task pane to display the parameters that you specified for the batch.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

Figure 83. Example task pane when you have completed the Acquisition mode
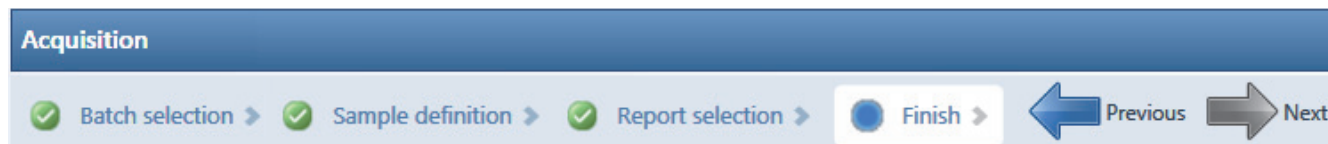
Hold your cursor over Batch Selection, Sample Definition,
or Report Selection to view the parameters for your batch.
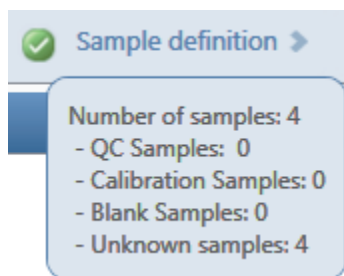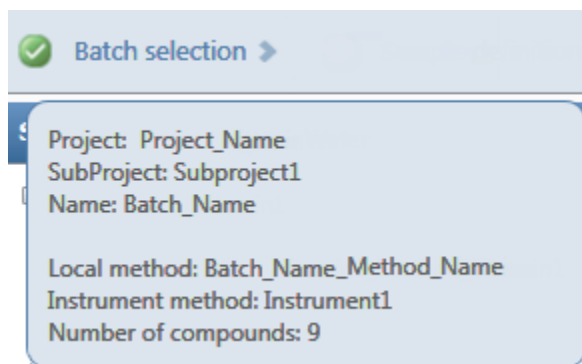
Categories in the Sample Definition list:

QC Samples: QC

Calibration Samples: Calibrator

Blank Samples: Negative

Unknown Samples: All other samples

Creating and Submitting Batches

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

1. Selecting a Batch

2. Defining the Sample List

3. Selecting and Reviewing Reports

4. Submitting the Batch

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

- To start a new quantitative batch

- To start a new screening batch

- To start a new batch from a template

- To select a prepared batch

- To reinject samples in a previously acquired batch

- To create a quantitative batch template

- To create a screening batch template

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

Workflow for Creating an Original Batch

Batch and Method

↓

Samples

↓

Reports

↓

Finish
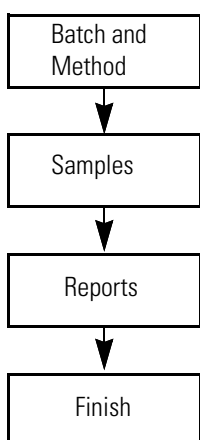
To create an original batch, start with the instructions "To start a new quantitative batch" on page 332 or "To start a new screening batch" on page 334.

Workflow for Acquiring a Prepared Batch

```
┌─────────────┐
│    Batch    │
└─────────────┘
       │
       ▼
┌─────────────┐        ┌─────────────┐
│   Finish    │◄──────►│   Samples   │
└─────────────┘        └─────────────┘
```
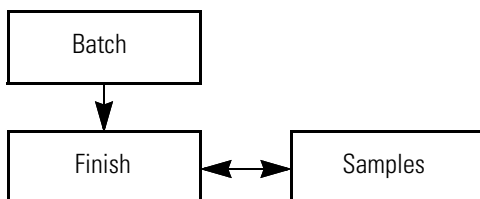
To acquire a prepared batch, start with the instructions "To select a prepared batch" on page 336.

Workflow for Reinjecting a Previously Acquired Batch

```
┌─────────────┐
│    Batch    │
└─────────────┘
       │
       ▼
┌─────────────┐
│   Samples   │
└─────────────┘
       │
       ▼
┌─────────────┐
│   Finish    │
└─────────────┘
```
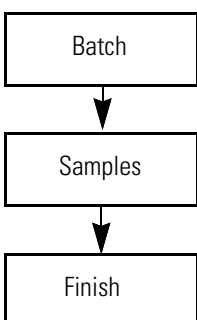
To process a previously acquired batch, start with the instructions "To reinject samples in a previously acquired batch" on page 337.

Workflow for Creating or Editing a Batch Template

```
┌─────────────┐
│ Template and│
│   Method    │
└─────────────┘
       │
       ▼
┌─────────────┐
│   Samples   │
└─────────────┘
       │
       ▼
┌─────────────┐
│   Finish    │
└─────────────┘
```
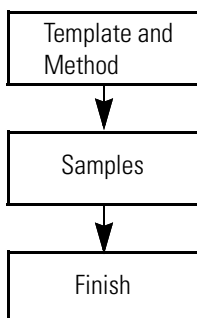
Note When user security is activated, in either the default LabDirector or default ITAdmin role, you can create a batch template.

To create a batch template, start with the instructions "To create a quantitative batch template" on page 338 or "To create a screening batch template" on page 339.

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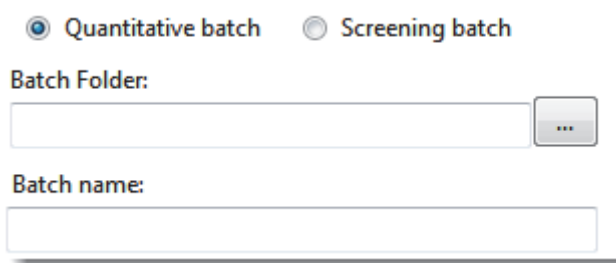
On a Batch Selection page of the Acquisition mode, you can create a new quantitative or screening batch in any of your current projects/subprojects. Or, you can submit a batch that you previously prepared and saved, reinject the samples in a batch that you previously acquired, or create a batch template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

Follow these procedures:

- To start a new quantitative batch
- To start a new screening batch
- To start a new batch from a template
- To select a prepared batch
- To reinject samples in a previously acquired batch
- To create a quantitative batch template
- To create a screening batch template
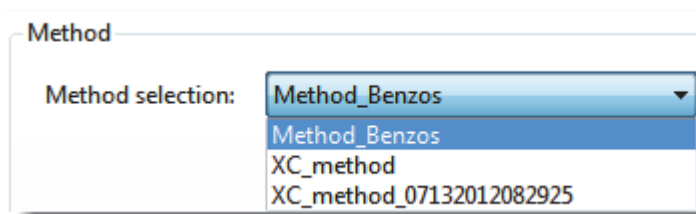
❖ **To start a new quantitative batch**

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

2. Select the **Quantitative Batch** option.

3. Select the batch folder where you want to create the new batch.

4. Type a unique name for the new batch in the Batch Name box.

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

5. Select a method from the Method Selection list.

The Method Compound Data pane displays the compounds in the method. You cannot edit the compounds list from the Acquisition mode.

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

The Sample Definition page opens. See "Defining the Sample List" on page 340.

❖ **To start a new screening batch**

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

2. Select the **Screening Batch** option.

3. Select the batch folder where you want to create the new batch.

4. Type a name for the new batch in the Batch Name box.

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

5. Select a method from the Method Selection list.

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

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

The Sample Definition page opens. See "Defining the Sample List" on page 340.

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

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

2. Select either the **Screening Batch** or the **Quantitative Batch** option.

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

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

Batch name:	
Benzos_template_083012_0955	
Available Templates	
Template name	Method
Benzos_template	Method_Benzos

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

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

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

Method	
Method selection:	Method_Benzos ▼
	Method_Benzos
	XC_method
	XC_method_07132012082925

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

   The Sample Definition page of the Acquisition mode opens. See "Defining the Sample List" on page 340.
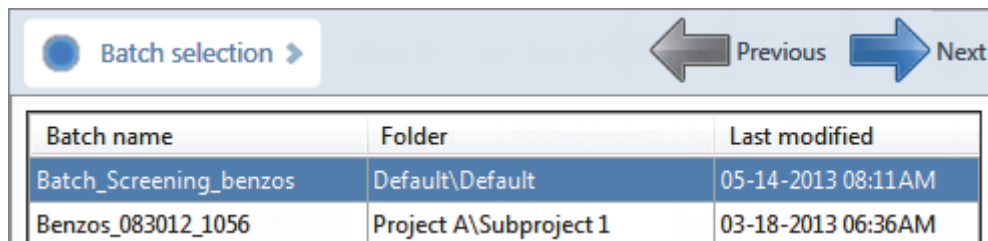
❖ **To select a prepared batch**

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

   The application displays all your unacquired, saved batches. The TraceFinder application stores all unacquired batches in the following folder:

   …\TraceFinderData\Projects\…

2. Select the batch that you want to acquire.

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

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

   - If the batch is unreadable, the application reports that the batch file is not valid and cannot be opened.

   - If a sample in the batch is unreadable, the application cannot open the sample. The application creates a new sample with the same name and flags the sample. You must complete the missing information such as Sample Type, Level, and so forth, and then save the batch before you submit it for acquisition. Or, you can browse in a new raw data file to replace the corrupt file.

4. Do one of the following:

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

     For detailed instructions, see "Defining the Sample List" on page 340.

   –or–

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

     For detailed instructions, see "Submitting the Batch" on page 358.

   –or–

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

     The TraceFinder application saves your batch in the following folder:

     …\TraceFinderData\Projects\...

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

❖ **To reinject samples in a previously acquired batch**

1. Click **Reinject Samples** in the navigation pane.

2. On the Batch page, select the batch that you want to reacquire.

   The Batch page displays all previously acquired batches, both quantitative and screening.

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

   The Sample Definition page of the Acquisition mode opens. See "Defining the Sample List" on page 340.

   • If the batch is unreadable, the application reports that the batch file is not valid and cannot be opened.

   • If a sample in the batch is unreadable, the application creates a new sample with the same name and flags the sample. You must complete the missing information, such as Sample Type, Level, and so forth, and then save the batch before you submit it for acquisition. Or, you can browse in a new raw data file to replace the corrupt file.

❖ **To create a quantitative batch template**

1. Click **Create or Edit a Template** in the navigation pane.
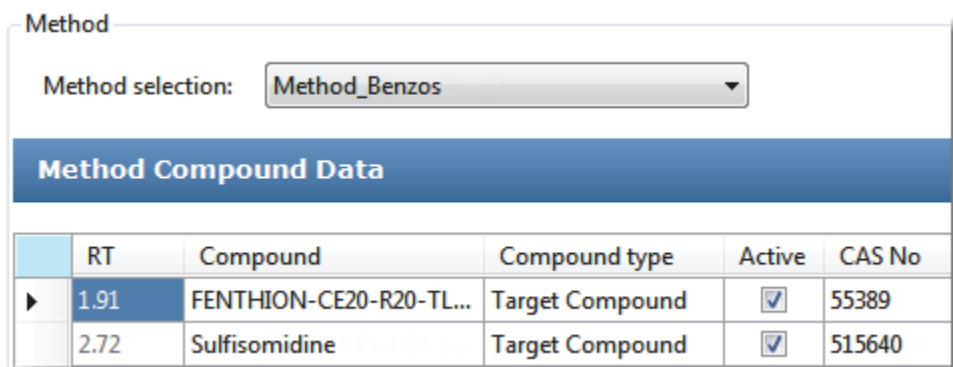
> **Note** When user security is activated, this page is available only to users assigned to a role with template editing permission.

2. Select the **Quantitative Batch** option.

3. Click [...] and select the folder where you want to create the new batch template.

4. Type a name for the new batch template in the Template Name box.

5. Select a method from the Method Selection list.

   The Method Compound Data pane displays the compounds in the method. You cannot edit the compounds list from the Acquisition mode.

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

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

❖ **To create a screening batch template**

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

> **Note** When user security is activated, this page is available only to users assigned to a role with template editing permission.

2. Select the **Screening Batch** option.

3. Click ⬚ ⋯ ⬚ and select the folder where you want to create the new batch template.

4. Type a name for the new batch template in the Template Name box.

5. Select a method from the Method Selection list.

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

6. Select the check box for each database that you want to use for screening.

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

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

Defining the Sample List

Use the Samples page on the Sample Definition page of the Acquisition mode, to create a list of samples for the batch. See "Samples" on page 350. You can add samples, insert samples, import a sample list, or remove samples from the list. You can use the Reference Sample page to select a reference sample to use as a reference peak in the Data Review. See "Reference Sample" on page 353.

To create the sample list, you can use either of two sets of function buttons (described in the following graphic) or you can use commands on the shortcut menu (see the Shortcut Menu section of the "Samples page parameters" on page 350).

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

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

- When you are creating a batch from scratch, creating a batch from a template, or editing a batch template and you click Next, the Report Selection page opens. See "Selecting and Reviewing Reports" on page 354.

- When you are editing a prepared batch or reinjecting samples and you click Next, the Finish Selection page opens. See "Submitting the Batch" on page 358.

Follow these procedures:
- To add samples to the list
- To insert samples into the list
- To import samples into the list
- To remove samples from the list
- To reinject a sample from a previously acquired batch
- To select channels for the batch
- To assign a specific channel to a sample
- To select a reference sample
- To add an auto sample type
- To specify different instrument methods for samples

❖ **To add samples to the list**

1. Select the number of sample rows to add $\boxed{1 \;\updownarrow}$ and then click the **Add** icon, $\boxed{\text{⬇}}$ or $\boxed{\text{Add}}$.

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

   Each file name must be unique.

3. Select a sample type from the Sample Type list for each sample.

Available sample types			
Specimen	Hydrolysis	Solvent	QC
Unextracted	Calibrator	Negative	

For a detailed description of each sample type, see "Sample Types" on page 384.

4. For each Calibrator or QC sample, select a level from the Level list.

The sample levels are defined in the master method. If there are no levels to select in the Level list, ask a user with Method Development permission to edit the method and specify the levels. Then return to the Acquisition mode, and begin the batch again. The application does not save a batch when you leave the Acquisition mode.

If you have Method Development permission, do the following:

a. Return to the Method Development mode.

b. Open the method.

c. Click the **Compounds** tab.

d. Click the **Calibration Levels** tab.

e. Add the levels.

f. Save the method.

For detailed instructions, see "Calibration Levels" on page 179.

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

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

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

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

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

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

For instructions to automatically copy or fill values in these columns, see Appendix C, "Using Copy Down and Fill Down."

❖ **To insert samples into the list**

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

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

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

   Insert .

   The application inserts the Specimen samples above the selected sample.

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

Inserted samples → (rows 2 and 3)

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

   Each file name must be unique.

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

Available sample types			
Specimen	Hydrolysis	Solvent	QC
Unextracted	Calibrator	Negative	

5. For each Calibrator or QC sample, click the Level cell and select a level from the list.

   The sample levels are defined in the master method. If there are no levels to select from the Level list, ask a user with Method Development permission to edit the method and specify the levels. Then return to the Acquisition mode, and begin the batch again. The application does not save a batch when you leave the Acquisition mode.

   If you have Method Development permission, follow the instructions in step 4 of the procedure "To add samples to the list" on page 340.

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

   Tip Use the Fill Down command to make entering vial positions easier.

7. For each sample, type a volume in the Injection Volume column.

   The minimum injection volume allowed is 0.1 µL; the maximum injection volume allowed is 5000 µL.

8. (Optional) Type or edit the values for the remaining columns.

   Note When you use the horizontal scroll bar at the bottom of the sample list, the Status, Filename, and Sample Type columns stay fixed while the other columns scroll right and left.

❖ **To import samples into the list**

1. Click **Import**, [Import] .

    The Sample Import Tool dialog box opens.
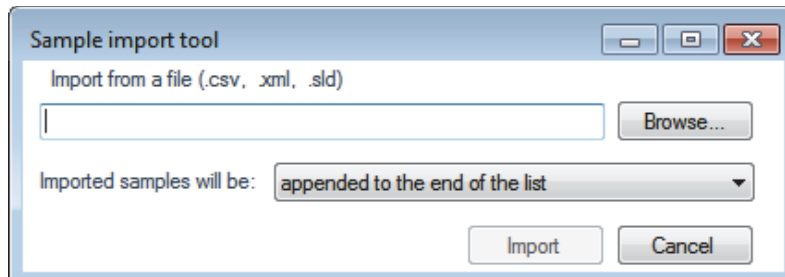
    Use this dialog box to import a sample list from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file with the sample definitions that you want to import.

    > **Note** The .csv, .xml, or .sld file format must match the TraceFinder file format.

3. From the Imported Samples Will Be list, select either **Appended to the End of the List** or **Inserted at the Selected Row**.

4. Click **Import**.

    The Sample Import Tool dialog box closes, and the application adds the specified samples to the sample list.

    When you import samples from an Xcalibur sequence file (.sld), the TraceFinder application makes the following column name substitutions.

Xcalibur column	TraceFinder column
Position	Vial position
Inj Vol	Injection volume
Dil Factor	Conversion Factor

    When you import samples from an Xcalibur sequence file (.sld), the TraceFinder application makes the following sample type substitutions.

Xcalibur sample type	TraceFinder sample type
Blank	Negative
Std Bracket	Calibrator

    For each imported sample, the application uses the Instrument Method specified in the local method.

5. For each Calibrator or QC sample, click the Level cell and select a level from the list.

   The sample levels are defined in the master method. If there are no levels to select from the Level list, ask a user with Method Development permission to edit the method and specify the levels. Then return to the Acquisition mode, and begin the batch again. The application does not save a batch when you leave the Acquisition mode.

   If you have Method Development permission, follow the instructions in step 4 of the procedure "To add samples to the list" on page 340.

   For detailed instructions about defining calibration levels, see "Calibration Levels" on page 179.

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 horizontal scroll bar at the bottom of the sample list, the Status, Filename, and Sample Type columns stay fixed while the other columns scroll right and left.

9. (Optional) When using multiplexing, select a channel for each imported sample.

   Imported samples default to Auto.

❖ **To remove samples from the list**

1. Select the samples that you want to remove.

   > **Tip** Use the CTRL or SHIFT keys to select multiple samples.

2. Right-click and choose **Remove Selected Samples** from the shortcut menu.

❖ **To reinject a sample from a previously acquired batch**

1. In the sample list, select the sample to reinject.

2. Right-click and choose **Reinject Selected Samples** from the shortcut menu.

   The TraceFinder application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth.

   The TraceFinder application copies all parameter values from the original sample.

A green status icon indicates previously acquired samples (acquired and processed) and the sample name is grayed out. A blue status icon indicates samples created for reinjection (not acquired).

🔵	cal_50_INJ001	Calibrator	10
🟢	cal_50	Calibrator	10
🔵	cal_10_INJ001	Calibrator	10
🟢	cal_10	Calibrator	10

When you submit this batch, the application acquires only the reinjection samples.

❖ **To select channels for the batch**

> **Note** These features are available only when you have activated multiplexing in the Configuration console. See "Multiplexing" on page 70.

To disable a configured channel, clear the check box for the channel in the Multiplexing Channels area at the bottom of the page.

Multiplexing Channels
☑ All Channels   ☑ Channel 1   ☑ Channel 2   ☑ Channel 3   ☑ Channel 4
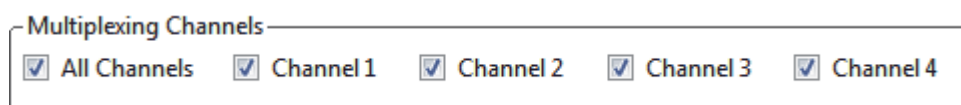
By default, all configured channels are selected. The configured channels are determined by the multiplexing settings in the Configuration console. See "Multiplexing" on page 70.

Clearing a channel in the Multiplexing Channels area does not remove this channel selection from the Channels list for each sample. When you assign a channel to a sample, be careful not to assign a channel that is not available.

❖ **To assign a specific channel to a sample**

1. Scroll to the Channel column.

> **Note** The Channel column is available only when you have activated multiplexing in the Configuration console. See "Multiplexing" on page 70.

All samples default to Auto.

2. Select a channel from the Channel list.

Auto ▼
Auto
Channel 1
Channel 2
Channel 3
Channel 4
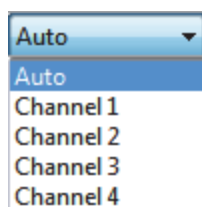
When you submit the batch, samples that are set to Auto run on any of the available channels and samples that are set to a specific channel run only on that channel.

If you select a channel that is not available for this batch, the application flags the sample sequence on the Finish page of the Acquisition mode. See the previous procedure, To select channels for the batch.
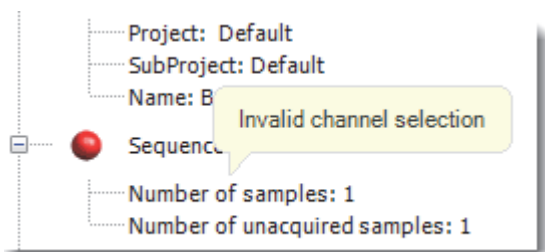
3. If you see this error, do the following:

a.   Click **Previous** to return to the Sample Definition page.

The incorrect sample is marked with an error flag.

b.   Correct the channel selection.

❖ **To select a reference sample**

1. Click the **Reference Sample** tab.

   The Reference Sample page in the Sample Definition page opens. See "Reference Sample" on page 353.

   You can select one reference sample to use as a reference peak in the Data Review.

2. Right-click the Reference Sample page and choose **Add Reference Sample** from the shortcut menu.

   The Open Chromatograph Reference Sample dialog box opens.
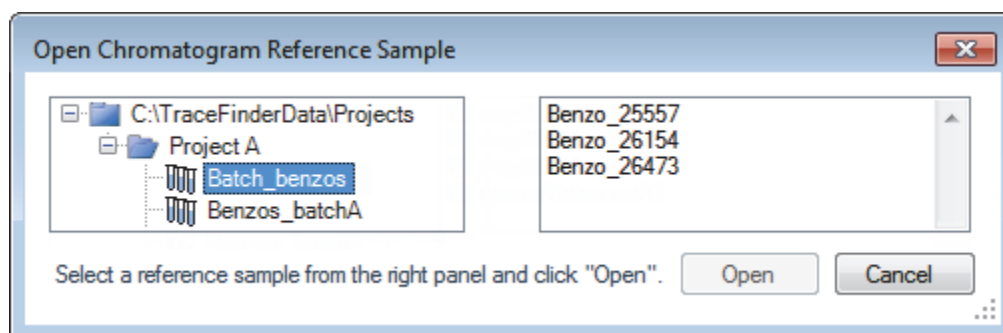
   Note If you are using a new method, you will not see any samples here. You must create and save a batch using the current method to see available samples in this list.

3. Select a project/subproject/batch from the list.

   The TraceFinder application displays only batches that were created using the current master method.

4. Select a sample from the list of processed samples on the right.

   The TraceFinder application displays all the processed samples in the selected batch. To use a sample as a reference sample, the sample must have been processed with the current master method.

5. Click **Open**.

6. The application adds the reference sample to the Reference Sample page.

7. (Optional) Enter values for Sample ID, Sample Name, Comment, and Barcode Actual.

8. (Optional) Change the Vial Position for the sample.

The application uses the peak in this sample as a reference peak in the Analysis mode. See "Reference Peak" on page 519.

❖ **To add an auto sample type**

1. Click the **Auto Samples** tab.

   The Auto Samples page opens. See "Auto Samples" on page 352.

2. Right-click and choose **Add Auto Sample** from the shortcut menu, or click the **Add New Auto Sample** icon, [1] .

   The application adds a Solvent sample to the sample list.

   You can add, insert, or remove samples from this list as you would any sample list.

3. To change the sample type to a Negative, click the Sample Type column and select Negative from the list.

4. In the Injection Volume column for the sample, type a volume.

   The minimum injection volume value allowed is 0.1 μL; the maximum injection volume value allowed is 5000 μL.

5. In the Number of Injections column, type the number of injections available in the designated Solvent or Negative vial.

   After auto sample injections have occurred, you can return to this page to view the number of Injections Used in each vial.

6. In the Vial Position column, type the vial position for the Solvent or Negative sample.

❖ **To specify different instrument methods for samples**

> **Note** By default, the Instrument Method column is not displayed on the Sample Definition page. See Instrument method column.

1. Display the Instrument Method column in the sample list:

   a. Right-click the sample list and choose **Modify Columns** from the shortcut menu.

      The Modify Columns dialog box opens.

   b. In the Available Columns pane, select **Instrument Method**.

   c. Click [>] to move the Instrument Method column to the Displayed Columns pane.

   d. Click **OK**.

   The application displays the Instrument Method column, defaulting to the instrument method specified in the master method.

2. Click the Instrument Method column and select an instrument method from the list.

   This list contains all the available instrument methods. The application prefixes instrument methods from external sources with "Ext:".

   You can specify a different instrument method for each sample.

Figure 84. 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**ExternalMethods*

Local instrument methods:

…\TraceFinderData\Projects\…*batch*\Methods*method*

Samples

Use the features on the Samples page to create a list of samples for the batch.

Figure 85. Samples page on the Sample Definition page

Table 57. Samples page parameters (Sheet 1 of 2)

Parameter	Definition
Previous	Returns you to the previous page.
Next	Takes you to the next page.
Status color codes	● Sample is not acquired.
	● Sample is acquired but not processed.
	● Sample is acquired and processed.
	● Sample is currently acquiring.
Sample Controls	
Add	Adds the specified number of empty rows to the sample grid.
Insert	Inserts the specified number of empty rows above the selected row.
Import	Opens the Sample Import Tool where you can import samples defined in a CSV file or an XML file.
Multiplexing Channels	These features are available only when you have activated multiplexing in the Configuration console. See "Multiplexing" on page 70.
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.

Table 57. Samples page parameters (Sheet 2 of 2)

Parameter	Definition
Reinject Selected Samples	Creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth.
Remove Selected Samples	Removes selected samples from the sample grid.
Import Samples	Opens the Sample Import Tool. See "To import samples into the list" on page 343.
Copy Down	Copies the value in the selected row to all rows below it. For detailed instructions about using the Copy Down command, see Appendix C, "Using Copy Down and Fill Down."
Fill Down	Enters sequential values in the column starting with the value in the selected row and ending with the last row in the column. For detailed instructions about using the Fill Down command, see Appendix C, "Using Copy Down and Fill Down."
Modify Columns	Opens the Modify Columns dialog box. See "Column Display" on page 393.
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 another application, such as an Excel spreadsheet. You cannot paste this data back into the Acquisition mode sample list.
Copy With Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information to another application, such as a Microsoft Excel spreadsheet. You cannot paste this data back into the Acquisition mode sample list.
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column.
Undo Last Paste	Removes the last pasted item in the Acquisition mode sample list.
Export to CSV File	Opens the Save As dialog box where you can save the current sample list to a CSV file.
Edit Instrument Method	Opens the Instrument Setup window where you can edit the parameters of the instrument method. • When you edit an external method, the application updates the method in the …\Xcalibur\methods folder. • When you edit an internal method, the application updates the method in the …\TraceFinderData\Projects*project**subproject**batch*\Methods*method* folder. For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 309.

Auto Samples

Use the features on the Auto Samples Sample page to identify the Solvent or Negative samples to use for any Auto Sample or Auto Sample and Reinject failure actions as specified on the Intelligent Sequencing page of the method. See "Editing the Intelligent Sequencing Page" on page 204.

Each sample type that you specify for a failure action on the Intelligent Sequencing page must be defined on the samples list on the Auto Samples page.

Figure 86. Auto Samples page on the Sample Definition page
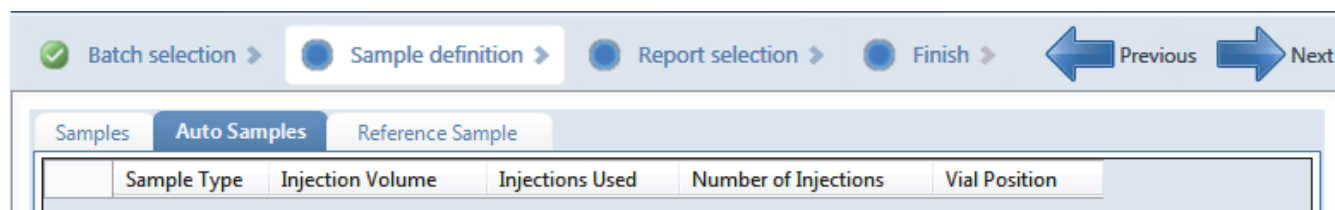
Table 58. Auto Samples page parameters

Column	Description
Sample Type	The sample type for the auto sample injection as specified on the Intelligent Sequencing page of the method—either Solvent or Negative. Default: Solvent
Injection Volume	The injection volume used for the sample acquisition as specified on the Samples page. Range: 0.1 through 5000 µL
Injections Used	The number of times a vial has been used. The count is cumulative across all batches.
Number of Injections	The number of injections available in the designated Solvent or Negative vial.
Vial Position	Vial position for this sample type as specified on the Samples page.

Reference Sample

Use the features on the Reference Sample page to select a sample to use as a reference peak in Data Review.

Figure 87. Reference Sample page in the Sample Definition page
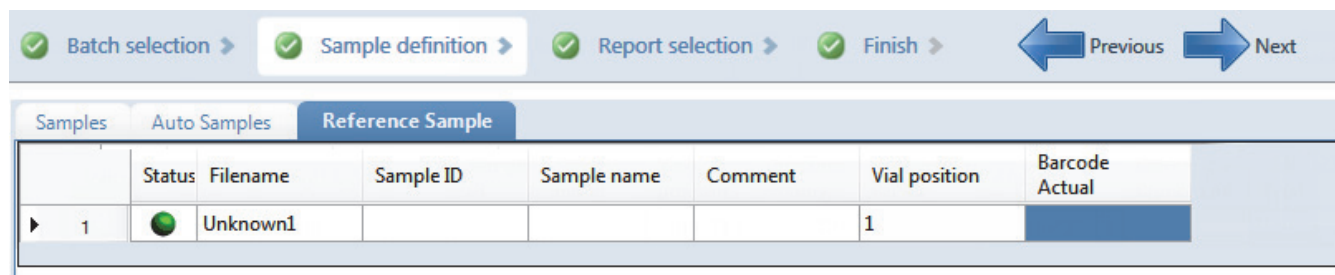
Table 59. Reference Sample page parameters

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 another application, such as an Excel spreadsheet. 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 another application, such as an Excel spreadsheet. You cannot paste this data back into the reference sample list.
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column.
Export to CSV File	Opens the Save As dialog box where you can save the current sample list to a CSV file.

Selecting and Reviewing Reports

On the Report Selection page, you can specify the types of reports that you want to create. See "Report Selection" on page 356. For a complete list of report types and examples of output files, see Appendix A, "Reports." In addition to the report type, you can specify a report description for each of your reports.

- For each standard report that you generate, you can create a hardcopy printout, a PDF file, or an XML file.

- For each custom report that you generate, you can create a hardcopy printout or an XLSM file.

- For each target screening report that you generate, you can create a hardcopy printout or a PDF file.

- For each ToxID report that you generate, you can create a hardcopy printout or a PDF file.

Use any of the following procedures to create a reports list. When you finish specifying your report options, click **Next** to go to the Finish page and submit your batch. See "Submitting the Batch" on page 358.

The application writes the resulting output files for your reports to the following folder:

…\TraceFinderData\Projects\…*batch*\Reports

Follow these procedures:

- To edit a report description
- To preview a standard report
- To specify a standard report in print format or as a PDF, an XML, or an XLSM file
- To specify a custom report in hardcopy or XLSM format
- To specify a ToxID or target screening report in hardcopy format or as a PDF file
- To export reports to a specific folder

❖ **To edit a report description**

Select the Report Title column and edit the default title.

The default report title is the same as the report name.

❖ **To preview a standard report**

1. Click (magnifier icon) to view an example of the report type as a PDF file.

   The right pane of the page displays an example PDF report with typical PDF viewer buttons.

2. To minimize the PDF viewer, click .

   > **Note** Only Standard report types have preview documents.

❖ **To specify a standard report in print format or as a PDF, an XML, or an XLSM file**

1. For each type of report that you want to create, select the check box in the Print, Create PDF, or Create XML columns.

2. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell. This action applies only to report types that make this output format available.

❖ **To specify a custom report in hardcopy or XLSM format**

1. For each custom report that you want to create, select the check box in the Print or Create XLSM columns.

2. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell. This action applies only to report types that make this output format available.

❖ **To specify a ToxID or target screening report in hardcopy format or as a PDF file**

1. For each target screening report that you want to create, select the check box in the Print or Create PDF columns.

2. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell. This action applies only to report types that make this output format available.

❖ **To export reports to a specific folder**

1. Select the **Export Results** check box at the lower left corner of the page.

☐ Export Results

The Browse For Folder dialog box opens.
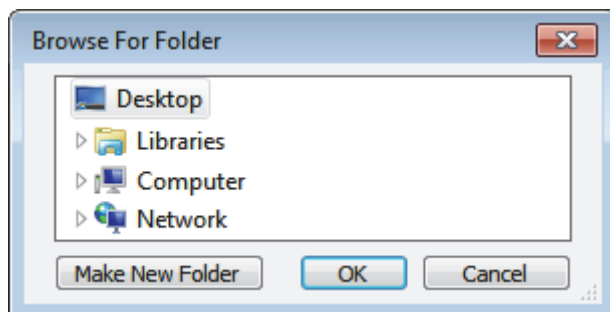
2. Locate and select the folder where you want to save the reports.

3. (Optional) To create a new reports folder within the selected folder, click **Make New Folder** and type the new folder name.

4. Click **OK**.

The application writes all reports to the specified folder in addition to the batch Reports folder.

Report Selection

Use the features on the Report Selection page to specify the types of reports that you want to create.

Figure 88. Report Selection page

Table 60. Report Selection page parameters (Sheet 1 of 2)

Parameter	Description
Example	Displays an example PDF file for the report type. This example provides a model of the report type only; it does not reflect your specific data. This is available for standard reports only.
Report Name	The name of a report.

Table 60. Report Selection page parameters (Sheet 2 of 2)

Parameter	Description
Report Title	User-editable description to be used on a report.
Report Type	The type of report: Standard, Custom, ToxID, or Target Screening.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files. Available only for standard, ToxID, and target screening reports.
Create XML	Reports to be exported in XML format. Available only for standard reports.
Create XLSM	Reports to be exported in Excel Macro-Enabled Workbook (.xlsm) format. Available only for custom reports.
Batch Level	Rather than creating separate reports for each sample, the application uses a composite of the data from all the samples to create a single report for the entire batch. Batch-level reports are prepended with a **B** to differentiate them. You cannot select this option from the Report Selection page. You must select the Batch Level option for the report in the report configuration. See "Specifying the Reports" on page 40.
Shortcut menu: Copy Down	Copies the selected or cleared state to all subsequent reports in the column.
Export Results	Writes all reports to the specified folder in addition to the batch Reports folder.

Submitting the Batch

In the Finish page of the Acquisition mode, you can specify a startup method, a shutdown method, or a calibration batch. You can save the batch to be acquired later, or you can acquire and process data and optionally create reports. See "Finish page" on page 365.

Note If you are working with a batch template, the only available function is Save.

Follow these procedures:

- To specify startup or shutdown methods
- To automatically update the timed SRM information
- To specify a calibration batch
- To specify device states
- To save a batch for later acquisition
- To start an acquisition
- To view the output files

❖ **To specify startup or shutdown methods**

1. Select a method from the System Startup Method list.

   The TraceFinder application runs this method before running the batch. No autosampler injection takes place. This feature is not available for all instruments.

2. Select a method from the System Shutdown Method list.

   The TraceFinder application runs this method after running the batch. This feature is not available for all instruments.

System startup method:

| AS Method 1 ▼ |

System shutdown method:

| AS Method 3 ▼ |

❖ **To automatically update the timed SRM information**

Select the **Auto TSRM Update** check box.

☐ Auto TSRM Update

When you submit the batch, the application updates the TSQ method with mass transitions, collision energy, and other appropriate data for TSRM functionality.

❖ **To specify a calibration batch**

1. In the Calibration area, select a calibration (.calx) file from the list.
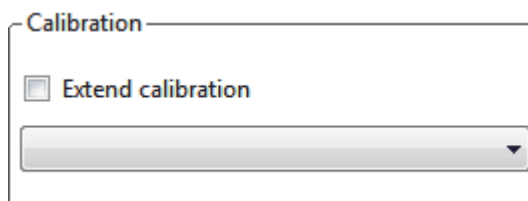
> **Note** You must acquire at least one batch with the current method to create a .calx calibration file.

2. To add calibration data from the current batch to the selected calibration file, select the **Extend Calibration** option.

❖ **To specify device states**

In the System Status area, select the name of the device, right-click, and then choose a device state from the shortcut menu.
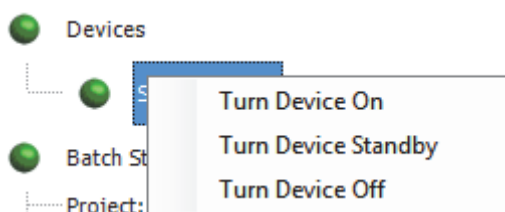
Table 61. Instrument states (Sheet 1 of 2)

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 61. Instrument states (Sheet 2 of 2)

Instrument state	Description
Turn Device Off	Keeps the system in the Off state when the current run finishes. The Off state indicates that all power to the instrument, which the TraceFinder application can control, is turned off. This includes power to all heaters and subassemblies, but in some cases not all subassemblies.
	Some devices do not have an Off feature. For devices that do have this feature, the device enters a power-saving or consumable-saving mode, and you can switch the device back on. When several runs are queued, the application uses the system power scheme of the last submitted run.
Instrument status indicators	
● (green)	Green indicates that the device is turned on or is running.
● (yellow)	Yellow indicates that the device is in standby mode or is waiting for contact closure.
● (red)	Red indicates that the device is turned off or that there is an error with the device.

❖ **To save a batch for later acquisition**

From the Finish page, click **Save**, 💾 Save .

The TraceFinder application saves your batch as a prepared file.

❖ **To start an acquisition**

1. Click **Submit**, 🧪➡ Submit .

   The Submit Options dialog box opens. For detailed descriptions of the parameters, see .

2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.

   • When all submitted samples have been previously acquired, this option is (by default) not selected.

   • When any of the submitted samples has not been acquired, this option is (by default) selected.

3. To process the submitted samples, select the **Process Data** check box.

   You can process the data with or without performing peak detection. You might, for example, want to turn off peak detection when reprocessing samples.

4. (Optional) Select the **Create Reports** check box.

5. (Optional with multiplexing activated) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.

6. (Optional without multiplexing activated) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   • Next Available Batch places the batch immediately after the currently acquiring batch.

   • Next Available Sample places the batch immediately after the currently acquiring sample.

   Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

7. Select the **Use** check box for the device that you want to use for this acquisition.

8. (Optional) Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

   This is usually the autosampler.

9. (Optional) Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

   When this is cleared, individual instruments can start at different times and then have to wait for the last instrument to be ready.

10. Do one of the following:

    To start the selected processes, click **OK**.

    The selected processes begin, and the TraceFinder application shows the real-time display at the bottom of the current window. You can begin another batch in the Acquisition mode while you watch the real-time display of the currently acquiring batch.

    –or–

    Click **Cancel** to exit the Acquisition mode without performing any tasks.

Figure 89. Submit Options dialog box

Acquire Data
selected

Acquire Data
not selected

Table 62. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Samples	Number of samples to be submitted for acquisition, processing, or reporting.
Acquire Data	Submits the current batch to acquisition. • When all submitted samples have been previously acquired, this option is (by default) not selected. • When any of the submitted samples has not been acquired, this option is (by default) selected.
Process Data	(Default) Processes the data for the current batch.
With Peak Detection	(Default) Processes the data with peak detection. When cleared, this option lets you reprocess samples without performing peak detection.

Table 62. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
Create Reports	Creates reports for the current batch.
Priority Sequence	With multiplexing activated, places the batch immediately after the currently acquiring batch.
	Without multiplexing activated, specifies one of the following priority options to place the batch in the queue:
	Next Available Batch: Places the batch immediately after the currently acquiring batch.
	Next Available Sample: Places the batch immediately after the currently acquiring sample.
	Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.
Acquisition pane	
Device Name	Lists all configured instruments.
	If the instrument that you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the TraceFinder application. You cannot configure an instrument while the TraceFinder application is running.
	Available only when the Acquire Data check box is selected.
Use	Specifies the instruments used for this acquisition.
	Available only when the Acquire Data check box is selected.
Start Device	Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler.
	Available only when the Acquire Data check box is selected.
Start When Ready	Starts the specified device when all the instruments are ready to acquire data. When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
Post-run System State	Specifies the system state after it acquires the last batch. On (default), Standby, or Off.
Hide/Show Details	Collapses or expands the acquisition details of the Submit Options dialog box.
OK	Begins the selected processes.
Cancel	Closes the Submit Options dialog box without submitting any tasks.

❖ **To view the output files**

Locate the files to view from the following directories:

- The TraceFinder application writes saved batches to the subproject 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*method*

- The application writes the reports to the batch Reports folder:

  …\TraceFinderData\Projects\…*batch*\Reports

Finish

Use the features on the Finish page to save the batch to be acquired later or acquire and process data and optionally create reports.

Figure 90. Finish page
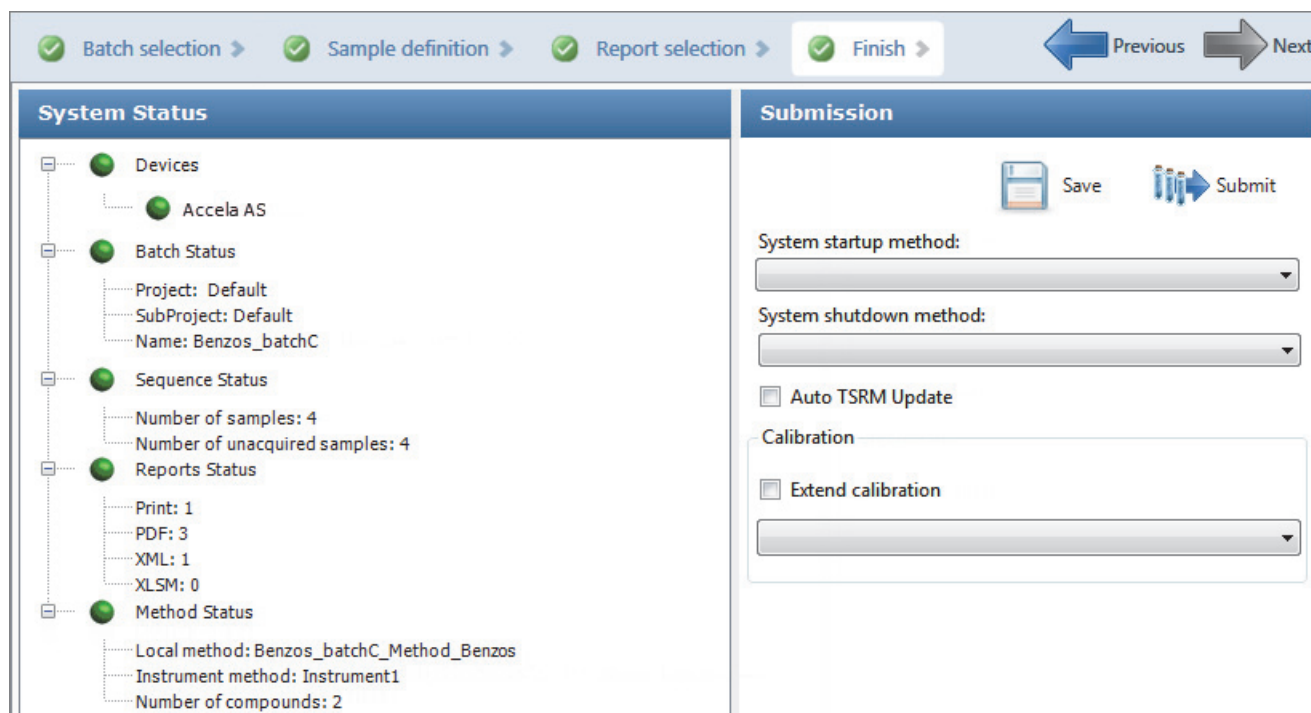
Table 63. Finish page parameters

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 standard and custom reports to be printed and saved as PDF, XML, or XLSM files • Local method and instrument method used for the batch • Number of compounds in the method
System Startup Method System Shutdown Method	The instrument methods that run before and after the batch. No autosampler injection takes place. These features are not available for all instruments.
Auto TSRM Update	Updates the TSQ method with mass transitions, collision energy, and other appropriate data for TSRM functionality.
Calibration	• Use calibration: Uses the selected calibration file to process the current data. • Extend calibration: Adds calibration data from the current batch to the selected calibration file.
Save	Saves the current batch as a prepared batch.
Submit	Opens the Submit Options dialog box where you can choose to generate reports.

Using Quick Acquisition
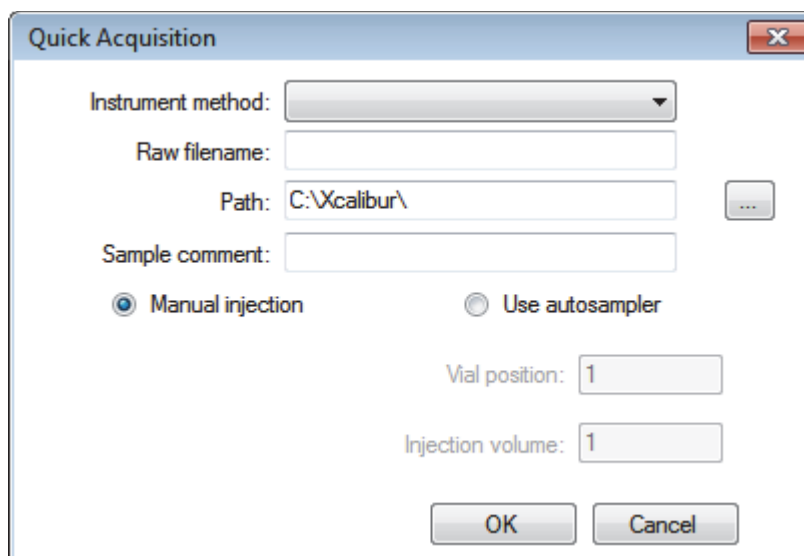
Use the quick acquisition feature to quickly submit a single sample from any view of the Acquisition mode.

> **Note** The Quick Acquisition feature is available only when you activate it in the Configuration console. See "Quick Acquisition" on page 65.

❖ **To run a quick acquisition**

1. Choose **Tools > Quick Acquire Sample** from the main menu or click the **Quick Acquire Sample** icon, 🔧 .

   The Quick Acquisition dialog box opens.

2. Select an instrument method.

3. Type a name for the raw data file that you acquire.

   Do not enter the .raw file extension.

4. For the path, browse to a folder where you want to write the acquired raw data file.

5. Select either the manual injection or the autosampler option:

   • To perform manual injection, do the following:

      i.   Select the **Manual Injection** option.

      ii. Click **OK**.

      The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 369.

- To perform autosampler injection, do the following:

  i.   Select the **Use Autosampler** option.

  ii. In the Vial Position box, type a vial position.

  iii. In the Injection Volume box, type an injection volume.

      The minimum injection volume allowed is 0.1 μL; the maximum injection volume allowed is 5000 μL.

  iv. Click **OK**.

      The Quick Acquisition dialog box opens.

  v.   Select the **Use** check box for the device that you want to use for this acquisition.

  vi. (Optional) Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

      This is usually the autosampler.

  vii. (Optional) Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

      When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.

  viii. (Optional) Select the **Priority** check box to place the sample immediately after any currently acquiring sample.

  ix. (Optional) Select a value for the Post-run System State: **Unknown**, **On** (default), **Off**, or **Standby**.

      The application sets the system to this state after it acquires the last sample.

  x.   Click **OK**.

  The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 369.

Real Time Status Pane

You can access the Real Time Status pane from any mode in the TraceFinder application.

❖ **To access the Real Time Status Pane from any mode**

Click **Real Time Status** in the upper right corner of the TraceFinder window.

Real time status

The Real Time Status pane opens at the bottom of the current view.

Figure 91. Real Time Status pane
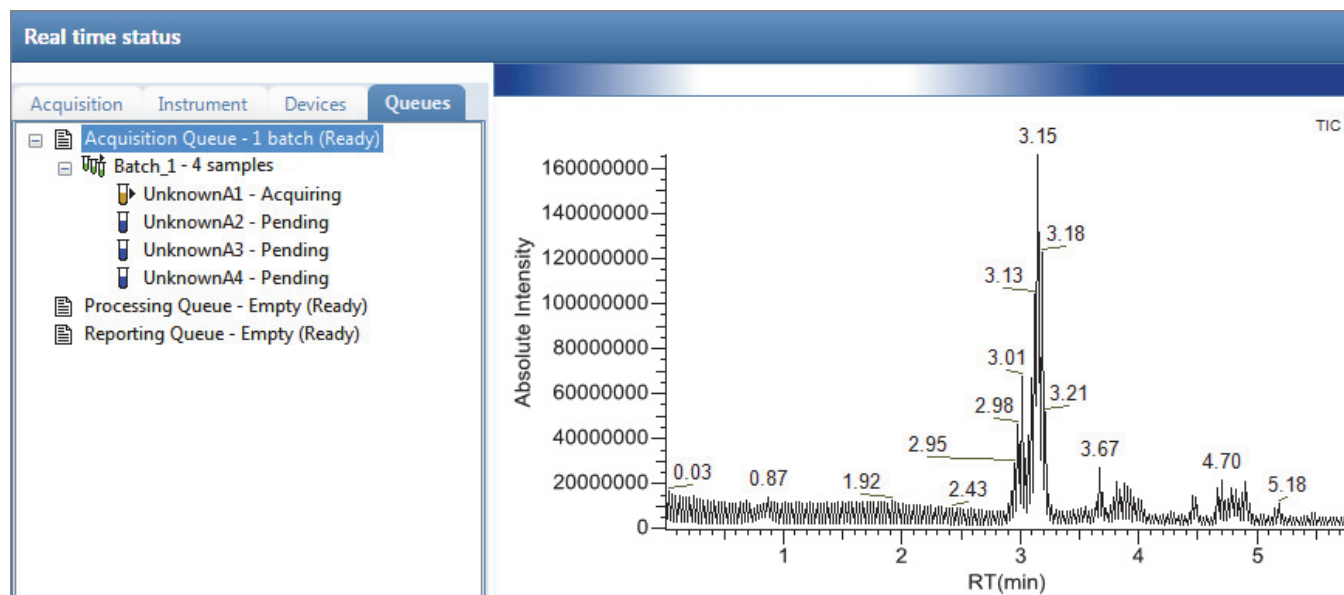
The Real Time Status pane has four pages of information and a real-time trace pane:

- Acquisition Page

- Instrument Page

- Devices Page

- Queues Page

- Real-Time Trace Display

Acquisition Page

Use the Acquisition page to monitor the progress as the application acquires the samples.

Acquisition	Instrument	Devices	Queues

Acquisition queue: ▶ ⬛ ⏸

⊟ UnknownA3
    UnknownA3

Bar code	
Bar code status	
Calib. file	C:\TraceFinderData\Projects\Project A\Subproject 1\Batch_06_123\Meth
Comment	
Dil. factor	1
Filename:	Unknown1
Inj. volume	1.25
Inst. method	C:\TraceFinderData\Projects\Project A\Subproject 1\Batch_06_123\Meth
ISTD amount	
Level	
Path	C:\TraceFinderData\Projects\Project A\Subproject 1\Batch_06_123\Data
Proc. method	Default
Revision	0
Sample ID	
Sample name	
Sample type	Unknown
Sample volume	0
Sample weight	0
Vial	1
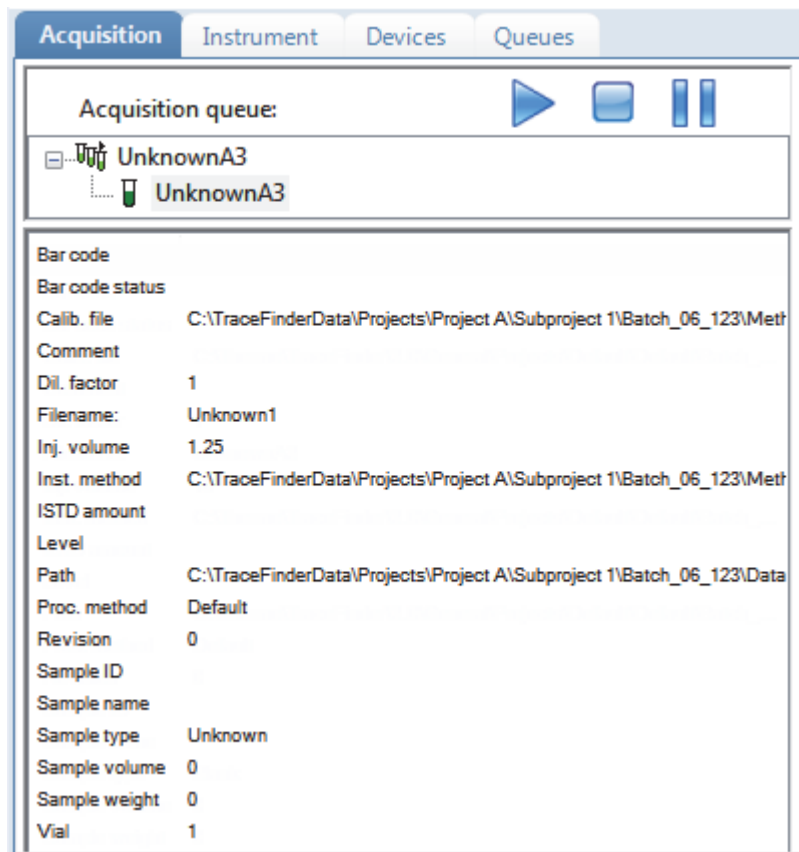
Use the **Start**, ▶, **Stop**, ⬛, or **Pause**, ⏸, icons to control batches in the Acquisition queue.

❖ **To view the last acquired file in the Qual Browser**

Right-click anywhere in the Acquisition page and choose **View Last File In Qual Browser** from the shortcut menu.

The Thermo Xcalibur Qual Browser window opens, displaying the last processed file.

❖ **To open the Instrument Setup window**

Right-click anywhere in the Acquisition page and choose **Open Instrument Method Editor** from the shortcut menu.

The Thermo Xcalibur Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 309.

> **Note** Changes you make and save to the instrument method do not affect the currently running batch.

Instrument Page

Use the Instrument page to monitor the currently acquiring sample.

When you run single sample submission, this displays the sample name instead of the batch name.

❖ **To view the last acquired file in the Qual Browser**

Right-click anywhere in the top pane of the Instrument page and choose **View Last File In Qual Browser** from the shortcut menu.

The Thermo Xcalibur Qual Browser window opens, displaying the last processed file.

❖ **To open the Instrument Setup window**

Right-click anywhere in the top pane of the Instrument page and choose **Open Instrument Method Editor** from the shortcut menu.

The Thermo Xcalibur Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 309.

> **Note** Changes you make and save to the instrument method do not affect the currently running batch.

Devices Page

Use the Devices page to monitor the status of the instrument. The feedback you see on the Devices page depends on the instrument you are using. The following examples show an Accela autosampler and an Aria™ multiplexing device.

Accela Autosampler Feedback

Acquisition	Instrument	**Devices**	Queues

Accela AS

Status

Status:	Stopped
Scan speed (x):	5
First scan:	1
Last scan:	534
Scan number:	534
Start time (min):	8.041820
Real time elapsed (min):	1.608350
Repeat count:	0

Aria Multiplexing Feedback

Acquisition	Instrument	**Devices**	Queues

Aria MX

Hold Autosampler   Direct Control

Status   Events   Pres

Autosampler 1
READY

Channel 1
READY
40   bar

Channel 3
READY

Detector
NOT READY

1	Inline

Status	**Events**	**Pres**

Time	Ch	Msg
11:40:38.48	1	Chan Status NOT READY
11:40:36.48	1	(Channel1\Pump1) Std Pump 1
11:35:38.76		Detector NOT READY
11:35:36.30	1	Chan Status READY
11:33:24.39		System Init

Status	Events	**Pres**

- Pres 1
- Pres 2
- Meth Avrgs
- Channel 1
- Channel 2
- Channel 3
- Channel 4
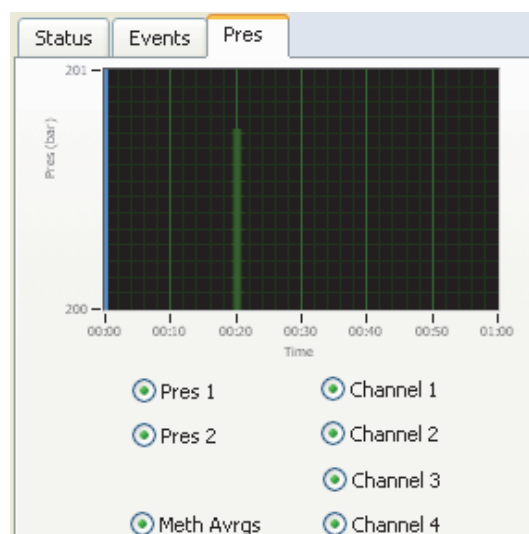
Follow these procedures:

- To pause the autosampler
- To control the channels
- To view the pressure trace
- To access the Aria multiplexing controls
- To view the last acquired file in the Qual Browser
- To open the Instrument Setup window

❖ **To pause the autosampler**

1. Click **Hold Autosampler**.

   The autosampler finishes the current autosampler step and then pauses. The LC pumps and autosampler continue.

2. To restart the autosampler, click **Hold Autosampler** again.

❖ **To control the channels**

Right-click the channel name and choose a command from the shortcut menu.
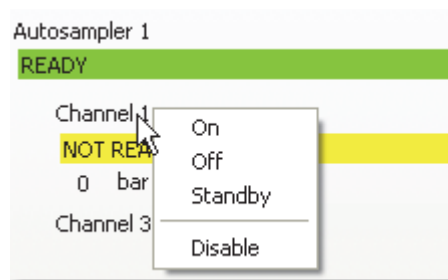
Table 64. Autosampler shortcut menu commands (Sheet 1 of 2)

Command	Description
On	Turns on a stopped pump and continues acquiring the sample list assigned to that channel.
Off	After the current sample completes, the application stops acquiring and the pump shuts down.

Table 64. Autosampler shortcut menu commands (Sheet 2 of 2)

Command	Description
Standby	After the current sample completes, the application stops acquiring. The pump continues to run.
Disable / Enable	**Disable**: Prevents the channel from receiving samples. When you choose **Disable** during a run, the application finishes the current sample on the channel and then stops.
	Enable: Allows the channel to receive samples.
	When you disable a channel that is set to **On**, the channel is highlighted in green and the status is READY. You can turn the channel to **Off** or **Standby**.

❖ **To view the pressure trace**

1. Click the **Pres** tab.

   The Pressure page displays a pump pressure graph for each sample in the batch. A fluctuation or change in the pump pressure could indicate a change in the chromatography conditions.
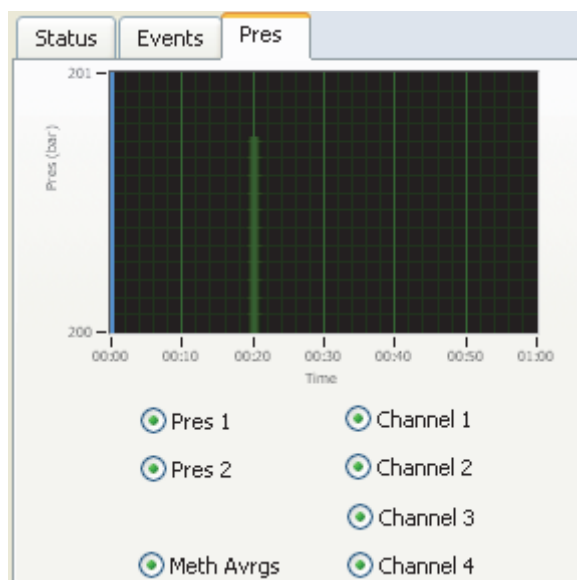
2. To view the pressure for a specific pump, select the **Pres 1** or **Pres 2** option.

   By default, the pressure for all pumps are displayed.

3. To view the pressure for a specific channel, select the corresponding channel number.

   By default, the pressure for all channels is displayed.

❖ **To access the Aria multiplexing controls**

Click **Direct Control**.

The Aria MX Direct Control dialog box opens.

For detailed descriptions of the features in this dialog box, refer to the *Transcend Systems with Xcalibur Software User Guide.*

❖ **To view the last acquired file in the Qual Browser**

Right-click in the header of the Devices page and choose **View Last File In Qual Browser** from the shortcut menu.

The Thermo Xcalibur Qual Browser window opens, displaying the last processed file.

❖ **To open the Instrument Setup window**

Right-click in the header of the Devices page and choose **Open Instrument Method Editor** from the shortcut menu.

The Thermo Xcalibur Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 309.

> **Note** Changes you make and save to the instrument method do not affect the currently running batch.

Queues Page

Use the Queues page to monitor and control the Acquisition, Processing, and Reporting queues.
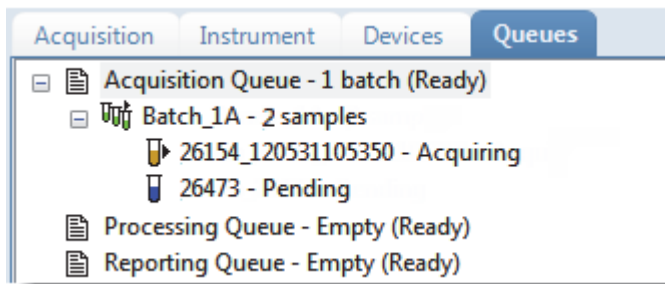
- Use the Queue-Level Commands to pause or remove batches in any of the queues.

- Use the Batch-Level Commands to pause or remove entire batches or samples within batches from any of the queues.

- Use Additional Commands to open the Qual Browser or the Instrument Setup window.

Queue-Level Commands

Use the queue-level commands to pause or remove batches in any of the queues on the Queues page. See "Queue-Level Shortcut Menu" on page 378.

Follow these procedures:

- To pause all batches in a queue
- To remove a single batch from a queue
- To remove all batches in a queue
- To remove all pending batches

❖ **To pause all batches in a queue**

1. Select a queue (Acquisition, Processing, or Reporting).

   Note When multiplexing is activated, you can have as many as four samples acquiring at once. Pausing the Acquisition queue does not affect any acquiring samples.

2. Right-click and choose **Pause Queue** from the shortcut menu.

   After the current sample completes, the application pauses all batches and samples in the specified queue. Only the selected queue is affected.
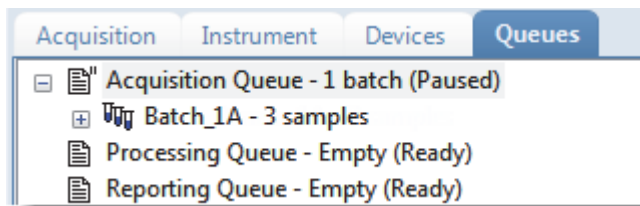
3. To restart a paused queue, select the queue, right-click, and choose **Resume Queue** from the shortcut menu.

❖ **To remove a single batch from a queue**

1. Select a queue (Acquisition, Processing, or Reporting).

2. Right-click and choose **Stop Active Batch** from the shortcut menu.

> **Note** This command is available only when there are active batches in the queue. Paused batches and batches that contain only pending samples are not "active."

The application confirms that you want to remove the active batch from the selected queue. After the current sample completes, the application removes the batch and all pending samples from the queue. Only the selected queue is affected.

❖ **To remove all batches in a queue**

1. Select a queue (Acquisition, Processing, or Reporting).

2. Right-click and choose **Stop All Batches** from the shortcut menu.

The application removes all batches with pending samples from the selected queue. The current sample continues to acquire. Only the selected queue is affected.

❖ **To remove all pending batches**

1. Select a queue (Acquisition, Processing, or Reporting).

2. Right-click and choose **Remove Pending Batches** from the shortcut menu.

> **Note** A pending batch is a batch in which all samples are pending. If any sample in the batch is active, the batch is not affected by this command.

The application removes all batches that contain only pending samples. Only the selected queue is affected.

Queue-Level Shortcut Menu

Use the commands on the shortcut menu to pause or remove batches in any of the queues on the Queues page.

Figure 92. Queue-level shortcut menu
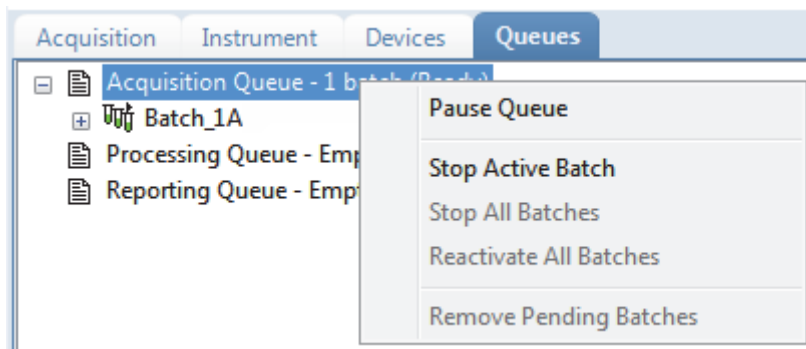
Table 65. Queue-level shortcut menu commands

Command	Description
Pause Queue	After the current sample completes, the application pauses the specified queue. Only the selected queue is affected.
Resume Queue	Returns the paused queue to active status.
Stop Active Batch	Removes all pending samples from the specified queue. The active sample is not affected.
Stop All Batches	Removes all pending samples and batches from the specified queue. The active sample is not affected.
Reactivate All Batches	Returns all paused batches to active status.
Remove Pending Batches	Removes all pending batches from the specified queue. The active batch is not affected.

Batch-Level Commands

Use the batch-level commands to pause or remove entire batches or samples within batches from any of the queues on the Queues page. See "Batch-level shortcut menu."

Follow these procedures:

- To remove a single pending sample from a batch

- To remove all pending samples from a batch

- To stop a batch

- To remove a pending batch

❖ **To remove a single pending sample from a batch**

1. Select a pending sample.

2. Right-click the sample and choose **Remove Sample** from the shortcut menu.
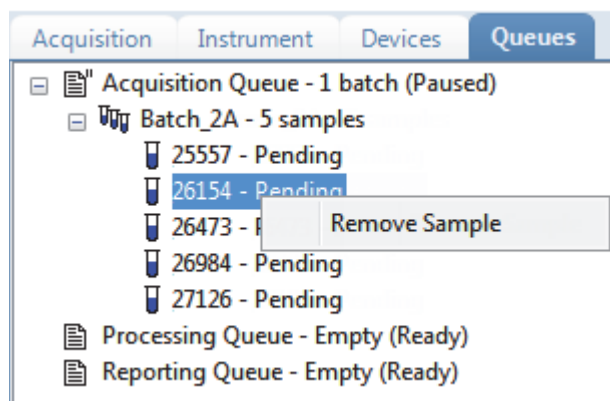
The application confirms that you want to remove the selected sample from the batch and then removes the sample.

❖ **To remove all pending samples from a batch**

1. Select a batch in any of the queues (Acquisition, Processing, or Reporting).

   The batch must have at least one pending sample.

2. Right-click and choose **Remove Pending Samples** from the shortcut menu.

   The application confirms that you want to remove all pending samples from the batch and then removes the samples. If the batch includes only pending samples, the application removes the batch from the queue.

❖ **To stop a batch**

1. Select an active batch in any of the queues (Acquisition, Processing, or Reporting).

   Note The batch must have at least one active sample and one pending sample.

2. Right-click and choose **Stop Batch** from the shortcut menu.

   The application confirms that you want to remove the selected batch from the queue. After the current sample completes, the application removes the batch and all pending samples from the queue.

❖ **To remove a pending batch**

1. Select a pending batch in any of the queues (Acquisition, Processing, or Reporting).

   Note A pending batch is a batch in which all samples are pending. If any sample in the batch is active, this command is not available.

2. Right-click and choose **Remove Pending Batch** from the shortcut menu.

   The application confirms that you want to remove the selected batch from the queue and then removes the batch from the queue.

Figure 93. Batch-level shortcut menu
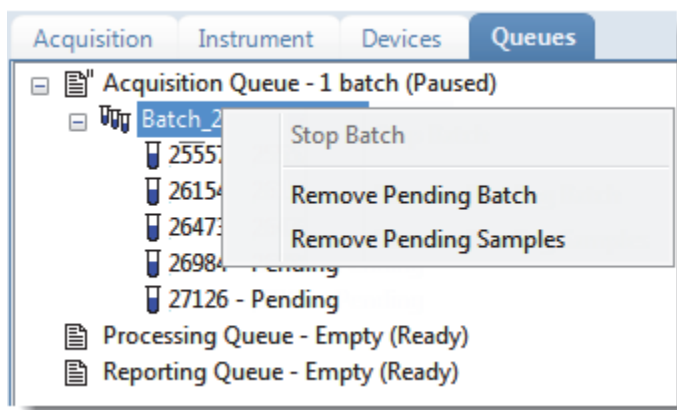
Table 66. Batch-level shortcut menu commands

Command	Description
Stop Batch	After the current sample completes, the application removes all samples in the selected batch.
Remove Pending Batch	Removes all samples from the selected pending batch.
Remove Pending Samples	Removes all pending samples from the selected batch.

Additional Commands

Use the commands on this shortcut menu to open the Qual Browser or the Instrument Setup window.

❖ **To view the last acquired file in the Qual Browser**

Right-click below the queues list in the Queues page and choose **View Last File In Qual Browser** from the shortcut menu.

> **Note** You must click in the white space below the list of queues. Clicking on or to the right of the queues displays queue-, batch-, or sample-level shortcut menus.

The Thermo Xcalibur Qual Browser window opens, displaying the last processed file.

❖ **To open the Instrument Setup window**

Right-click below the queues list in the Queues page and choose **Open Instrument Method Editor** from the shortcut menu.

> **Note** You must click in the white space below the list of queues. Clicking on or to the right of the queues displays queue-, batch-, or sample-level shortcut menus.

The Thermo Xcalibur Instrument Setup window opens, displaying the currently running instrument method.

For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 309.

> **Note** Changes you make and save to the instrument method do not affect the currently running batch.

Real-Time Trace Display

As each sample acquires, the real-time chromatogram pane shows the retention time and intensity of the TIC trace.
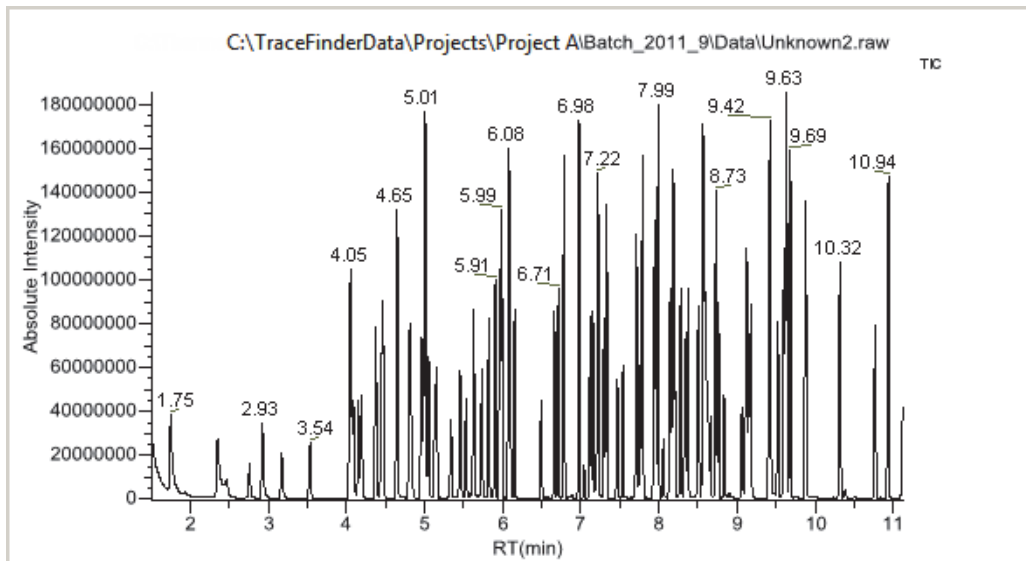
By default, the Real Time Status pane shows only the TIC trace as each sample acquires. To observe specific traces, such as the internal standard, use the RTV Display Traces function to display multiple traces.

When you create your method, you can specify additional traces to display in the real-time viewer and in which order the traces are displayed. The application always displays the TIC trace in the top pane. See "Real Time Viewer" on page 186.

❖ **To display multiple traces**

Right-click the chromatogram pane and choose the number of traces to display.

RTV display traces:	▶	TIC only
		TIC + 1
		TIC + 2
		TIC + 3
		TIC + 4
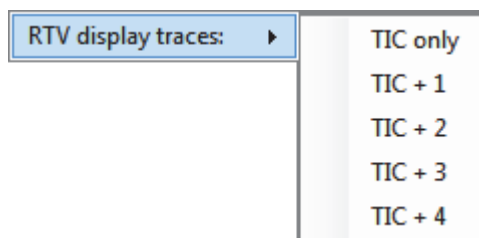
The chromatogram pane displays real-time chromatograms for the selected number of traces.

The TIC is always displayed at the top. When there are more traces than can fit in the pane, you can scroll through the traces.

For each trace, the application displays the mass or precursor mass.

Figure 94. Real-time trace display with multiple traces
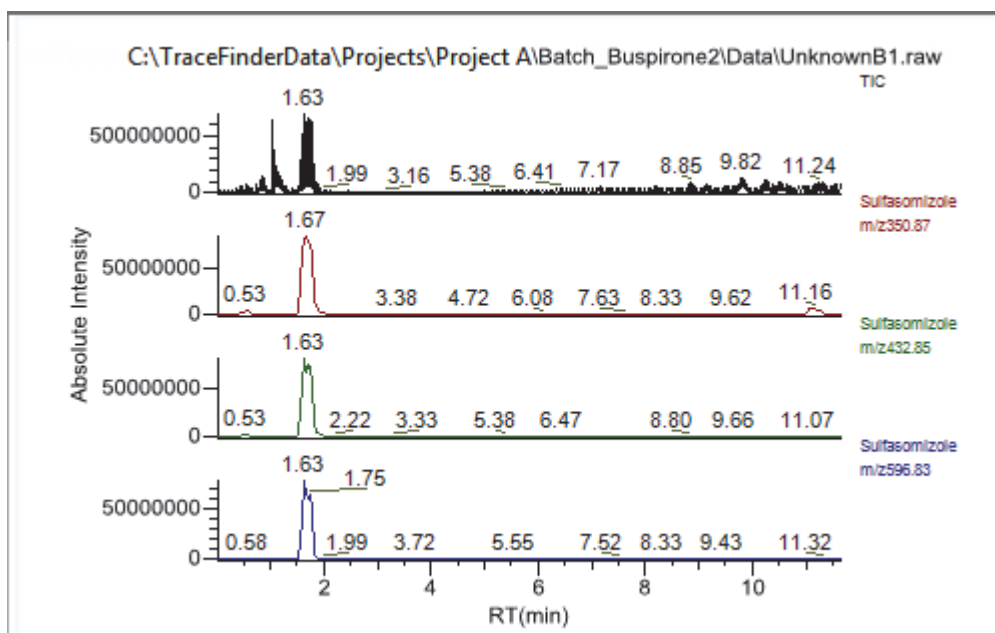
Sample Types

The TraceFinder application uses the following sample types in all sample definitions and reports. To view example standard reports specific to a sample type, see Appendix A, "Reports."

Table 67. Sample type definitions

Sample type	Definition
Negative	Contains no target compounds but might contain an ISTD when you use the internal standard quantitative analysis technique. By analyzing a blank sample, you can confirm that there are no residual compounds in the solvent system that can cause erroneous results.
Unextracted	Similar to a Negative sample, but contains target compounds. By analyzing a sample, you can confirm that there are no residual compounds in the solvent system that can cause erroneous results.
Calibrator	(Calibration standard) Contains known amounts of all target compounds. The purpose of a standard is to measure the response of the instrument to the target compounds so that the processing software can generate a calibration curve for each compound.
QC	(Quality Check) Contains a known amount of one or more specific target compounds. The application places check standard samples in the sequence so that it can test quantitative analysis results for quality assurance purposes. After the application analyzes the QC sample, it compares the measured quantity with the expected value and an acceptability range. The quantitative analysis of a QC sample is classified as *passed* if the difference between the observed and expected quantities is within the user-defined tolerance. A QC sample is classified as *failed* if the difference between the observed and expected quantities is outside the user-defined tolerance.
Solvent	Contains only solvent.
Specimen	Used for quantitative analysis of samples.
Hydrolysis	Checks the degradation of compounds dissolved in water.

Using the Analysis Mode

This chapter includes instructions about using the features of the Analysis mode.

Contents

- Using Quick Acquisition
- Working in the Batch View
- Creating a Batch Using the Batch Wizard
- Working in Data Review for Quantitation Methods
- Working in Data Review for Target Screening Methods
- Working in the Report View
- Working in the Local Method View
- Working in the Batch Template Editor

Use the Analysis mode to do the following:

- Submit a single sample for quick acquisition.
- Submit batches for acquisition, processing, or reports.
- Review batches, batch data, reports, and local methods.

❖ **To access the Analysis mode**

Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.

Using Quick Acquisition

Use the quick acquisition feature to quickly submit a single sample from any view of the Acquisition mode.

> **Note** The Quick Acquisition feature is available only when you activate it in the Configuration console. See "Quick Acquisition" on page 65.

❖ **To run a quick acquisition**

1. Choose **Go > Quick Acquire Sample** from the main menu or click the **Quick Acquire Sample** icon, ⬚ .

   The Quick Acquisition dialog box opens.

2. Select an instrument method.

3. Type a name for the raw data file that you acquire.

   Do not enter the .raw file extension.

4. For the path, browse to a folder where you want to write the acquired raw data file.

5. Select either the manual injection or the autosampler option:

   • To perform manual injection, do the following:

   i.   Select the **Manual Injection** option.

   ii.   Click **OK**.

   The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 369.

- To perform autosampler injection, do the following:

  i.   Select the **Use Autosampler** option.

  ii. In the Vial Position box, type a vial position.

  iii. In the Injection Volume box, type an injection volume.

       The minimum injection volume allowed is 0.1 µL; the maximum injection volume allowed is 5000 µL.

  iv. Click **OK**.

       The Quick Acquisition dialog box opens.

  v.   Select the **Use** check box for the device that you want to use for this acquisition.

  vi. (Optional) Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

       This is usually the autosampler.

  vii. (Optional) Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

       When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.

  viii.(Optional) Select the **Priority** check box to place the sample immediately after any currently acquiring sample.

  ix. (Optional) Select a value for the Post-run System State: **Unknown**, **On** (default), **Off**, or **Standby**.

       The application sets the system to this state after it acquires the last sample.

  x.   Click **OK**.

  The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 369.

Working in the Batch View

In the Batch View, you can manually create and edit a new batch or open and edit a previously saved batch. When you submit a batch, you can acquire and process data and optionally create reports for the submitted samples.

The Analysis mode includes a toolbar:

Use the toolbar or the equivalent commands on the Batch View shortcut menu to create the sample list and submit samples for acquisition. See "Toolbar" on page 401 or "Batch View Shortcut Menu" on page 405.

This section includes the following topics:

- Samples Page

- Auto Samples Page

- Reference Samples Page

- Threshold Samples Page

❖ **To open the Batch View**

1. Click **Analysis** in the navigation pane of the current mode.

2. In the Analysis navigation pane, click **Batch View**.

The Batch View navigation pane opens.

Available only for quantitative batches when you activate Intelligent Sequencing in the Configuration console.

Available only for quantitative batches.
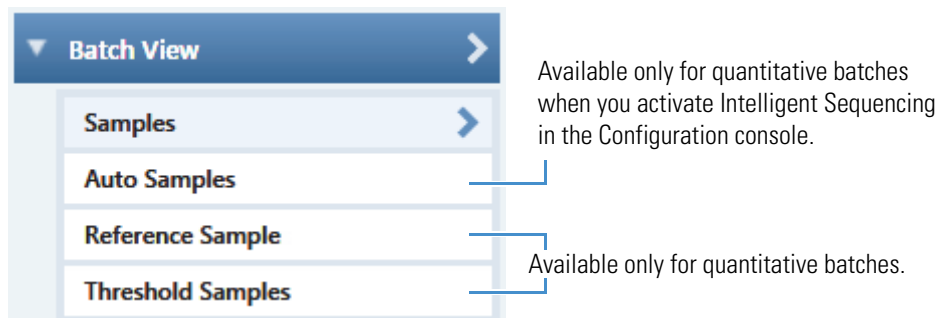
Samples Page

To open the Samples page, click **Samples** in the Batch View navigation pane.

This section contains information about the following topics:

- Samples Page Features
- Creating a New Batch
- Editing a Batch
- Submitting a Batch

Samples Page Features

The Samples page is divided into three panes:

- Samples pane

  Use the sample list pane to create a batch. See "Samples Pane" on page 392.

- Automated Batch Reports pane

  Use the Automated Batch Reports pane to select the type of output formats that you want to generate for the reports. See "Automated Batch Reports Pane" on page 407.

- Compound Active Status pane

  Use the Compound Active Status pane to make specific compounds active or inactive. See "Compound Active Status Pane" on page 409.

Samples pane

Automated Batch Reports pane   Compound Active Status pane

Tip To resize the panes, drag the separators that divide the panes.

Samples Pane

The samples pane includes the following features:

- Column Display

- Status Indicators

- Groups

- Blank Subtraction in Target Screening Batches

- Sample Weight Calculation

- Instrument Methods

- Toolbar

- Batch View Sample List

- Batch View Shortcut Menu

Column Display

The sample list contains many columns of information. You can scroll to see all the columns of information, and you can customize which columns to display and their display order.

Follow these procedures:

- To scroll the sample list

- To customize the column display

❖ **To scroll the sample list**

Use the horizontal scroll bar at the bottom of the sample list to view all the information.

When you use the scroll bar at the bottom of the sample list, the Status, Filename, and Sample Type columns stay fixed while the other columns scroll right and left.

❖ **To customize the column display**

1. Right-click the sample list and choose **Modify Columns** from the shortcut menu.

   The Modify Columns dialog box opens. See "Modify Columns dialog box."

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

   These columns are displayed after the Status, Filename, and Sample Type, columns.

3. To arrange the order of the columns, do the following:

   a. In the Displayed Columns pane, select a column name.

   b. Use **Up** or **Down** to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Batch View sample list, and the last column in the list represents the rightmost column in the Batch View sample list.

      > **Note** You cannot move the Status, Filename, Sample Type, or Level column.

4. To change the width of a column, do the following:

   a. In the Displayed Columns pane, select the column width.

5	Sample ID	100
▶ 6	Sample name	100
7	Vial position	100

   b. Type a new value for the width.

5. Repeat step 4 for all columns whose widths you want to change, and click **OK**.

   The columns in the sample list immediately reflect your changes. The application uses these settings for all sample lists in the Batch View.

Figure 95. Modify Columns dialog box
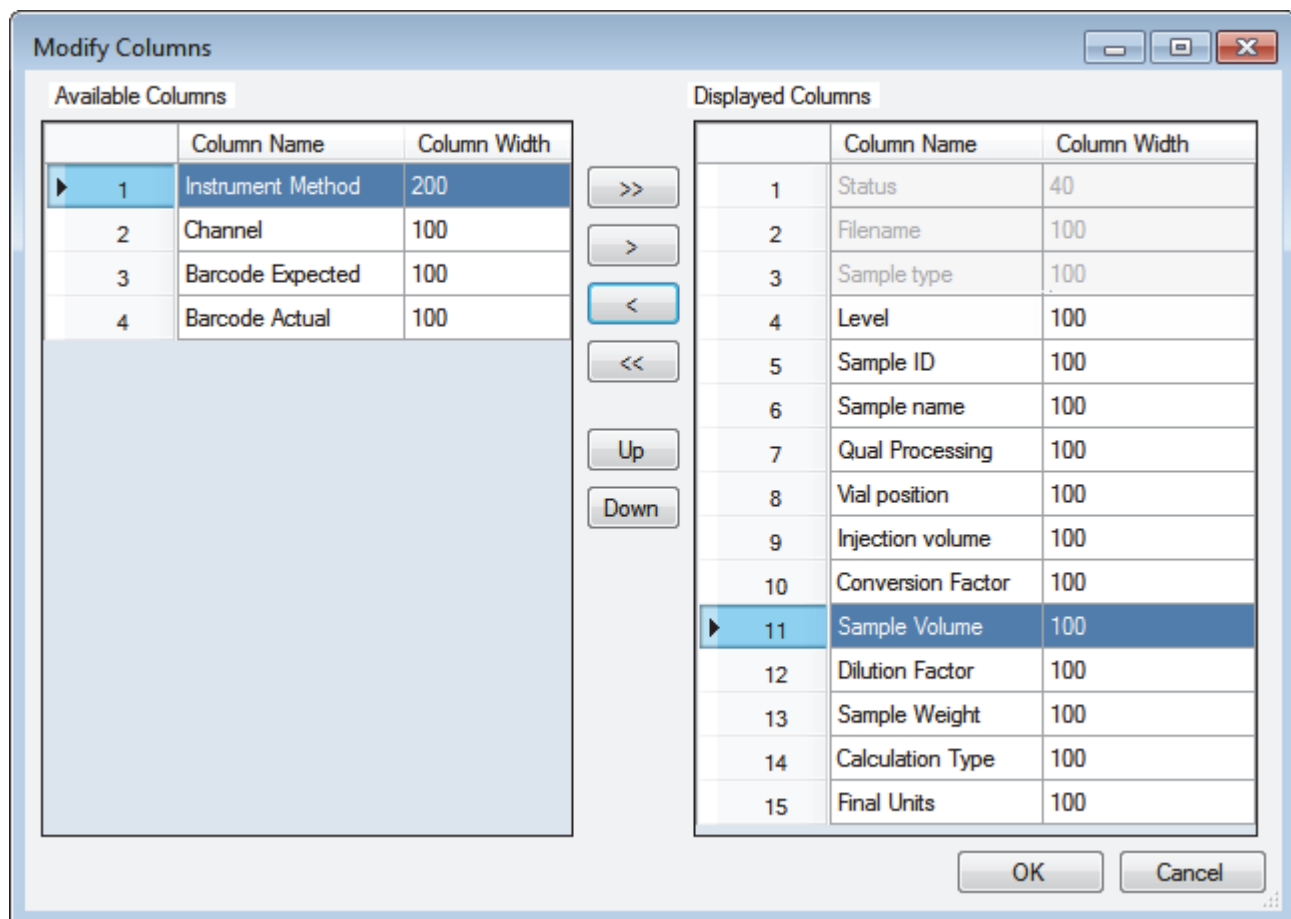
Table 68. Modify Columns function buttons

Function	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
<	Moves the selected column to the Available Columns pane. You cannot move the Status, Filename, or Sample Type column.
<<	Moves all columns except Status, Filename, and Sample Type to the Available Columns pane.
Up	Moves the selected column name in the Displayed Columns pane one row up in the column order. You cannot move the Status, Filename, or Sample Type column.
Down	Moves the selected column name in the Displayed Columns pane one row down in the column order. You cannot move the Status, Filename, or Sample Type, column.

Note In target screening batches only, a Blank Subtraction column is added to the fixed columns.

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

Groups

Use the Groups feature to assign samples to a group.

After you create groups, you can choose one of the samples as a threshold sample for the group and then view the samples in the group in the Comparative View in the Analysis mode.

❖ **To create a group**

1. For each sample, click the Groups column and type the name of a group.

   > **Note** Group names are not case sensitive and are always interpreted as lowercase. For example, if you assign one sample to "GroupA" and another sample to "groupa", both samples will be assigned to "groupa" on the Threshold Samples page.

2. Repeat step 1 for each sample you want to include in a group.

3. Create as many groups as you want.

   > **Note** To assign a sample to multiple groups, separate the groups with a comma.

Status	Filename	Groups
🟢	Benzo26473	groupB, groupA
🟢	Benzo25557	groupB
🟢	Benzo26154	groupB, groupA

For information about specifying a threshold sample for a group of samples, see "Threshold Samples Page" on page 434.

For information about viewing grouped samples in Data Review, see "Comparative View" on page 474.

Blank Subtraction in Target Screening Batches

In target screening batches only, use the Blank Subtraction feature to select which negative samples you want to use for peak subtraction. The application subtracts the areas of the peaks in the selected negative samples from the matching areas in the specimen samples.

Status	Filename	Sample type	Blank Subtraction
🟡	Benzo25557	Negative	☑
🟡	Benzo25558	Specimen	☐
🟡	Benzo25559	Negative	☑
🟡	Benzo25560	Specimen	☐

When you process the batch sequence, the application subtracts the peaks in a selected negative sample from all specimen samples that follow it, until it encounters another negative sample.

To activate the Blank Subtraction feature, see "To specify peak filter settings" on page 232.

Sample Weight Calculation

Use the sample weight features to calculate the conversion factor for a sample. The application uses different methods to calculate the conversion factor for liquid or solid calculation types.

Liquid: *SampleVolume ÷ DilutionFactor*

Solid: (*SampleVolume × DilutionFactor*) ÷ *SampleWeight*

Manual: The application does not calculate the Conversion Factor. Instead, you can enter the Conversion Factor value.

Follow these procedures:

- To display the features for calculating sample weight
- To calculate the conversion factor for a liquid sample
- To calculate the conversion factor for a solid sample
- To manually specify the conversion factor for a sample

❖ **To display the features for calculating sample weight**

If the Conversion Factor, Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns are not visible, right-click and choose **Enable Sample Weight Calculation** from the shortcut menu.

Conversion Factor	Sample Volume	Dilution Factor	Sample Weight	Calculation Type	Final Units
1.000	1	1	1	Liquid ▼	
1.000	1	1	1	Solid ▼	
1.000	1	1	1	Manual ▼	

❖ **To calculate the conversion factor for a liquid sample**

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, on the Active View page in the Report View, or in reports.

The application uses the following formula to calculate the Conversion Factor:

SampleVolume ÷ DilutionFactor

❖ **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, on the Active View page in the Report View, or in reports.

The application uses the following formula to calculate the Conversion Factor:

$(SampleVolume \times DilutionFactor) \div SampleWeight$

❖ **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, on the Active View page in the Report View, or in reports.

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.

❖ **To specify instrument methods for samples**

1. Display the Instrument Method column in the sample list:

   a. Right-click the sample list and choose **Modify Columns** from the shortcut menu.

      The Modify Columns dialog box opens.

   b. In the Available Columns pane, select **Instrument Method**.

   c. Click [>] to move the Instrument Method column to the Displayed Columns pane.

   d. Click **OK**.

   The application displays the Instrument Method column, defaulting to the instrument method specified in the master method.

2. Click the Instrument Method column and select an instrument method from the list.

   This list contains all the available instrument methods. Instrument methods from external sources are prefixed with "Ext:".

   You can specify a different instrument method for each sample.

   When you submit the batch for acquisition, the application saves a copy of the selected instrument methods to the following folders:

   External instrument methods:

   …\TraceFinderData\Projects\…*batch*\Methods*method**ExternalMethods*

   Local instrument methods:

   …\TraceFinderData\Projects\…*batch*\Methods*method*

Toolbar

The Analysis mode includes this toolbar for creating and submitting a batch.

Table 69. Toolbar functions

Icon	Description
1 ⬍ ▯⊕	Adds the specified number of new, empty samples to the end of the sample list. See the instructions "To add samples to the list" on page 413.
1 ⬍ ▯⬇	Inserts a new, empty sample or samples above the selected sample. See the instructions "To insert samples into the list" on page 413.
▯—	Removes the selected samples from the sample list. See the instructions "To remove samples from the list" on page 414.
▯⬇	Adds imported samples from a CSV, an XML, or an SLD file to the sample list. See the instructions "To import samples into the list" on page 413.
⬥⬆	Submits only the selected samples for acquisition, processing, or report generation. See the instructions "To submit samples in the batch" on page 423.
⬜⬆	Submits the batch for acquisition, processing, or report generation. See the instructions "To submit samples in the batch" on page 423.
🜹	Opens the Batch Wizard 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 "Creating a Batch Using the Batch Wizard" on page 435.
⬥	Opens the Batch Template Editor where you can create a batch template that contains the basic settings and sample types for your batches. See "Working in the Batch Template Editor" on page 581.
⬛	Opens the Quick Acquisition dialog box where you can quickly submit a single sample. See "Using Quick Acquisition" on page 387.

Batch View Sample List

The sample list displays all the quantitative data for the samples of a batch.

Status indicators for each sample indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The sample list includes the following columns of information:

Figure 96. Batch View sample list

Note

- In target screening batches only, the sample list includes a Blank Subtraction column after the Sample Type column.

- Cells in the sample list that are not editable, such as Barcode Actual, are shaded and empty.

Table 70. Batch View sample list columns (Sheet 1 of 2)

Column	Description
Status	🔵 Sample is not acquired.
	🟡 Sample is acquired but not processed.
	🟢 Sample is acquired and processed.
	🟠 Sample is currently acquiring.
Groups	Threshold group to which a sample belongs. Samples can be viewed by group in the Comparative View of Data Review.
Filename	Name of the raw data file that contains the sample data.
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative. Default: Specimen
Qual Processing	Indicates samples to be processed with the qualitative peak processing criteria specified in the method. The Qualitative View displays processed data for the selected samples.
Blank Subtraction	Specifies a negative sample to use for blank subtraction.
Level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined, alphanumeric string that identifies a sample.
Sample Name	A user-defined name that identifies a sample.
Vial Position	The tray vial number used for an autosampler acquisition.
Injection Volume	The injection volume (in microliters) of the injected sample. When you are using an autosampler, you can set the default injection volume in the Autosampler dialog box in the Instrument View. The minimum and maximum injection volumes that you can use depend on the Autosampler you configure. The usable range depends on the injection mode and might be smaller than the displayed range. The Injection Volume value set in the master method overwrites the value in the instrument method. Range: 0.1 through 5000 μL

Table 70. Batch View sample list columns (Sheet 2 of 2)

Column	Description
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, on the Active View page in the Report View, or in reports. Default: 1
Instrument Method	Specifies the instrument to use for the acquisition. This column is hidden by default. To display this column, see "To customize the column display" on page 393.
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. The Channel column is available only when you have activated multiplexing in the Configuration console. See "Multiplexing" on page 70.
Barcode Expected	A user-entered barcode for the vial.
Barcode Actual	An actual barcode for the vial. This value is not editable.
Comment	A user-defined comment for the sample.
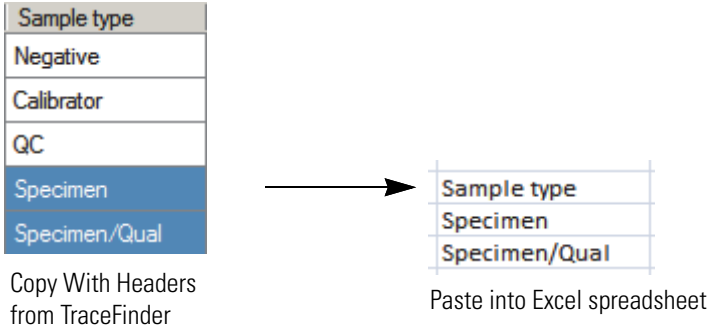
Batch View Shortcut Menu

The Batch View includes a shortcut menu for creating a batch.

Table 71. Batch View shortcut menu commands (Sheet 1 of 2)

Command	Description
Add Sample	Adds a single empty row to the sample grid.
Insert Sample	Inserts a single empty row to the sample grid above the selected row.
Insert Copy Sample	Copies the currently selected row and inserts a copy above the row.
Reinject Selected Samples	Creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth.
Remove Selected Samples	Removes selected samples from the sample grid.
Import Samples	Opens the Sample Import Tool. See "To import samples into the list" on page 413.
Browse In Raw File (Move)	Opens a dialog box where you can select a raw data file to use for the selected sample row. The application removes the raw data file from the source location.
Browse In Raw File (Copy)	Opens a dialog box where you can select a raw data file to use for the selected sample row. The application copies the raw data file from the source location.
Map Raw Files to Samples	Opens a dialog box where you can select multiple raw data files to use for the selected sample rows.
Copy Down	Copies the value in the selected row to all rows below it. This command is available only when you have selected a value that can be copied down.
Fill Down	Enters sequential values in the column starting with the value in the selected row and ending with the last row in the column. This command is available only when you have selected a value that can be filled down.
Modify Columns	Opens the Modify Columns dialog box. See "Column Display" on page 393.
Disable Sample Weight Calculation	
Copy	Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information to another application, such as an Excel spreadsheet. You cannot paste this data back into the Batch View sample list.

Table 71. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
Copy With Headers	Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy sample information to another application, such as an Excel spreadsheet. You cannot paste this data back into the sample list. For example Copy With Headers from TraceFinder Paste into Excel spreadsheet
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column.
Undo Last Paste	Removes the last pasted item in the Batch View.
Export to CSV File	Opens the Save As dialog box where you can save the current sample list to a CSV file.
Edit Instrument Method	Opens the Instrument Setup window where you can edit the parameters of the instrument method. • When you edit an external method, the application updates the method in the …\Xcalibur\methods folder. • When you edit an internal method, the application updates the method in the …\TraceFinderData\Projects\…*batch*\Methods*method* folder. For detailed information about editing instrument methods, see "Working with Instrument Methods" on page 309.

Automated Batch Reports Pane

In the Automated Batch Reports pane, you can view the reports that are selected for this batch and modify which output formats are generated for each report.

❖ **To edit the sample-level output formats**

1. Click the **Sample Level** tab.

   The application displays reports and the output formats as they were specified in the method.

Automated Batch Reports

		Report Name	Type	Print	Create PDF	Create XML	Create XLSM
▶	1	Sample Report	Standard	☐	☐	☐	☐
	2	Sample Report Long	Standard	☐	☐	☐	☐
	3	Chromatogram Report	Standard	☐	☐	☐	☐

   For detailed instructions about specifying which reports and output formats are generated, see "Specifying the Reports" on page 40.

2. Select or clear any of the check boxes for your reports.

3. To duplicate an output format for all reports for this sample, right-click the cell and choose **Copy Down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell. You can duplicate the output type only for reports that have this output format available.

4. To duplicate the output format for all samples in the batch, right-click the cell and choose **Apply Selection to All Samples** from the shortcut menu.

> **Tip** In the Batch View, you can change the output formats but you cannot change which reports are available.

❖ **To edit the batch-level output formats**

1. Click the **Batch Level** tab.

   The application displays the reports and the output formats as they were specified in the method.

   Automated Batch Reports

	Report Name	Type	Print	Create PDF	Create XML	Create XLSM
▶ 1	Batch Summary Report	Standard	☐	☐	☐	☐
2	Calibration Curve Report	Standard	☐	☐	☐	☐
3	Batch Report	Standard	☐	☐	☐	☐

   For detailed instructions about specifying which reports and output formats are generated and which reports are batch-level, see "Specifying the Reports" on page 40.

2. Select or clear any of the check boxes for your reports.

3. To duplicate the output format for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell. You can duplicate the output type only for reports that have this output format available.

   Tip In the Batch View, you can change the output formats but you cannot change which reports are available.

Compound Active Status Pane

In the Compound Active Status pane, you can choose specific compounds to be active or inactive.

❖ **To set a compound as active or inactive**

1. In the sample list, select a sample.

   All compounds in the selected sample are listed in the Compound Active Status pane.

   Compound Active Status

		RT	Compound	Active
▶	1	1.91	FENTHION-CE20-R20-TL75-QED	☑
	2	2.72	Sulfisomidine	☑

   The default active/inactive status is determined by the identification settings in the local method. For information about setting the identification parameters, see "Identification" on page 123.

   - To display compounds alphabetically, right-click and choose **Sort by Compound Name** from the shortcut menu.

   - To display compounds from shorter to longer retention time, right-click and choose **Sort by Retention Time** from the shortcut menu.

2. Select or clear the **Active** check box for the compound.

   For instructions about changing the active/inactive status in the Data Review view, see "Inactive and Excluded Compounds" on page 504.

Compound Active/Inactive Status

You can specify which compounds are active or inactive in the Local Method View or the Batch View.

Figure 97. Active and inactive compounds in the Local Method View

For details about setting the status on the Identification page, see "Identification" on page 123.

Figure 98. Active and inactive compounds in the Batch View

For details about setting the status in the Batch View, see "Compound Active Status Pane" on page 409.

Creating a New Batch

In the Batch View, you can create a new batch.

Follow these procedures:

- To create a new batch
- To add samples to the list
- To insert samples into the list
- To import samples into the list
- To remove samples from the list
- To copy a sample
- To reinject a sample
- To edit sample values
- To browse in raw data files
- To customize the column display

❖ **To create a new batch**

1. Choose **File > New > Batch** from the main menu.

   The Create New Batch dialog box opens, displaying all drives that contain projects. See "Create New Batch" on page 418.

2. Select a drive from the list.

   ```
   ▼ 📁 C:\TraceFinderData\Projects
      ▶ 📁 Default
      ▼ 📁 Project A
            📁 Subproject 1
         📁 Project B
   ▶ 📁 B:\TraceFinderData\Projects
   ```
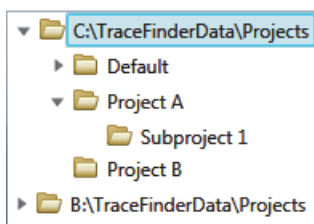
   Tip The application displays all configured and enabled repositories.

3. Select the folder where you want to store your batch.

   Tip To activate the Create button, you must enter a unique batch name. If the Create button is not activated, you have entered a batch name that is already used.

   To create a new folder for the storage location, see "Editing Folders for Batches" on page 420.

4. Select either **Quan** or **Screening** from the Type list.

   The batch list displays all batches in the selected folder. The Method list displays all methods for the selected type: quantitative or target screening.

5. Select a master method from the Method list.

   The list displays all available methods of the selected type, either quantitative or target screening.

Type: Quan ▼	Method	Alprazolom1 ▼
		Alprazolom1
		VitaminWater
		Benzos

Type: Screening ▼	Method	Alprazolom1 ▼
		Alprazolom1_screening
		VitaminWater_screening
		Benzos_screening
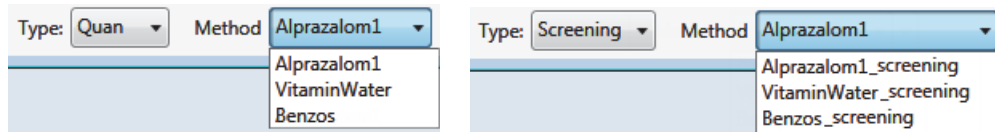
6. Click **Create**.

   A new batch opens with one Specimen sample.

   Batch View – Batch_13 [Quan]

   Local Method: Method_Benzos ▼   [Update]

	Status	Groups	Filename	Sample type	Qual Processing	Level	Sample ID	Sample name	Vial position
▶1	🔵		Unknown1	Specimen	☐				
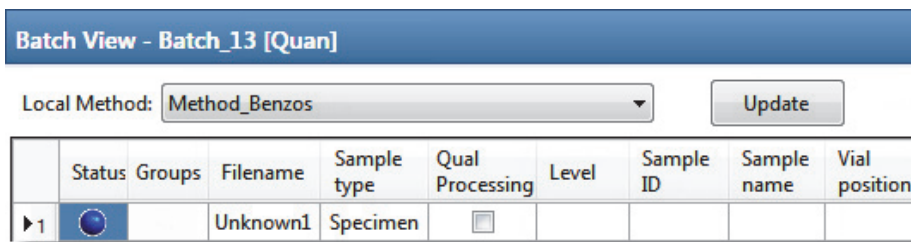
   The batch name in the title bar indicates that you are creating either a quantitative or a target screening batch.

❖ **To add samples to the list**

1. To add a single sample row, right-click the sample list and choose **Add Sample** from the shortcut menu.

2. To add multiple sample rows, select the number of rows and then click the **Add Sample** icon, [1] [⊞] .

   The application adds the specified number of new, empty samples to the end of the sample list.

❖ **To insert samples into the list**

Select the sample above which you will insert new, Specimen samples, and then do one of the following:

- To insert a single sample row, right-click and choose **Insert Sample** from the shortcut menu.

- To insert multiple sample rows, select the number of rows and then click the **Insert Sample** icon [1] [⊞] .

The application inserts the Specimen samples above the selected sample.

	Status	Filename	Sample type	Groups	Qual Processing	Level
1	🟡	cal_std_5	Calibrator		☐	5
2	🔵	Unknown2	Specimen		☐	
3	🔵	Unknown1	Specimen		☐	
4	🟡	cal_std_10	Calibrator		☐	10

Inserted samples ⎯ (pointing to rows 2 and 3)

❖ **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.

   Sample import tool

   Import from a file (.csv, .xml, .sld)

   [   ] [Browse...]

   Imported samples will be: [appended to the end of the list ▼]

   [Import] [Cancel]
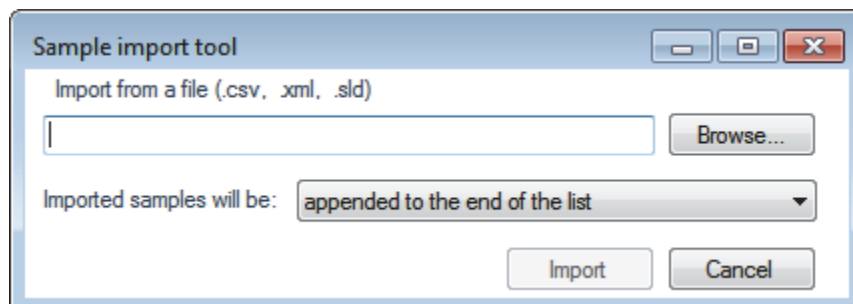
   From this dialog box, you can import samples from a CSV, an XML, or an SLD file.

2. Click **Browse** and select a CSV, an XML, or an SLD file that contains the samples to import.

3. From the Imported Samples Will Be list, select **Appended to the End of the List** or **Inserted at the Selected Row**.

4. Click **Import**.

   The Sample Import Tool dialog box closes, and the application adds the specified samples to the sample list.

   When you import samples from an Xcalibur sequence file (SLD), the TraceFinder application makes the following column name substitutions:

Xcalibur column	TraceFinder column
Position	Vial Position
Inj Vol	Injection Volume
Dil Factor	Conversion Factor

   When you import samples from an Xcalibur sequence file (.sld), the TraceFinder application makes the following sample type substitutions:

Xcalibur sample type	TraceFinder sample type
Blank	Negative
Std Bracket	Calibrator

5. (Optional) When using multiplexing, select a channel for each imported sample.

   Imported samples default to Auto.

   > **Note** The Channel column is available only when you have activated multiplexing in the Configuration console. See "Multiplexing" on page 70.

❖ **To remove samples from the list**

1. Select the samples that you want to remove.

   > **Tip** Use the CTRL or SHIFT keys to select multiple samples.

2. Right-click and choose **Remove Selected Samples** from the shortcut menu.

❖ **To copy a sample**

1. Select the sample that you want to copy.

2. Right-click and choose **Insert Copy Sample** from the shortcut menu.

   The TraceFinder application inserts the copy above the selected sample.

❖ **To reinject a sample**

1. In the sample list, select the sample that you want to reinject.

2. Right-click and choose **Reinject This Sample** from the shortcut menu.

   The TraceFinder application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth. The TraceFinder application copies all parameter values from the original sample.

❖ **To edit sample values**

1. For each sample, do one of the following:

   Type a new file name over the current filename.

   –or–

   Double-click the Filename column and locate a raw data file to use for the sample.

   –or–

   Right-click and choose **Browse in Raw File** from the shortcut menu, and then locate a raw data file to use for the sample.

   By default, the application sets the Sample Type to Unknown.

2. For each sample, click the Sample Type column and select a sample type from the list.

Available sample types			
Specimen	Hydrolysis	Solvent	QC
Unextracted	Calibrator	Negative	

3. For each Calibrator or QC sample, select a level from the Level list.

   The sample levels are defined in the master method. If there are no levels to select in the Level list, do the following:

   a. Return to the Method Development mode.
   b. Open the method.
   c. Click the **Compounds** tab.
   d. Click the **Calibration Levels** tab.
   e. Add the levels.
   f. Save the method.
   g. Return to the Analysis mode, and then click **Update**.

   Local Method: Method_Benzos ▾ Update

   The application updates the local method with the new sample levels.

   For detailed instructions, see Chapter 4, "Using the Method Development Mode."

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 horizontal scroll bar at the bottom of the sample list, the Status, Filename, and Sample Type columns stay fixed while the other columns scroll right and left.

For instructions to automatically copy or fill values in these columns, see Appendix C, "Using Copy Down and Fill Down."

❖ **To browse in raw data files**

1. Do one of the following:

Double-click the Filename column.

–or–

Right-click and choose **Browse in Raw File** from the shortcut menu.

The What Raw File Would You Like to Use dialog box opens.

2. Select a raw data file to use for the sample or use the CTRL key to select multiple files, and then click **Open**.

The application overwrites the selected, unacquired sample in the batch with the first "browsed in" file and adds any additional browsed in files below the selected sample.

For all browsed-in raw data files, the application sets the Status to Acquired, ⬤ , and sets the Sample Type to Specimen.

> **Note** You cannot overwrite an acquired sample. When you select a sample that is acquired, the application adds all browsed in files below the selected sample.

❖ **To customize the column display**

1. Right-click the Batch View sample list and choose **Modify Columns** from the shortcut menu.

   The Modify Columns dialog box opens.
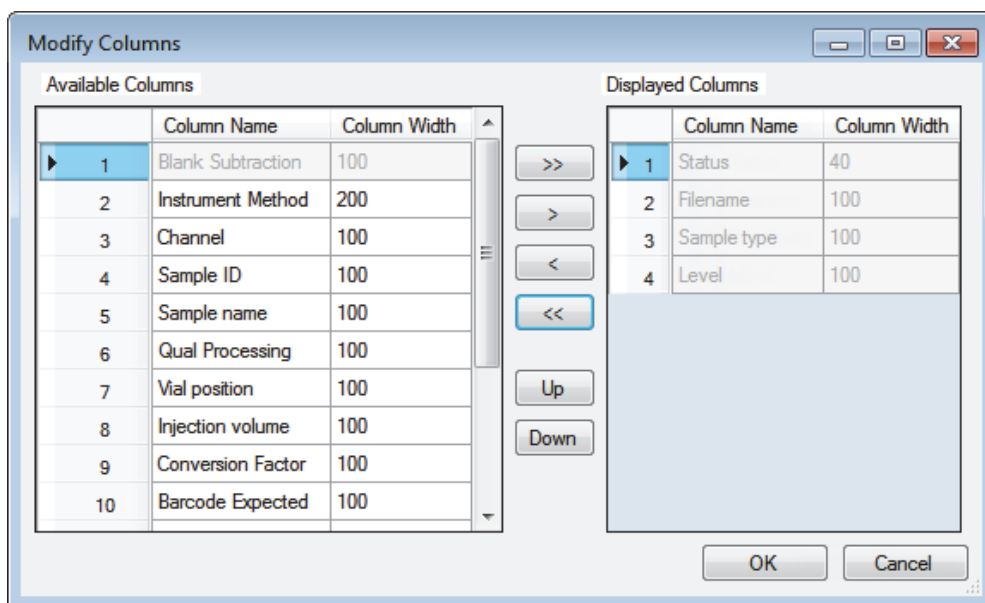
Table 72. Modify Columns dialog box function buttons

Function	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
<	Moves the selected column to the Available Columns pane. You cannot move the Status, Filename, Sample Type, or Level columns.
<<	Moves all columns except Status, Filename, Sample Type, or Level to the Available Columns pane.
Up	Moves the selected column name in the Displayed Columns pane one row up in the column order. You cannot move the Status, Filename, Sample Type, or Level columns.
Down	Moves the selected column name in the Displayed Columns pane one row down in the column order. You cannot move the Status, Filename, Sample Type, or Level columns.

2. Use the arrow buttons to move all the columns that you want displayed to the Displayed Columns pane.

   All the columns you select are displayed after the Status, Filename, Sample Type, or Level columns.

3. To arrange the order of the columns, do the following:

   a. In the Displayed Columns pane, select a column name.

   b. Use **Up** or **Down** to move the selected column up or down in the list.

      The first column in the list represents the leftmost column in the Batch View sample list, and the last column in the list represents the rightmost column in the Batch View sample list.

      > **Note** You cannot move the Status, Filename, or Sample Type columns.

4. To change the width of a column, do the following:

   a. In the Displayed Columns pane, select the column width.

7	Vial position	69
▶ 8	Injection volume	100
9	Calculation Type	100

   b. Type a new value for the width.

5. When you have completed your changes, click **OK**.

   The columns in the sample list immediately reflect your changes. The application uses these settings for all sample lists in the Batch View.

Create New Batch

Use the Create New Batch dialog box to select a folder and method for your batch and to name the new batch.
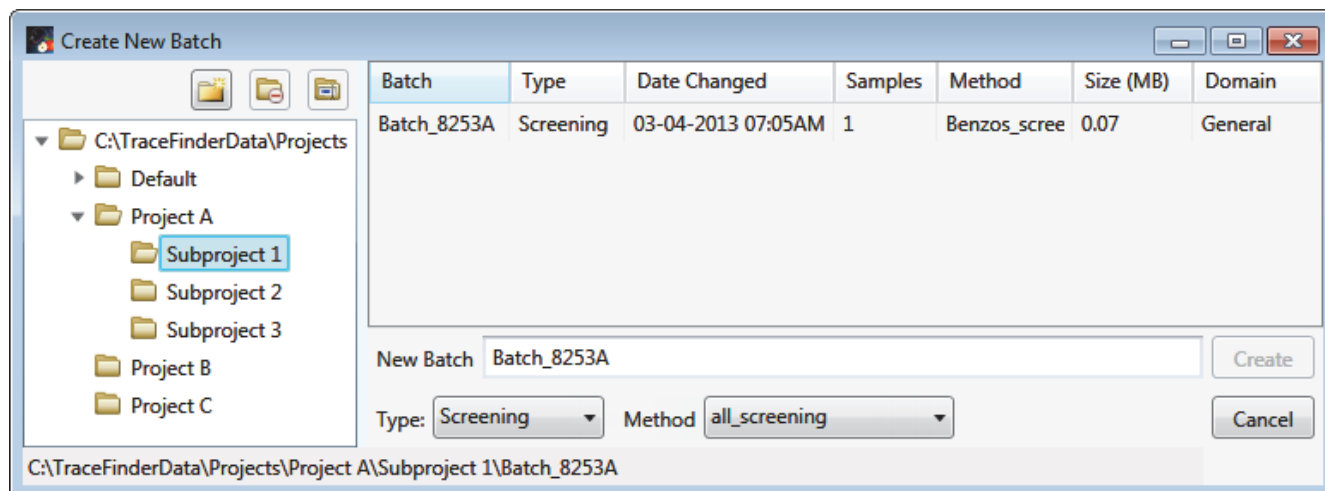
Table 73. Create New Batch dialog box parameters

Parameter	Description
 Create New Folder	Adds one of the following: • When a drive is selected, adds a new project-level folder to the drive. • When a project folder is selected, adds a subproject-level folder to the selected project. • When a subproject folder is selected, adds a lower-level folder to the subproject. Or, right-click and choose **Create Folder** from the shortcut menu.
 Delete Folder	With no confirmation prompt, immediately removes the selected folder. You cannot delete a folder that contains lower-level folders; you must delete the lower-level folders first. Or, right-click and choose **Delete** from the shortcut menu.
 Rename Folder	Renames the selected folder. Or, right-click and choose **Rename** from the shortcut menu.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan or Screening.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.
Method	Name of the method used to create the batch.
Size	Size of the batch in megabytes.
Domain	TraceFinder domain in which the batch was created: General, EFS, Clinical, or Forensic.
New batch parameters	
New Batch	Name of the new batch to create. **Note** If the Create button is not activated, you have entered a name that is already used or you have not selected a method.
Type	Type of batch to create: Quan or Screening.
Method	Method used to create the new batch.
Path	Path to the project in the TraceFinderData\Projects folder where the batch is created.
Function Buttons	
Create	Creates the specified batch and opens the Batch View for the new batch.
Cancel	Closes the Create New Batch dialog box without creating a batch.

Editing Folders for Batches

From the Create New Batch dialog box, you can create new folders for your batches. You can also delete or rename folders.

Use these procedures:

- To create new project folders
- To delete project folders
- To rename project folders

❖ **To create new project folders**

1. In the Create New Batch dialog box. select the folder for which you will create a new lower-level folder.

    - You can select the main TraceFinderData\Projects folder and create a new folder under it.

    - You can select one of the existing folders and create a lower-level folder under it.

2. Click the **Create Folder** icon, 🗀.

    The application adds a new lower-level folder to the selected folder.

3. Select the new folder name and type a name for the folder.

    Folder names are limited to 30 characters and can contain spaces and special characters, except for the following special characters: \ / : + ? ” < >

    > **Note** After you add a lower-level folder, you cannot rename the parent folder.

❖ **To delete project folders**

1. In the Create New Batch dialog box. select the folder to delete.

2. Click the **Delete Folder** icon, 🗀.

    With no confirmation prompt, the application immediately removes the selected folder.

    > **Note** You cannot delete folders that contains lower-level folders; you must delete the lower-level folders first.

❖ **To rename project folders**

1. In the Create New Batch dialog box, select the folder to rename.

2. Click the **Rename Folder** icon, 🗀.

    > **Note** You cannot rename folders that contain lower-level folders.

3. Type a new name for the folder and press ENTER.

    The application saves the new folder name.

Editing a Batch

In the Batch View, you can open a saved batch and edit the sample list. You can add samples, edit samples, or remove samples. If the batch has already been acquired, you can select specific samples for reinjection. If the batch has unacquired samples when you complete your edits, you can save it as a "ready to acquire" batch.

Follow these procedures:

- To open a saved batch
- To open a recent batch
- To edit samples in a batch
- To reinject a sample from a previously acquired batch

❖ **To open a saved batch**

1. Choose **File > Open > Batch** from the main menu.

   The Open Batch dialog box opens. See Open Batch dialog box.

2. Select a project and a subproject.

3. Select **Quan**, **Screening**, or **Any** from the Type list.

   The batch list displays all batches created with the selected type of method.

4. Select a batch from the list.

5. Click **Open**.

   The selected batch opens in the Batch View.

Figure 99. Open Batch dialog box

Open Batch							
▾ 📁 C:\TraceFinderData\Projec	Batch	Type	Date Changed	Samples	Method	Size (MB)	Domain
▸ 📁 Default	▸ Benzos_1	Screening	02-07-2013	3	BenzosA	29.20	General
▾ 📁 Project A							
📁 Subproject 1							
📁 Project B							
📁 Project C							Open
	Type: Screening ▾						Cancel

C:\TraceFinderData\Projects\Project A\Subproject 1\Benzos_1
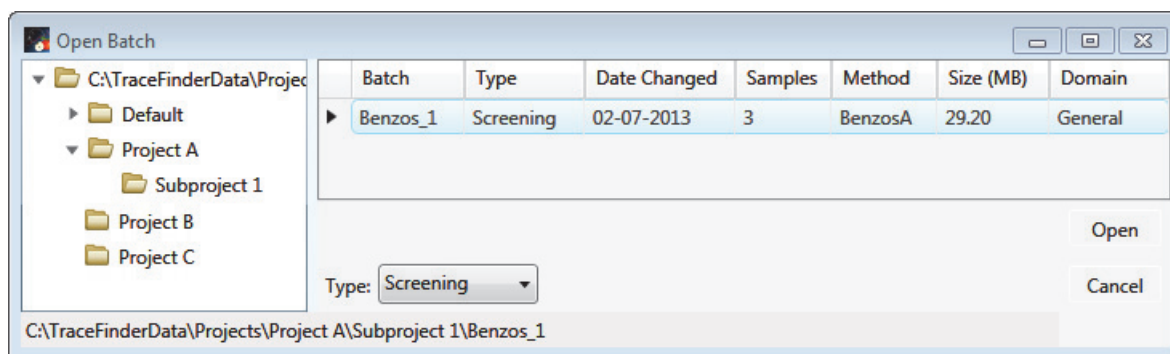
Table 74. Open Batch dialog box parameters (Sheet 1 of 2)

Parameter	Description
Batch	Name of batches in the selected project.
Type	Type of batch: Quan or Screening.

Table 74. Open Batch dialog box parameters (Sheet 2 of 2)

Parameter	Description
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: General, EFS, Clinical, or Forensic.
Path	Path to the project in the TraceFinderData\Projects folder where the batch is stored.
Function Buttons	
Type	Type of batch to display in the Batch list: Quan, Screening, or Any.
Open	Opens the Batch View for the selected batch.
Cancel	Closes the Open Batch dialog box without opening a batch.

❖ **To open a recent batch**

Choose **File > Recent Files > *batch*** from the main menu.
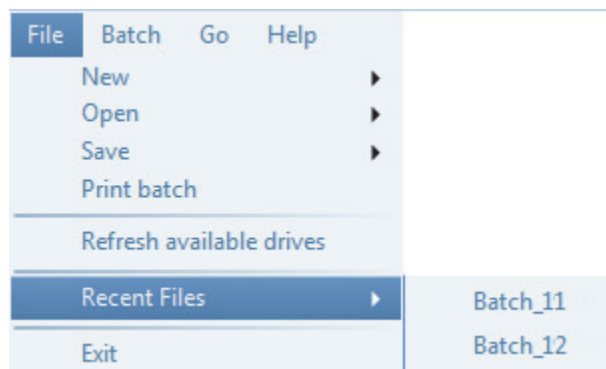
The selected batch opens in the Batch View.

❖ **To edit samples in a batch**

Use the commands described in "Working in the Batch View" on page 389.

You can add new samples, edit samples, or delete samples.

❖ **To reinject a sample from a previously acquired batch**

1. In the sample list, select the sample that you want to reinject.

2. Right-click and choose **Reinject This Sample** from the shortcut menu.

   The TraceFinder application creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth.

   The TraceFinder application copies all parameter values from the original sample.

   A green status icon indicates previously acquired samples (acquired and processed), and the sample name is grayed out. A blue status icon indicates samples created for reinjection (not acquired).

🔵	cal_50_INJ001	Calibrator	10
🟢	cal_50	Calibrator	10
🔵	cal_10_INJ001	Calibrator	10
🟢	cal_10	Calibrator	10

   When you submit all samples in this batch, the application acquires all samples (including previously acquired samples).

3. To save this batch with the new samples for reinjection, choose **File > Save > Batch** from the main menu.

   The batch is saved as a prepared batch that is ready to submit. You can open this batch from the Reinject Samples page in the Acquisition mode and submit the batch. The application acquires only the samples that have not been previously acquired.

Submitting a Batch

In the Batch View, you can submit an entire batch or only selected samples in the batch. When you submit a batch for acquisition and processing, you can choose to create reports for the submitted samples. See "Submit Options dialog box" on page 425.

For a description of commands on the shortcut menu, see "Batch View shortcut menu commands" on page 405.

❖ **To submit samples in the batch**

1. Do one of the following:

   • To submit all samples in the batch, click the **Submit Batch** icon, ⬛▶.

   • To submit specific samples, select the samples and click the

     Submit Selected Samples icon, ⬛▶.

   The Submit Options dialog box opens. See "Submit Options dialog box" on page 425.

2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.

   • When all submitted samples have been previously acquired, this option is not selected by default.

   • When any of the submitted samples have not been acquired, this option is selected by default.

3. To process the submitted samples, select the **Process Data** check box.

   You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

4. (Optional) Select the **Create Reports** check box.

5. (Optional with multiplexing activated) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.

6. (Optional without multiplexing activated) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   • **Next Available Batch** places the batch immediately after the currently acquiring batch.

   • **Next Available Sample** places the batch immediately after the currently acquiring sample.

7. (Optional) Click **Show Details** to display additional Acquisition parameters.

8. Select the **Use** check box for the device that you want to use for this acquisition.

9. (Optional) Select the **Start Device** check box to indicate the device that will initiate the communication with the other instruments.

   This is usually the autosampler.

10. (Optional) Select the **Start When Ready** check box to have all instruments start together when they are all ready.

    When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.

11. To start the selected processes, click **OK**.

Figure 100. Submit Options dialog box

Acquire Data selected

Acquire Data not selected

Table 75. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Samples	Range of samples to be submitted for acquisition, processing, or reporting.
Acquire Data	Submits the current batch to acquisition. • When all submitted samples have been previously acquired, this option is (by default) not selected. • When any of the submitted samples has not been acquired, this option is (by default) selected.
Process Data	(Default) Processes the data for the current batch.
With Peak Detection	(Default) Processes the data with peak detection. When cleared, this option lets you reprocess samples without performing peak detection.

Table 75. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
Create Reports	Creates reports for the current batch.
Priority Sequence	With multiplexing activated, places the batch immediately after the currently acquiring batch.
	Without multiplexing activated, specifies one of the following priority options to place the batch in the queue: • **Next Available Batch** places the batch immediately after the currently acquiring batch. • **Next Available Sample** places the batch immediately after the currently acquiring sample.
Acquisition pane	
Device Name	Lists all configured instruments.
	If the instrument that you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the TraceFinder application. You cannot configure an instrument while the TraceFinder application is running.
	Available only when the Acquire Data check box is selected.
Use	Specifies the instruments used for this acquisition.
	Available only when the Acquire Data check box is selected.
Start Device	Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler.
	Available only when the Acquire Data check box is selected.
Start When Ready	Starts the specified device when all the instruments are ready to acquire data. When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
Post-run System State	Specifies the system state after it acquires the last batch. On (default), Standby, or Off.
Function buttons	
Hide/Show Details	Collapses or expands the acquisition details of the Submit Options dialog box.
OK	Begins the selected processes.
Cancel	Closes the Submit Options dialog box without submitting any tasks.

Saving a Batch to a New Location

You can move the current batch to a different project folder, or you can make a copy of the current batch and save the copy to a different project folder.

Follow these procedures:

- To save a batch to another project folder
- To move a batch to another folder
- To create new project folders
- To delete project folders
- To rename project folders

❖ **To save a batch to another project folder**

1. Choose **File > Save > Save Batch As** from the main menu in the Analysis mode.

   The Save Batch As dialog box opens. See "Save Batch As Dialog Box" on page 429.

2. Select a storage location.

   The default storage location is C:\TraceFinderData\Projects.

3. Select or create a project folder.

4. Type a name for the new batch.

   If you are saving the batch to a different folder, you must give it a unique name. You cannot overwrite an existing batch in a folder.

5. Click **Save**.

   When you save the batch to a different folder, the reports reflect the original project folders and the application does not save the calibration history.

❖ **To move a batch to another folder**

1. Choose **File > Save > Move Batch** from the main menu in the Analysis mode.

   The Save Batch As dialog box opens. See "Save Batch As Dialog Box" on page 429.

2. Select a storage location.

   The default storage location is C:\TraceFinderData\Projects.

3. Select or create a project folder.

4. Type a name for the new batch.

   You must give the batch a unique name in the new subproject folder. You cannot overwrite an existing batch.

5. Click **Save**.

When you move the batch, the reports reflect the original project and subproject folders and the application does not save the calibration history.

❖ **To create new project folders**

1. In the Save Batch As dialog box. select the folder for which you will create a new lower-level folder.

   • You can select the main TraceFinderData\Projects folder and create a new folder under it.

   • You can select one of the existing folders and create a lower-level folder under it.

2. Click the **Create Folder** icon, .

   The application adds a new lower-level folder to the selected folder.

3. Select the new folder name and type a name for the folder.

   Folder names can contain spaces and special characters, except for the following special characters: \ / : + ? ” < >

   Note After you add a lower-level folder, you cannot rename the parent folder.

❖ **To delete project folders**

1. In the Save Batch As dialog box. select the folder to delete.

2. Click the **Delete Folder** icon, .

   With no confirmation prompt, the application immediately removes the selected folder.

   Note This feature is not available for folders that contain lower-level project or batch folders; you must first delete the lower-level project or batch folders.

❖ **To rename project folders**

1. In the Save Batch As dialog box. select the folder to rename.

2. Click the **Rename Folder** icon, .

   Note This feature is not available for folders that contain lower-level project or batch folders; you must first delete the lower-level project or batch folders.

3. Type a new name for the folder and press ENTER.

   The application saves the new folder name.

Save Batch As Dialog Box

Use the features on the Save Batch As dialog box to save a batch to a new name or to move a batch to a different project folder.

Figure 101. Save Batch As dialog box

Table 76. Save Batch As dialog box parameters (Sheet 1 of 2)

Parameter	Description
Create New Folder	Adds one of the following: • When a drive is selected, adds a new project-level folder to the drive. • When a project folder is selected, adds a subproject-level folder to the selected project. • When a subproject folder is selected, adds a lower-level folder to the subproject. Or, right-click and choose **Create Folder** from the shortcut menu.
Delete Folder	With no confirmation prompt, immediately removes the selected folder. You cannot delete a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders. Or, right-click and choose **Delete** from the shortcut menu.
Rename Folder	Renames the selected folder. You cannot rename a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders. Or, right-click and choose **Rename** from the shortcut menu.
Batch table	
Batch	Name of batches in the selected project.
Type	Type of batch: Quan or Screening.
Date Changed	Date that the batch was last updated.
Samples	Number of samples in the batch.

Table 76. Save Batch As dialog box parameters (Sheet 2 of 2)

Parameter	Description
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: General, EFS, Clinical, or Forensic.
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.
Function 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	Lets you rename the selected folder. You cannot rename a folder that contains lower-level project or batch folders; you must first delete the lower-level project or batch folders.
Expand Child Nodes	Expands all project and subproject folders in the Project tree.
Collapse Child Nodes	Collapses all project and subproject folders in the Project tree.

Auto Samples Page

The Auto Samples page identifies the Solvent or Negative samples to use for any Auto Sample or Auto Sample and Reinject failure actions as specified on the Intelligent Sequencing page of the method. See "Editing the Intelligent Sequencing Page" on page 204.

Each sample type that you specify for a failure action on the Intelligent Sequencing page must be defined on the samples list on the Auto Samples page.

❖ **To open the Auto Samples page**

Click **Auto Samples** in the Batch View navigation pane.

The Auto Samples page opens. See Auto Samples page.

❖ **To add an auto sample type**

1. Right-click and choose **Add Auto Sample** from the shortcut menu, or click the **Add New Auto Sample** icon, 1 ▸.

   The application adds a Solvent sample to the sample list.

   You can add, insert, or remove samples from this list as you would any sample list. See "Samples Page" on page 390.

2. To change the sample type to a Negative, click the Sample Type column and select Negative from the list.

3. In the Injection Volume column for the sample, type a volume.

   The minimum injection volume value allowed is 0.1 µL; the maximum injection volume value allowed is 5000 µL.

4. In the Number of Injections column, type the number of injections available in the designated Solvent or Negative vial.

   After auto sample injections have occurred, you can return to this page to view the number of Injections Used in each vial.

5. In the Vial Position column, type the vial position for the Solvent or Negative sample.

Figure 102. 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 77. Auto Samples page parameters

Column	Description
Sample Type	The sample type for the auto sample injection as specified on the Intelligent Sequencing page—either Solvent or Negative. Default: Solvent
Injection Volume	The injection volume used for the sample acquisition as specified on the Samples page. Range: 0.1 through 5000 µL
Injections Used	The number of times a vial has been used. The count is cumulative across all batches.
Number of Injections	The number of injections available in the designated Solvent or Negative vial.
Vial Position	Vial position for this sample type as specified on the Samples page.

Reference Samples Page

The Reference Samples page displays the reference samples that you selected for this batch.

❖ **To specify a chromatogram reference sample**

1. In the Batch View, click **Reference Samples**.

   An empty reference sample table opens.
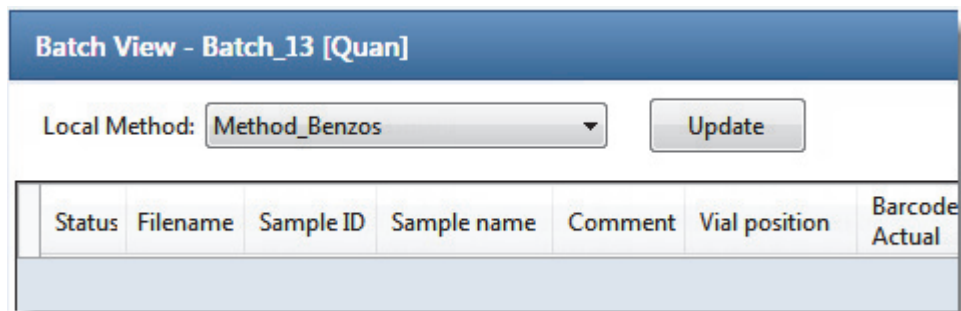
2. Click the **Add Reference Sample** icon, , or right-click and choose **Add Reference Sample** from the shortcut menu.

   The Open Chromatogram Reference Sample dialog box opens.
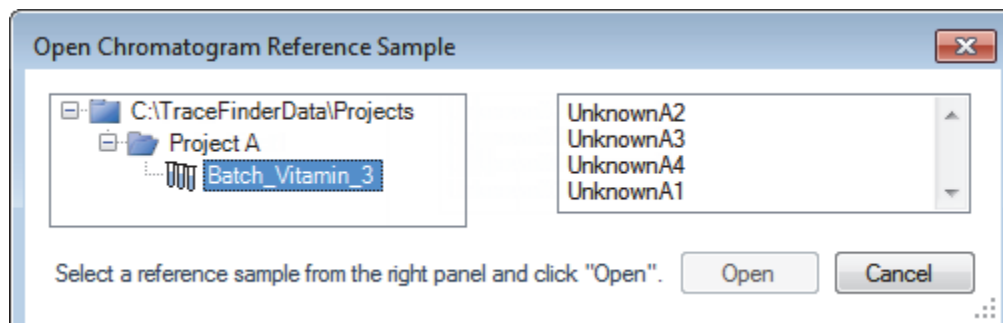
   Note If you are using a new method, no reference samples appear here. You must first process a batch using the current method to see the reference samples in this list.

3. Select a project from the list of projects.

4. Select a subproject from the list of subprojects.

5. Select a batch from the list of batches.

   The application displays only batches that were created using the current master method.

6. Select a sample from the list of processed samples.

   The application displays all the processed samples in the selected batch. Before using a sample as a reference sample, you must have processed the sample with the current master method.

7. Click **Open**.

Threshold Samples Page

For each group in a batch, you can specify a sample in the group as the threshold sample to use in the Comparative View.

❖ **To specify a threshold sample**

1. In the Batch View, click **Threshold Samples**.

2. Click the Sample list for each group and select a sample in the group to be the threshold sample.

Group	Sample
▶ groupb	Benzo26473 ▼
	Benzo26473
	Benzo25557
	Benzo26154

The Comparative View uses the threshold method and amount you specified in the method, the group you created on the Samples page, and the threshold sample you selected on this page to define the threshold guide that it displays on the sample peak plots.

For information about specifying the method to use for creating a threshold guide, see "Threshold" on page 197.

For information about creating groups, see "Groups" on page 396.

For information about using the threshold guide in the Comparative View, see "Comparative View" on page 474.

Creating a Batch Using the Batch Wizard

Using the Batch Wizard, you can define a sequence composed of various sample types to be assembled into a batch of samples. Before you can create a batch with the Batch Wizard, you must have a master method and a batch template. See "Creating a New Master Method" on page 86 and "Working in the Batch Template Editor" on page 581.

> **Note** This batch wizard is available only when you select the Batch Template Wizard (EnviroLab/ToxLab/QuanLab forms) style in the Configuration console. See "Batch Wizard Style" on page 66.

Follow these procedures in the Batch Wizard to create and submit a batch:

- Selecting a Batch Template

- Specifying a Batch

- Submitting the Batch

- (Optional) Selecting Calibration Files and Compounds

The Batch Wizard workflow uses the following pages:
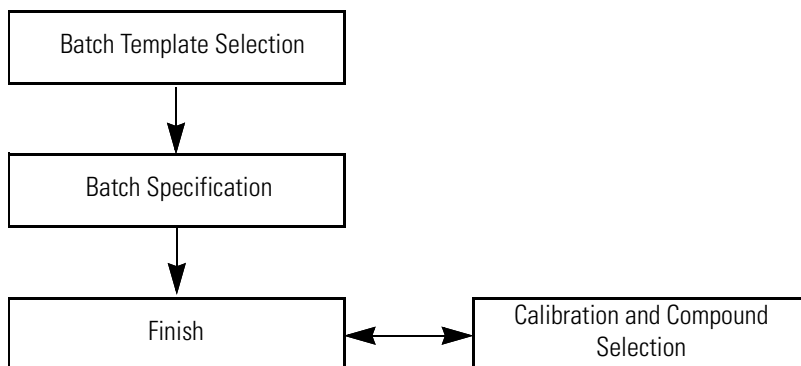
❖ **To open the Batch Wizard**

Choose **File > New > Batch Using Wizard** from the main menu in the Analysis mode, or click the **Batch Wizard** icon, .

> **Note** Creating a batch using the Batch Wizard requires that you have previously created at least one batch template. See "Working in the Batch Template Editor" on page 581.

The Batch Template Selection page of the Batch Wizard opens. For descriptions of the parameters on the Batch Template Selection page, see "Batch Template Selection page" on page 437.

Selecting a Batch Template

From the Batch Template Selection page, you can create a list of samples to acquire or process. For descriptions of the parameters on the Batch Template Selection page, see "Batch Template Selection page."

❖ **To create a sample list**

1. From the Project list, select a project.

2. From the Subproject list, select a subproject.

   The Available Templates area lists all the templates in the specified subproject.

3. Select a starting vial position.

   The default is vial position 1, but you can choose to start your acquisition at any vial position.

4. (Optional) To simplify the sample list, select the **Quick Mode** check box.

   Quick Mode limits the columns of information on the Batch Specification page to the following:
   - Sample Type
   - Sample ID
   - Injection Volume
   - Conversion Factor

5. From the Available Templates list, select a template that defines your layout preference.

   The Template Layout area displays sample information in the selected batch template and a list of methods that use the same assay type as your template.

6. Select an available method.

   By default, the application selects the method used to create the batch template, but you can choose any method in the Available Methods list.

7. To go to the next wizard page, click **Next**.

   From the Batch Specification page of the wizard, you can customize the batch.

Figure 103. Batch Template Selection page
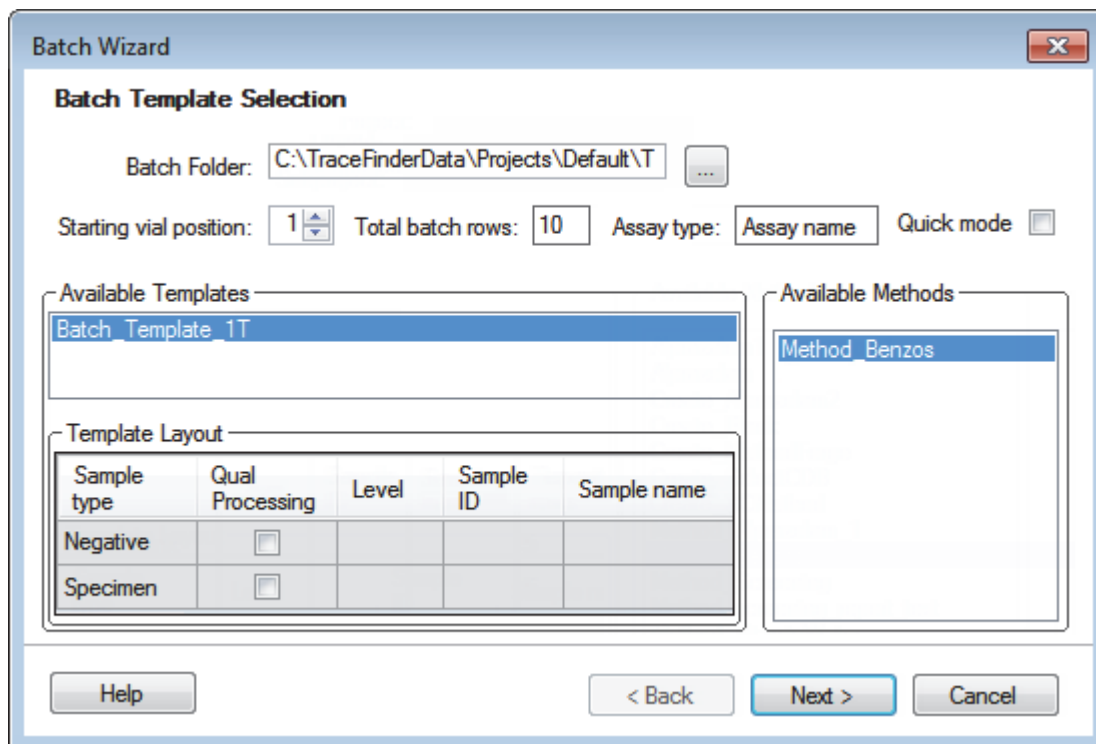
Table 78. Batch Template Selection page parameters (Sheet 1 of 2)

Parameter	Description
Batch Folder	The project folder for the batch.
Starting Vial Position	The vial position where you want to begin acquiring samples. Default: 1
Total Batch Rows	The number of sample rows in the batch template.
Assay Type	The assay type specified in the master method used to create the batch template.
Quick Mode	Limits the columns of information on the Batch Specification page to the following: • Sample Type • Sample ID • Injection Volume • Conversion Factor
Available Templates	All batch templates are saved in the following folder: …\TraceFinderData\Templates\Batches
Template Layout	Displays sample information in the selected batch template.
Available Methods	Lists all master methods created with the same assay type as the selected batch template.

Table 78. Batch Template Selection page parameters (Sheet 2 of 2)

Parameter	Description
Help	Opens the "Creating a Batch Using the Batch Wizard" topic (this topic) in the application Help tool.
Next	Returns you to the Batch Specification page where you can enter a sample ID, a sample name, or a comment. You can also add or remove samples from the sample list or edit the column values for the samples. See "Specifying a Batch" on page 439.
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.

Specifying a Batch

From the Batch Specification page, you must enter either a sample ID, sample name, or comment. You can also add or remove samples from the sample list or edit the column values for the samples. The batch template might contain many samples that you do not want to use for your batch. If you do not enter a sample ID, sample name, or comment for these samples, the application discards them when you save the batch. For descriptions of the parameters on the Batch Specification page, see "Batch Specification page" on page 443.

❖ **To enter a required sample ID, sample name, or comment**

1. In the Sample ID column, type an identifier.

   The identifier can be any text string.

2. In the Sample Name column, type a name.

   The name can be any text string.

3. In the Comment column, type a comment.

   The comment can be any text string.

> **Note** The application requires a value in at least one of these fields to acquire a sample. When the batch begins acquisition, it discards any sample that does not have a value in at least one of these fields.

❖ **To simplify the sample list**

Select the **Quick Mode** check box.

In Quick Mode, the Batch Specification page displays only the following columns:
- Sample Type
- Sample ID
- Injection Volume
- Conversion Factor

In Quick Mode, you cannot add or remove samples from the sample list. You can only edit these four column values for the samples specified in the template.

When you are not using Quick Mode, follow these procedures:
- To change the file names
- To remove samples from the batch
- To insert samples into the batch
- To copy a sample
- To move a sample up or down in the sample list
- To browse in a raw data file

❖ **To change the file names**

1. Select the file name.

Filename	Sample type		Filename	Sample type
9262012_a001	Matrix Blank ▾		9262012_a001	Matrix Blank ▾

Selected for renaming   Not selected for renaming

By default, all samples specified on the Batch Template Selection page are named with a date stamp and the designation "a*NNN*" as in this example: 9262012_a001.

2. Type a new file name.

> **Note** Or, you can right-click and choose **Browse in Raw File** from the shortcut menu. Follow the instructions "To browse in a raw data file" on page 442.

❖ **To add samples to the batch**

1. Right-click and choose **Add Sample** from the shortcut menu, or click the add sample icon, 🔣 .

   The application adds a new Specimen sample to the end of the sample list.

2. In the Filename column for each sample, do one of the following:

   - Accept the default file name: Unknown*N*.

   - Change the default file name. Follow the instructions "To change the file names."

   - Browse in a raw data file name. Follow the instructions "To browse in a raw data file" on page 442.

3. Select a sample type from the Sample Type list for each sample.

Available sample types		
Specimen	QC	Hydrolysis
Solvent	Calibrator	
Unextracted	Negative	

4. For detailed descriptions of sample types, see "Sample Types" on page 384.

5. For each Calibrator or QC sample, select a level from the Level list.

   The sample levels are defined in the master method. If there are no levels to select from the Level list, do the following:

   a. Click **Cancel** in the Batch Wizard.

   b. Return to the Method Development mode.

   c. Open the method.

   d. Click the **Compounds** tab.

    e.   Click the **Calibration Levels** tab.

    f.   Add the levels.

    g.   Save the method.

    h.   Return to the Analysis mode, open the Batch Wizard, and begin your batch again.

    For detailed instructions about defining sample levels, see Chapter 4, "Using the Method Development Mode."

6. In the Vial Position column for the new sample, type a vial position.

7. In the Injection Volume column for the new sample, type a volume.

    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** The Add Sample function is not available in Quick Mode.

❖ **To remove samples from the batch**

1. Select the samples to remove.

2. Right-click and choose **Remove Selected Samples** from the shortcut menu, or click the remove samples icon, [icon].

    The application removes the selected samples from the sample list.

> **Note** The Remove Selected Samples function is not available in Quick Mode.

❖ **To insert samples into the batch**

1. Select the sample above where you want to insert a new sample.

2. Right-click and choose **Insert Sample** from the shortcut menu.

    The application inserts a new Specimen sample above the selected sample.

> **Note** The Insert Sample function is not available in Quick Mode.

❖ **To copy a sample**

1. Select the sample that you want to copy.

2. Right-click and choose **Insert Copy Sample** from the shortcut menu.

    The application inserts the copy above the selected sample.

> **Note** The Insert Copy Sample function is not available in Quick Mode.

❖ **To move a sample up or down in the sample list**

1. Select the sample that you want to move.

2. Right-click and choose **Move Sample Up** or **Move Sample Down** from the shortcut menu.

   The application moves the selected sample up or down one row in the sample list.

   Note The Move Sample functions are not available in Quick Mode.

❖ **To browse in a raw data file**

1. Double-click the Filename column, or right-click and choose **Browse in Raw File** from the shortcut menu.

   A dialog box opens where you can select a raw data file to use for the sample. You can also browse in multiple raw data files to create multiple samples.

2. Locate the raw data file to use for the sample and click **Open**.

   Note The Browse in Raw File function is not available in Quick Mode.

Batch Specification

Use the features on the Batch Specification page to create a batch sequence from the batch template.

Figure 104. Batch Specification page
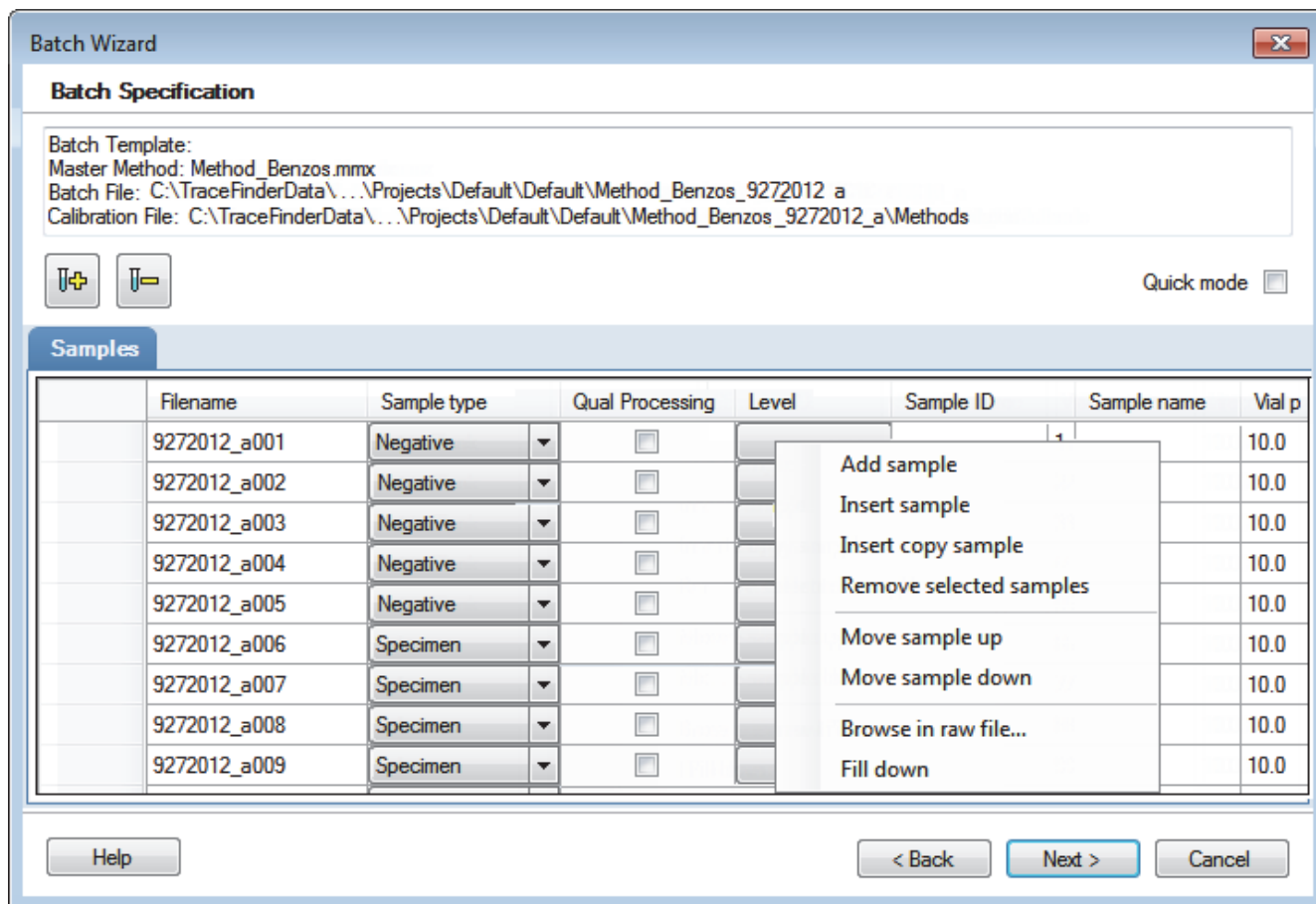
Table 79. Batch Specification page parameters (Sheet 1 of 2)

Parameter	Description
Batch Template Master Method Batch File Calibration File	Displays the path names of the batch template, master method, batch file, and calibration file used to create this batch.
[icon]	Adds a new, Specimen sample to the end of the sample list. This function is not available in Quick Mode.
[icon]	Removes the selected sample. This function is not available in Quick Mode.

Table 79. Batch Specification page parameters (Sheet 2 of 2)

Parameter	Description
Quick Mode	Limits the columns of information in the Batch Specification page to the following: • Sample Type • Sample ID • Injection Volume • Conversion Factor In Quick Mode, the shortcut menu and add/remove sample icons are unavailable.
Help	Opens the "Creating a Batch Using the Batch Wizard" topic (this topic) in the application Help tool.
Back	Returns you to the Batch Template Selection page where you can choose a different batch template, master method, or starting vial position.
Next	Takes you to the Finish page where you can submit the batch for acquisition or processing. See "Submitting the Batch."
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.
Shortcut Menu	
Add Sample	Adds a single empty row to the sample list.
Insert Sample	Inserts a new, Specimen sample above the selected row.
Insert Copy Sample	Copies the currently selected row and inserts a copy above the row.
Remove Selected Samples	Removes selected samples from the sample list.
Move Sample Up	Moves the selected sample up one row in the sample list.
Move Sample Down	Moves the selected sample down one row in the sample list.
Browse In Raw File	Opens a dialog box where you can select a raw data file to use for the sample row. You can also browse in multiple raw data files to create multiple samples.
Fill Down	Enters sequential values in the column, starting with the value in the selected row and ending with the last row in the column. For detailed instructions about using the Fill Down command, see Appendix C, "Using Copy Down and Fill Down."
Renumber Vial Positions	Renumbers vial positions for all samples after the currently selected sample. The selected sample retains its vial position. All subsequent samples are renumbered sequentially. Available only after you add or move samples.

Submitting the Batch

From the Finish page, you can change the name of the batch, access the Calibration and Compound Selection page to edit the calibration file or edit the list of compounds to identify, or save the batch and open it in Batch View. For descriptions of the parameters on the Finish page, see "Finish Page."

Follow these procedures:

- To change the name of the batch

- To save the batch

- To edit the calibration file

- To identify specific compounds or groups of compounds

❖ **To change the name of the batch**

Edit the name in the Batch Name box.

You cannot overwrite an existing batch name. If you enter a name for a batch that already exists, when you click Finish, the Batch Save dialog box asks you to enter another name.

❖ **To save the batch**

Click **Finish**.

The application saves the batch and displays it in the Batch View. From the Batch View, you can submit the batch for acquisition, processing, or report generation. See "Submitting a Batch" on page 423.

❖ **To edit the calibration file**

1. Select the **Modify Calibrations or Active Compounds by Group** check box.

   The application replaces the Finish button with a Next button.

2. Click **Next**.

   The Calibration and Compound Selection page opens. See "Selecting Calibration Files and Compounds" on page 448.

❖ **To identify specific compounds or groups of compounds**

1. Select the **Modify Calibrations or Active Compounds by Group** check box.

   The application replaces the Finish button with a Next button.

2. Click **Next**.

   The Calibration and Compound Selection page opens. See "Selecting Calibration Files and Compounds" on page 448.

Finish Page

Use the features on the Finish page to change the name of the batch, access the Calibration and Compound Selection page to edit the calibration file or edit the list of compounds to identify, or save the batch and open it in Batch View.

Figure 105. Finish page

Table 80. Finish page parameters (Sheet 1 of 2)

Parameter	Description
Modify Calibrations or Active Compounds by Group	Activates the Next button that lets you access the Calibration and Compound Selection page. When you have already used the Calibration and Compound Selection page, this option is not available.
Batch Name	Name of the default batch in this form: *MasterMethod_MMDDYYYY_*
Help	Opens the Creating a Batch Using the Batch Wizard topic (this topic) in the application Help tool.
Back	Returns you to the Batch Specification page where you can enter a sample ID, sample name, or comment. You can also add or remove samples from the sample list or edit the column values for the samples. See "Specifying a Batch" on page 439.
Finish	Saves the batch and displays it in Batch View. From Batch View, you can submit the batch for acquisition, processing, or report generation. See "Submitting a Batch" on page 423.

Table 80. Finish page parameters (Sheet 2 of 2)

Parameter	Description
Next	Opens the Calibration and Compound Selection page where you can edit the calibration file or edit the list of compounds that you want to identify.
	Available only when Modify Calibrations or Active Compounds by Group is checked.
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.

Selecting Calibration Files and Compounds

From the Calibration and Compound Selection page, you can edit the calibration file or edit the list of compounds that you want to identify. For descriptions of the parameters on the Calibration and Compound Selection page, see "Calibration and Compound Selection Page."

Follow these procedures:

- To add calibration data to the calibration file
- To identify specific compounds or groups of compounds

❖ **To add calibration data to the calibration file**

1. To add calibration data from another batch to the current calibration file, click **Extend Calibrations**.

   The Select a Calibration File to Use dialog box opens. The dialog box lists only calibration batches that use the same master method as the current batch.

2. Select a calibration file to append to the current calibration file and click **OK**.

   The application appends the selected calibration file to the current file.

3. To save calibration data from both files into a single file for this batch, click **Create New**.

4. When you are finished with the Calibration and Compound Selection page, click **Next**.

   The Finish page opens. See "Submitting the Batch" on page 445.

❖ **To identify specific compounds or groups of compounds**

1. In the Compound Groups area, select the groups that include the compounds to identify in the samples.

2. In the Included Compounds area, select the **Active** check box for each compound that you want to identify in the samples.

3. When you are finished with the Calibration and Compound Selection page, click **Next**.

   The Finish page opens. See "Submitting the Batch" on page 445.

Calibration and Compound Selection Page

Use the features on the Calibration and Compound Selection page to edit the calibration file or edit the list of compounds that you want to identify.

Figure 106. Calibration and Compound Selection page
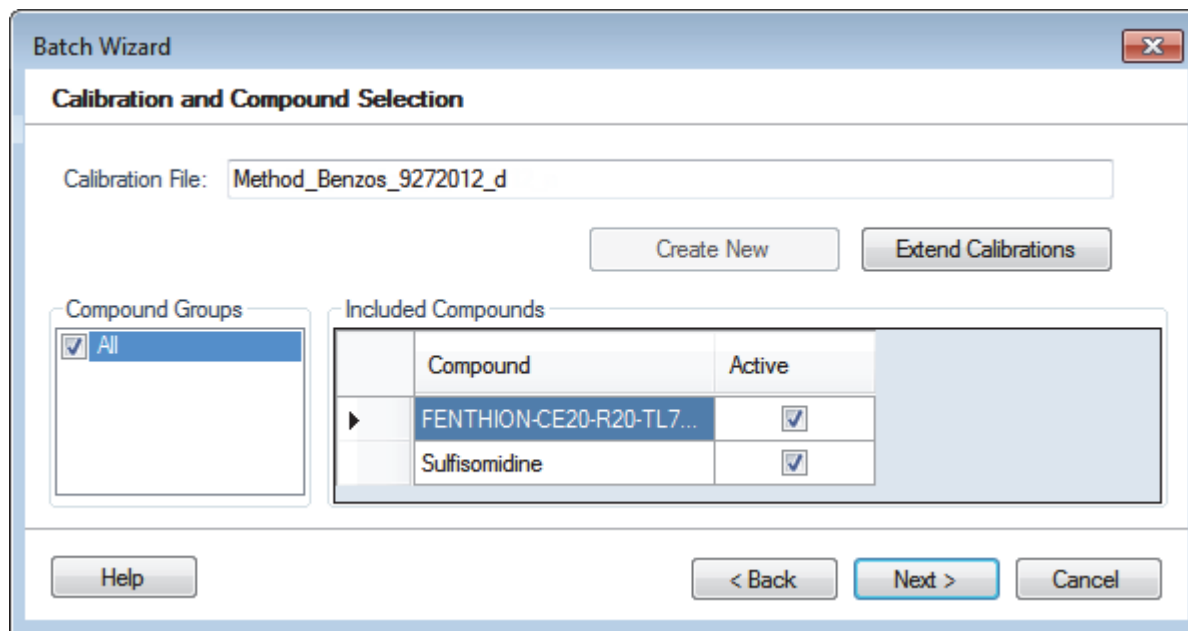
Table 81. Calibration and Compound Selection page parameters (Sheet 1 of 2)

Parameter	Description
Calibration File	Name of the current batch in this form: *MasterMethod_MMDDYYYY_*
Create New	Saves calibration data from all calibration files to the current calibration file. Available only after you use Extend Calibrations to append calibration data from another calibration file.
Extend Calibrations	Adds calibration data from the current batch to the selected calibration file.
Compound Groups	Displays all available groups defined on the Groups page of the Method View. See "Editing the Groups Page" on page 201.
Included Compounds	Displays all available compounds that you can identify in the samples. Compounds marked as Active are identified in the batch samples.
Help	Opens the "Creating a Batch Using the Batch Wizard" topic (this topic) in the application Help tool.
Back	Returns you to the Batch Specification page where you can enter a sample ID, sample name, or comment. You can also add or remove samples from the sample list or edit the column values for the samples. See "Specifying a Batch" on page 439.

Table 81. Calibration and Compound Selection page parameters (Sheet 2 of 2)

Parameter	Description
Next	Opens the Finish page where you can change the name of the batch or save the batch to the Batch View. See "Submitting the Batch" on page 445.
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.

Working in Data Review for Quantitation Methods

In the Data Review view, you can view the data generated by the quantitation master method. Use Data Review to verify the data for a compound before you generate reports.

❖ **To open the Data Review view**

1. Click **Analysis** in the navigation pane.

> **Analysis**

The Analysis navigation pane opens.

2. Click **Data Review**.

> ▶ **Data Review**

The Data Review navigation pane opens.

> ▼ **Data Review** >
>> **Sample View** >
>> **Compound View**
>> **Comparative View**
>> **Qualitative View**
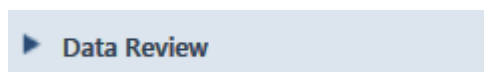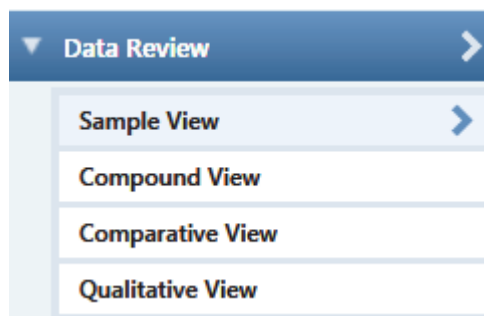
Choose from a Sample View, Compound View, Comparative View, or Qualitative View to analyze the data generated by the master method.

This section includes the following topics:

- Sample View

- Compound View

- Comparative View

- Qualitative View

- Features Common to All Data Review Pages

Sample View

The Sample View uses three different panes to display a list of all samples in the current batch, the compound results for all compounds in the method, and peak plots for all compounds found in the currently selected sample.

These are the default panes and their locations:

Sample Peaks pane   Samples pane   Compound Results pane
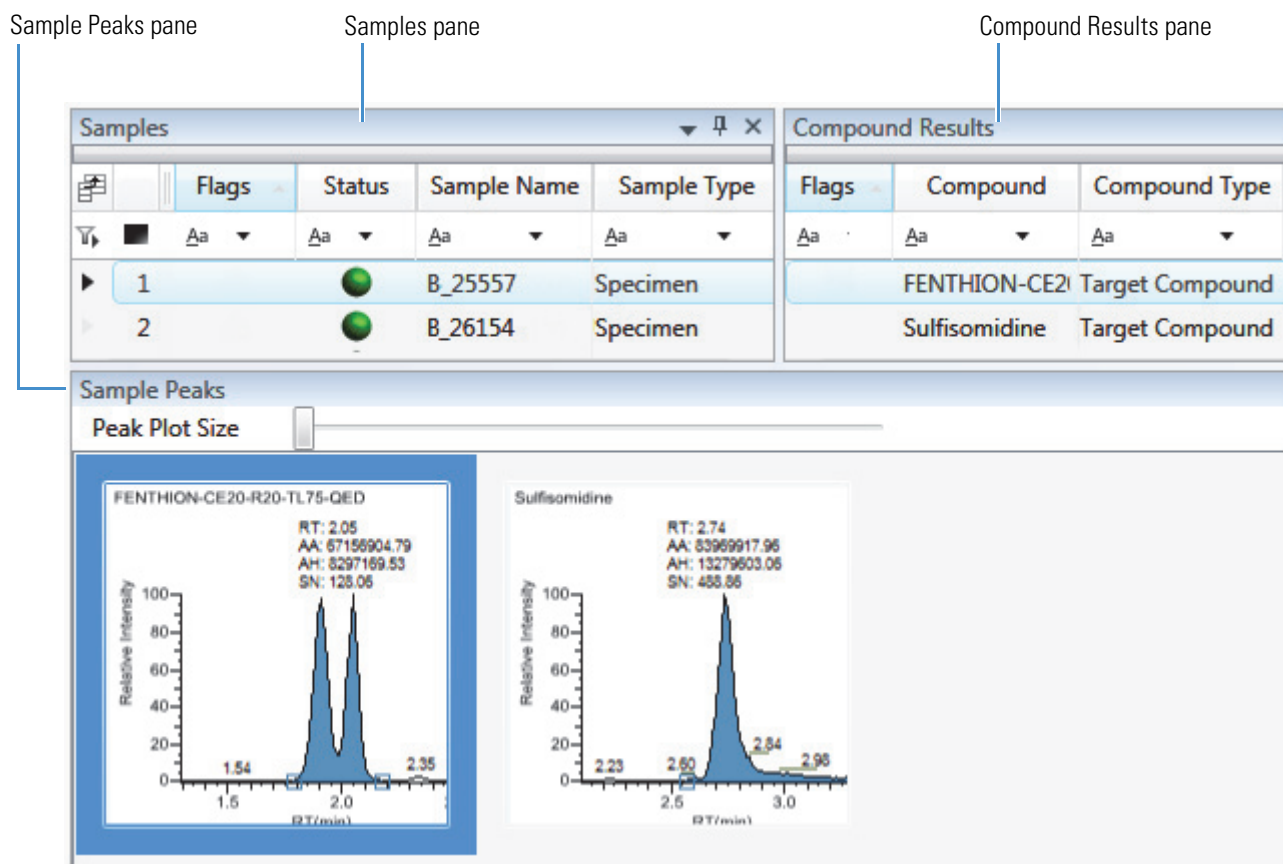
When you select a sample in the Samples Pane, the associated Compound Results Pane flags any compound with errors in the selected sample. The associated Sample Peaks Pane displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the selected sample. The Sample Peaks pane highlights the compound selected in the Compound Results pane.

The Sample View display includes the following features:

- Samples Pane
- Compound Results Pane
- Sample Peaks Pane
- Caution Flags
- Viewing Sample View Panes

Samples Pane

Use the Samples pane in the Sample View to select a specific sample. The associated Compound Results Pane displays all compounds in the method and flags any compound with errors in the selected sample.

❖ **To hide or display columns in the Samples pane**

1. Click the **Field Chooser** icon, ⊞, in the upper left corner of the pane.

   The Field Chooser displays all available columns of data for the Samples pane.
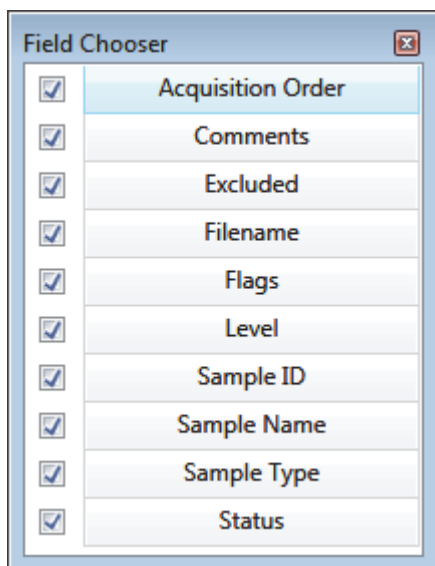
2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   The application immediately displays or hides the column in the Samples pane.

3. When you are finished modifying the column display, click ⊠ to close the Field Chooser.

Figure 107. Samples pane

Selected sample

Compound error in the selected sample

No compound error in the selected sample
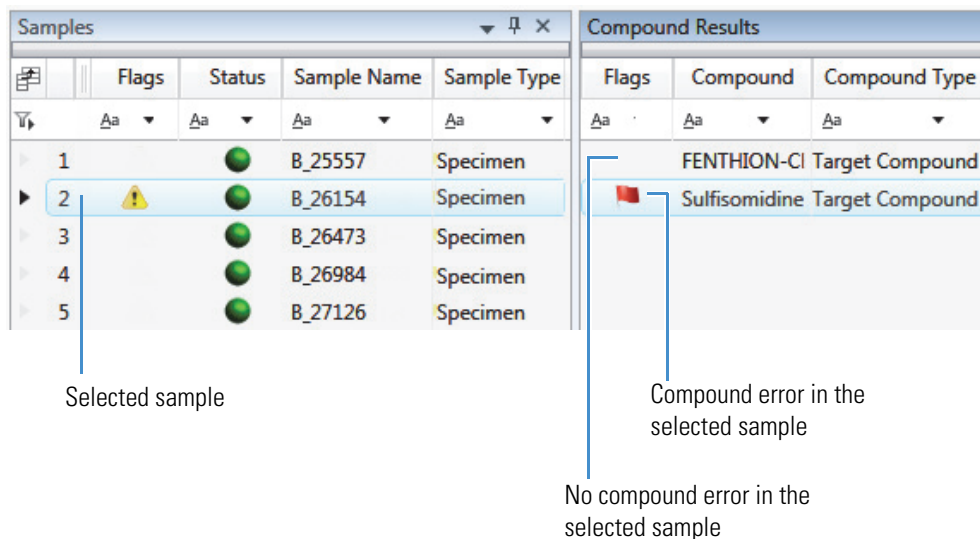
Table 82. Samples pane columns

Column	Description
Flags	Caution flag displayed when a compound in the sample has an error. See "Caution Flags" on page 458.
Status	● Sample is not acquired. ● Sample is acquired but not processed. ● Sample is acquired and processed. ● Sample is currently acquiring.
Sample Name	A user-defined name that identifies a sample.
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative.

Compound Results Pane

Use the Compound Results pane in the Sample View to select a specific compound in the selected sample. The associated Sample Peaks Pane highlights the selected compound.

❖ **To hide or display columns in the Compound Results pane**

1. Click the **Field Chooser** icon, ⊞ , in the upper left corner of the pane.

The Field Chooser displays all available columns of data for the Compound Results pane.
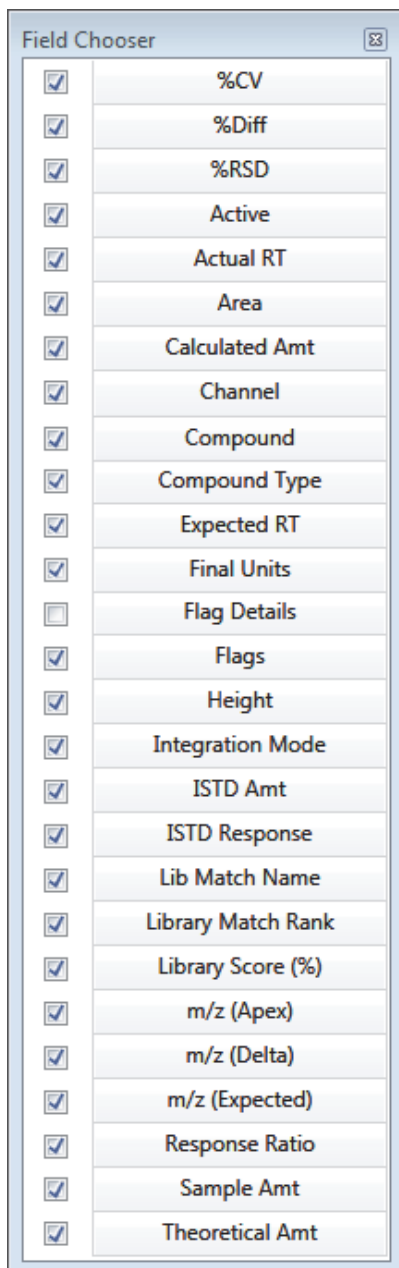
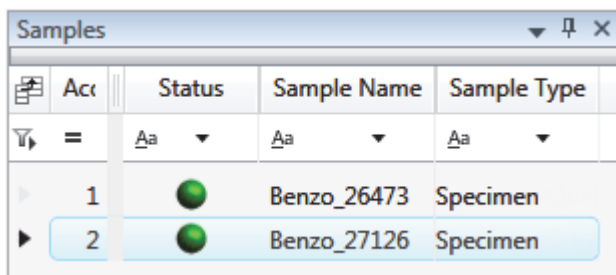| Field Chooser	⊠
☑	%CV
☑	%Diff
☑	%RSD
☑	Active
☑	Actual RT
☑	Area
☑	Calculated Amt
☑	Channel
☑	Compound
☑	Compound Type
☑	Expected RT
☑	Final Units
☐	Flag Details
☑	Flags
☑	Height
☑	Integration Mode
☑	ISTD Amt
☑	ISTD Response
☑	Lib Match Name
☑	Library Match Rank
☑	Library Score (%)
☑	m/z (Apex)
☑	m/z (Delta)
☑	m/z (Expected)
☑	Response Ratio
☑	Sample Amt
☑	Theoretical Amt

2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   The application immediately displays or hides the column in the Compound Results pane.

3. When you are finished modifying the column display, click ▣ to close the Field Chooser.

Figure 108. Compound Results pane
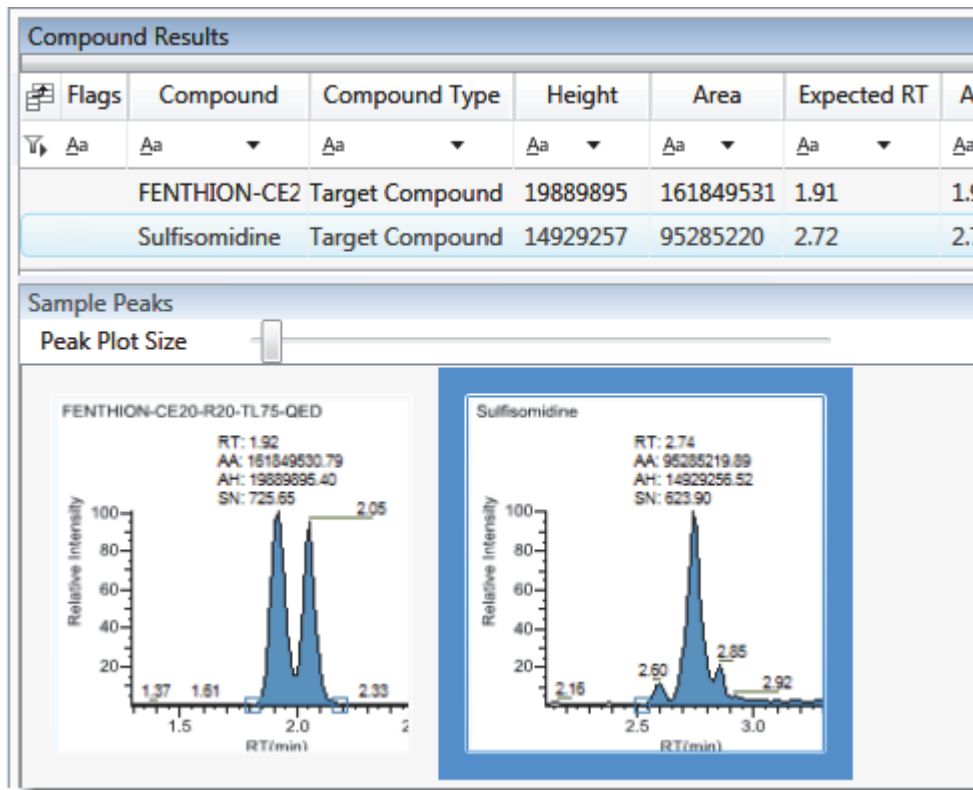
Table 83. Compound Results pane columns

Column	Description
Flags	Caution flag displayed when the compound has an error. See "Caution Flags" on page 458.
Compound	Compound names as identified in the library.
Compound Type	Specified compound type: Target Compound or Internal Standard.

The remainder of the columns in the results list are common to the Compound Results pane in the Sample View and the Sample Results pane in both the Compound View and the Comparative View. See "Common Column Parameters" on page 500.

Sample Peaks Pane

The Sample Peaks pane in the Sample View displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the Compound Results pane. The application highlights the chromatogram for the compound that is currently selected in the Compound Results pane.
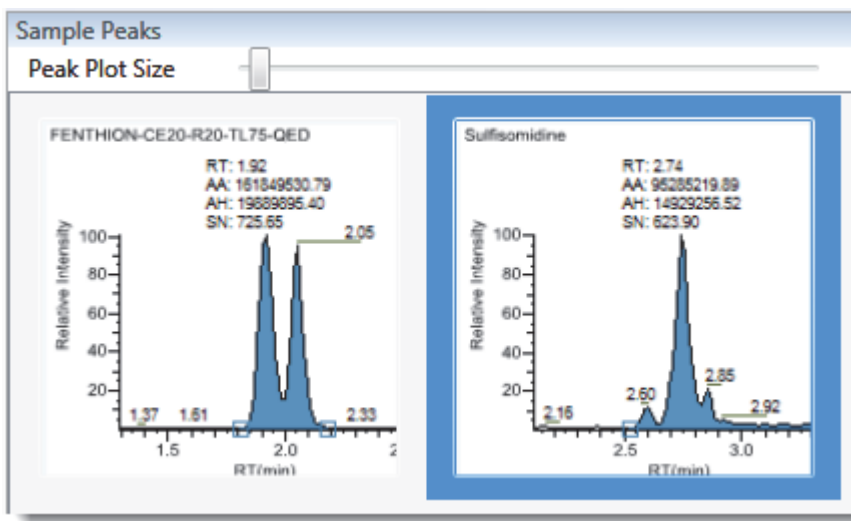
❖ **To display details for a compound**

Double-click the chromatogram in the Sample Peaks pane.

The Compound Details pane opens.
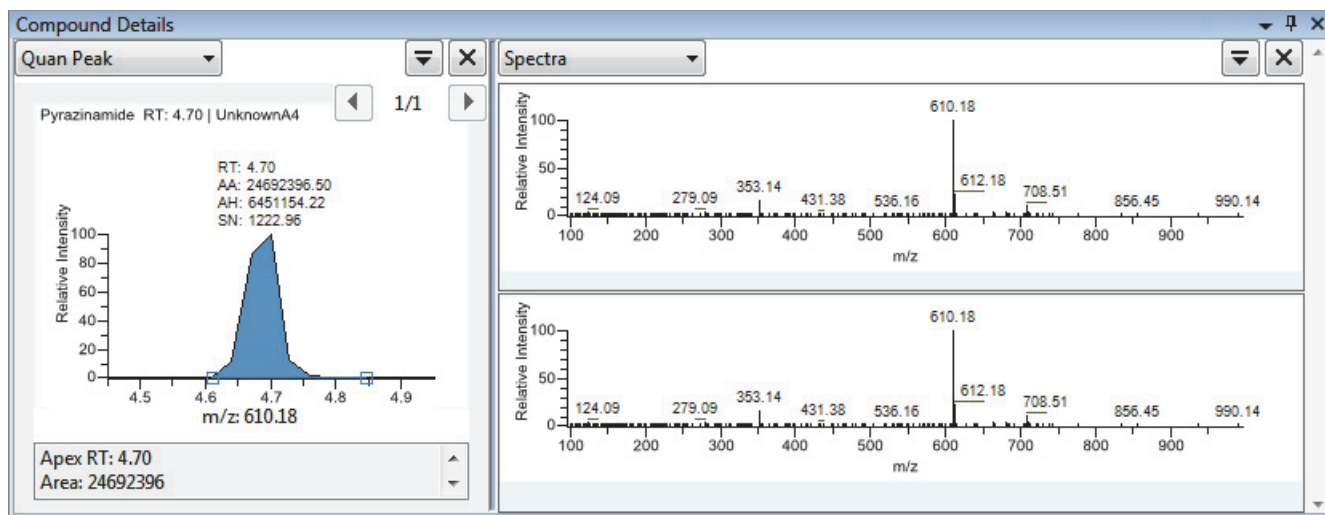
The Compound Details pane displays information about the quantitative peak, calibration curve, confirming ion, internal standard, reference peak, ion overlay, and spectra for the compound.

For a detailed description of the available information in the Compound Details pane, see "Compound Details" on page 506.

Caution Flags

In the Sample View, the application displays caution flags in both the Samples pane and the Compound Results pane.

This section includes the following topics:

- Flags in the Samples Pane
- Flags in the Compound Results Pane
- Error Indicators in the Sample Peaks Pane

Flags in the Samples Pane

The Flags column in the Samples pane displays a caution flag if any compound in the sample is not in compliance with the method criteria.

Click the caution flag icon, ⚠, to display the details. Information in the pop-up box shows the compound that is in error and describes the exact error condition.

Error condition

Compound name
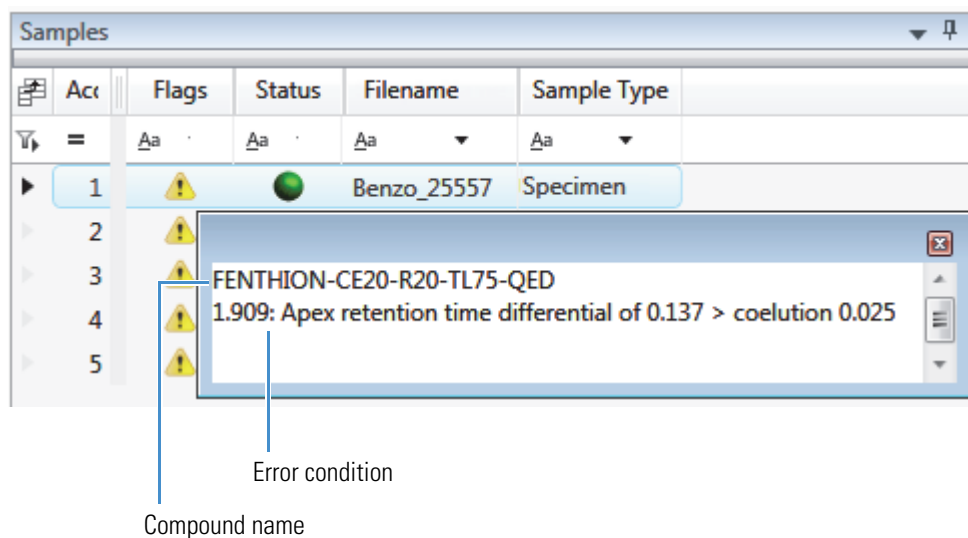
Flags in the Compound Results Pane

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.

Selected sample   Error condition of the Sulfisomidine
                                    compound in the selected sample
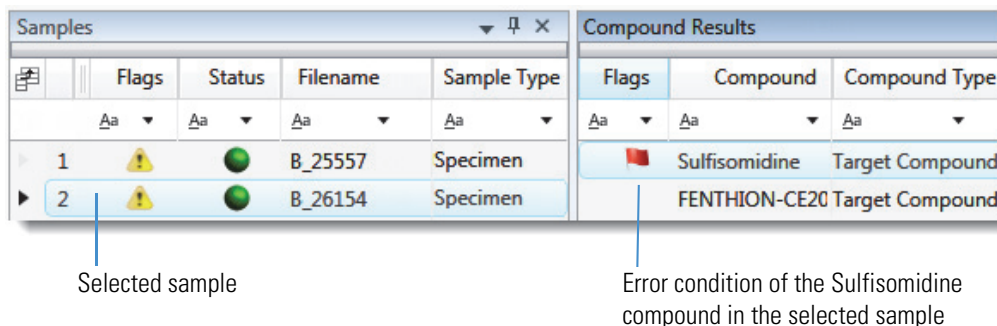
Hold your cursor over the flag icon, , to display details for the compound in the selected sample.
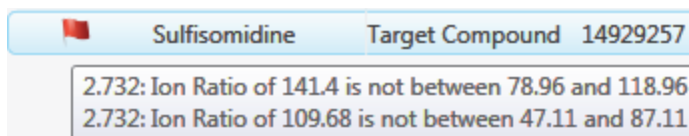
Flags in the Compound Results pane are displayed in these situations:

- A red flag for compounds that have violated (or are activated by) any of the values set in the method. See "Editing the QAQC Page" on page 190.

- A red flag for compounds that are outside the specified ion ratio range. See Ion ratio failure flag.

- An orange flag for compounds that are below the LOQ, below the LOD, or between the LOD and LOQ values specified in the method. For descriptions of these limits, see "Limits" on page 191.

- A green flag for "found" compounds that are over the LOR amount specified in the method. For a description of the LOR limit, see "Limits" on page 191.

- A yellow flag for compounds that are equal to or below the LOR amount specified in the method.

- A yellow flag for compounds that are not found in Calibrator or QC sample types.

  The Compound Results pane does not flag compounds that are not found in Specimen sample types.

- No flag for compounds that have no errors or where no report options are selected.

Note These criteria for flag states do not apply to Negative sample types when the compound is an internal standard.

Error Indicators in the Sample Peaks Pane

In the Sample Peaks pane, peak plots are outlined with the color of their associated error flag. In the following example, the FENTHION peak plot is highlighted in blue to indicate that FENTHION is the selected compound, and the Sulfisomidine peak plot is outlined in red to indicate that the Sulfisomidine compound in the selected sample is outside the specified ion ratio range.

Figure 109. Ion ratio failure flag
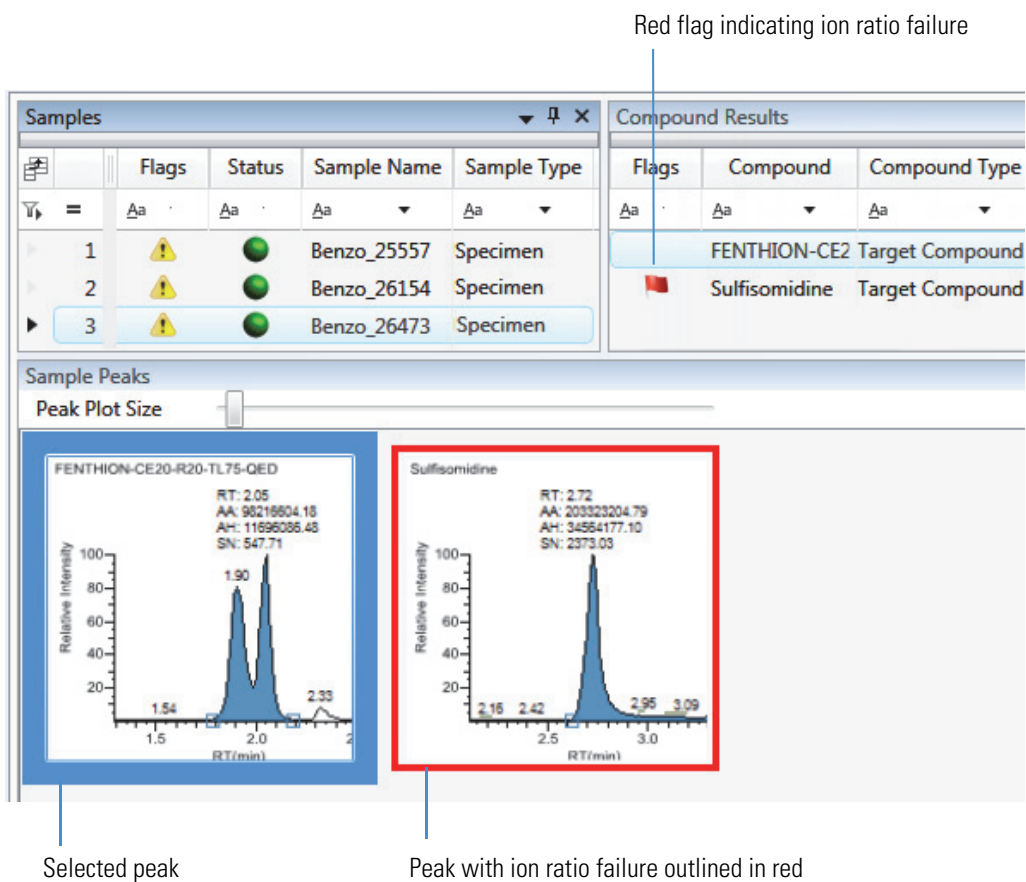
Viewing Sample View Panes

The Sample View display uses multiple panes to display data: Sample Results, Compound Results, Sample Peaks, and Compound Details. You can display, hide, or move any of these panes.

❖ **To display or hide a Sample View pane**

From the View menu, choose from the following:

- **Compounds with Data**: Displays or hides the Compound Results pane.

- **Sample View Peaks**: Displays or hides the Sample Peaks pane.

- **Compound Details**: Displays or hides the Compound Details pane.

> **Note** The Sample Results pane is required for the Sample View display. You cannot hide the Sample Results pane.

Displayed panes are indicated with a check mark.
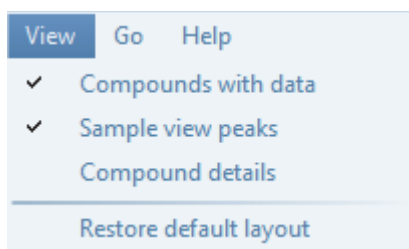
Data Review Pane Display Features

The following procedures are common to all Data Review displays.

- To dock a pane

- To make a pane floating or dockable

- To change a pane from a docked pane to a tabbed pane

- To restore the default layout

❖ **To dock a pane**

1. Grab the title bar of the pane and begin dragging the pane.

   The application displays docking arrows.

2. Drag the pane over one of the arrows.

   As you hold the cursor over a docking arrow, the application displays a blue region indicating where this arrow will place the pane.

3. Drop the pane onto one of the arrows.

❖ **To make a pane floating or dockable**

Do one of the following:

- To make a dockable pane floating, right-click the title bar of the pane and choose **Floating**.

  While a pane is set as floating, you cannot use the docking arrows to dock it or make it a tabbed pane.

- To make a floating pane dockable, right-click the title bar of the pane and choose **Dockable**.

❖ **To change a pane from a docked pane to a tabbed pane**

1. Grab the title bar of the pane and begin dragging the pane.

    The application displays docking arrows.

2. Hold the cursor over the center of the docking arrows to display a blue region indicating the location of the tabbed pane.

3. Drop the pane over the center of the docking arrows.

> **Note** To change a floating pane to a tabbed pane, you must first make the pane a dockable pane, and then you can make it a tabbed pane.

❖ **To restore the default layout**

Choose **View > Restore Default Layout**.

The Sample View, Compound View, and Qualitative View each have their own defaults for which panes are displayed and in which location.

Compound View

The Compound View uses three different panes to display a list of all compounds available in the method, all samples in the current batch, and the peak plots for all compounds found in each sample.

These are the default panes and their locations:
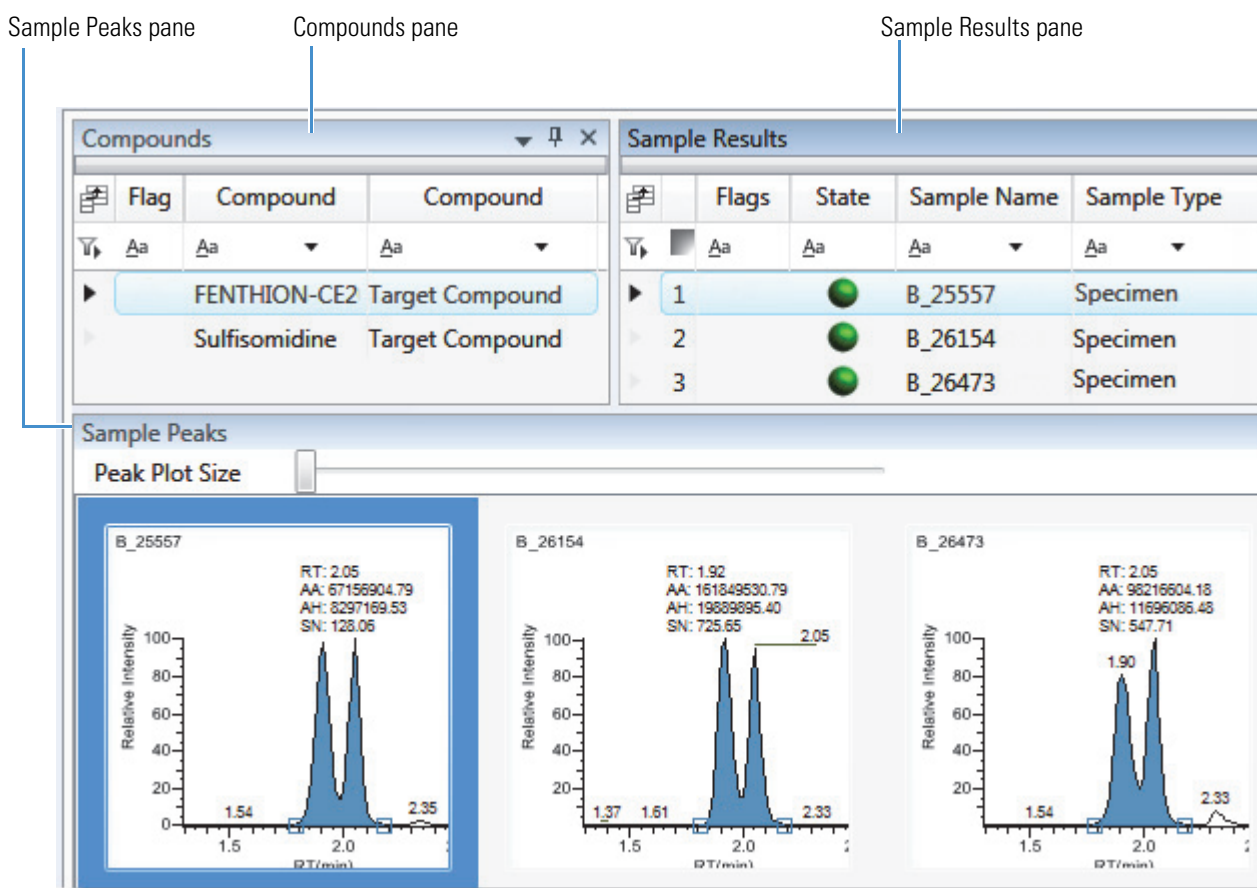
When you select a compound in the Compounds Pane, the Sample Results Pane flags any sample that contains errors with the selected compound. The Sample Peaks Pane highlights the selected compound and displays the name of the sample in which the compound was found and the following information about the compound: chromatogram, retention time, area, height, and signal-to-noise ratio.

The Compound View includes the following features:

- Compounds Pane
- Sample Results Pane
- Sample Peaks Pane
- Caution Flags

Compounds Pane

Use the Compounds pane in the Compound View to select a specific compound. The Sample Results Pane displays all samples in the batch and flags any sample that contains errors with the selected compound.

❖ **To hide or display columns in the Compounds pane**

1. Click the **Field Chooser** icon,   , in the upper left corner of the pane.

   The Field Chooser displays all available columns of data for the Compounds pane.

Field Chooser	
☑	Compound
☑	Compound Type
☑	Expected RT
☑	Flags
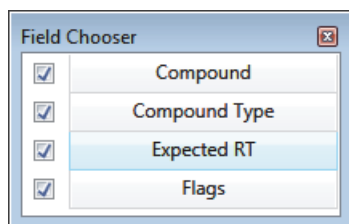
2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   The application immediately displays or hides the column in the Compounds pane.

3. When you are finished modifying the column display, click ☒ to close the Field Chooser.

Figure 110. Compounds pane

Selected compound

No error associated with the selected compound in these samples

Error associated with the selected compound in this sample
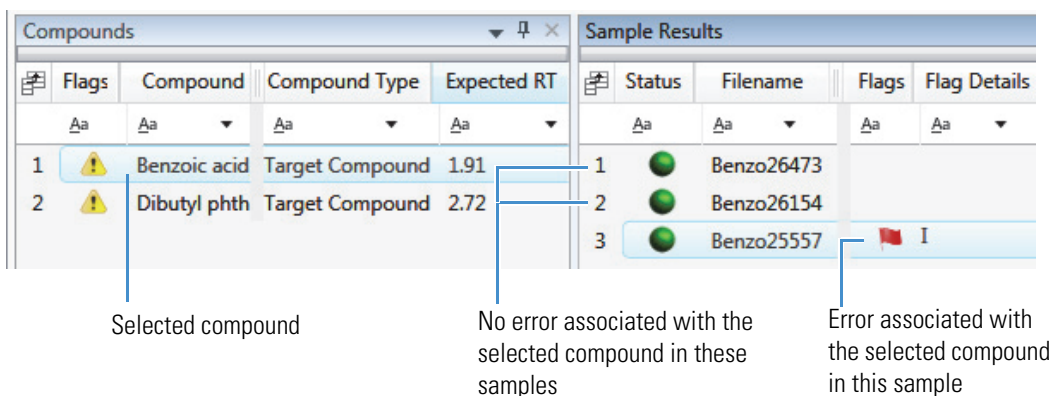
Table 84. Compounds pane columns

Column	Description
Flags	Caution flag displayed when a compound has an error in any of the samples.
Compound	Compound names as identified in the library. If there is no library selected in the method template, the compound name is identified as *peak@RT.*
Compound Type	Specified compound type: Target Compound or Internal Standard.
Expected RT	Expected retention time for the compound.

Sample Results Pane

Use the Sample Results pane in the Compound View to select a specific compound in a specific sample. The Sample Peaks pane highlights the selected compound and displays the name of the sample in which the compound was found and the following information about the compound: chromatogram, retention time, area, height, and signal-to-noise ratio. See Sample Results pane.

❖ **To hide or display columns in the Sample Results pane**

1. Click the **Field Chooser** icon, ⊞ , in the upper left corner of the pane.

   The Field Chooser displays all available columns of data for the Sample Results pane.
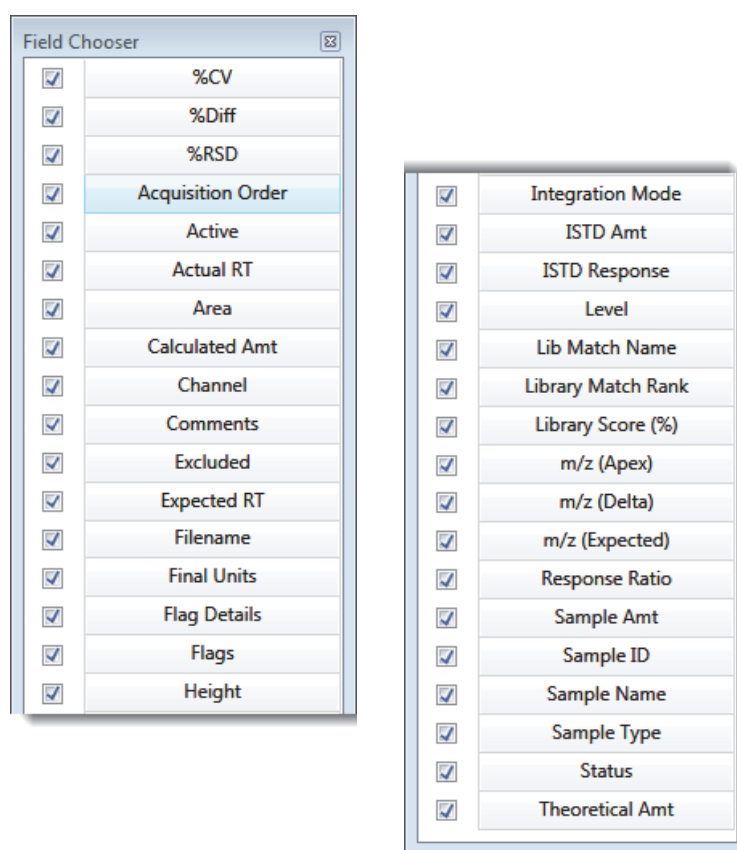
Field Chooser	⊠
☑	%CV
☑	%Diff
☑	%RSD
☑	Acquisition Order
☑	Active
☑	Actual RT
☑	Area
☑	Calculated Amt
☑	Channel
☑	Comments
☑	Excluded
☑	Expected RT
☑	Filename
☑	Final Units
☑	Flag Details
☑	Flags
☑	Height

☑	Integration Mode
☑	ISTD Amt
☑	ISTD Response
☑	Level
☑	Lib Match Name
☑	Library Match Rank
☑	Library Score (%)
☑	m/z (Apex)
☑	m/z (Delta)
☑	m/z (Expected)
☑	Response Ratio
☑	Sample Amt
☑	Sample ID
☑	Sample Name
☑	Sample Type
☑	Status
☑	Theoretical Amt

2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   The application immediately displays or hides the column in the Sample Results pane.

3. When you are finished modifying the column display, click ⊠ to close the Field Chooser.

Figure 111. Sample Results pane

Table 85. Sample Results pane columns (Sheet 1 of 2)

Column	Description
Acquisition Order	Sequentially numbers the samples.
Flags	Caution flag displayed when a compound within the sample has an error.
Flag Details	Indicates the type of error: • I: Confirming ion coelution failure or Ion ratio failure • A: Amount error • B: Matrix blank error • H: Peak not found
Status	● Sample is not acquired. ● Sample is acquired but not processed. ● Sample is acquired and processed. ● Sample is currently acquiring.
Filename	A user-defined name that identifies a sample.

Table 85. Sample Results pane columns (Sheet 2 of 2)

Column	Description
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative.

The remainder of the columns in the Sample Results pane are common to both the Sample View and the Compound View displays. See "Common Column Parameters" on page 500.

Sample Peaks Pane

The Sample Peaks pane in the Compound View displays the compound chromatogram, retention time, area, height, and signal-to-noise ratio for the selected compound in each of the samples in the batch. The application highlights the compound chromatogram for the sample that is currently selected in the Sample Results pane.
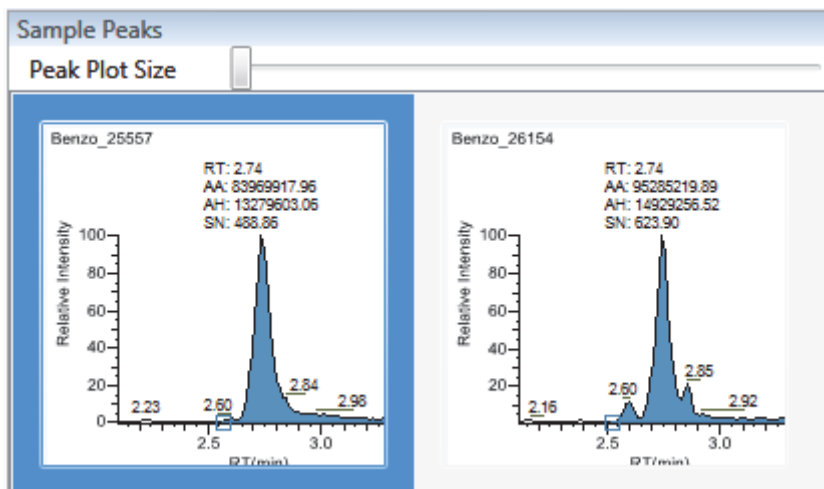
❖ **To display details for a compound**

1. Double-click the chromatogram in the Sample Peaks pane.

The Compound Details dialog box opens.
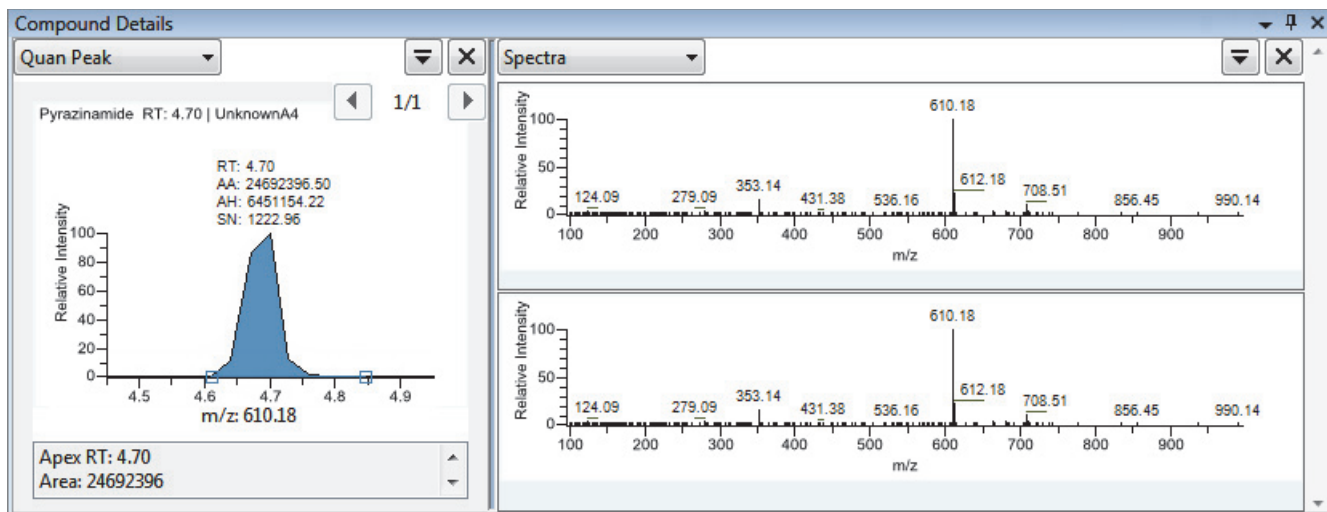
The Compound Details dialog box displays information about the quantitative peak, calibration curve, confirming ion, internal standard, reference peak, ion overlay, and spectra for the compound.

For details about the available information in the Compound Details dialog box, see "Compound Details" on page 506.

Caution Flags

In the Compound View, the application displays caution flags in both the Compounds pane and in the Sample Results pane.

This section includes the following topics:

- Flags in the Compounds Pane
- Flags in the Sample Results Pane
- Error Indicators in the Sample Peaks Pane

Flags in the Compounds Pane

The Flags column in the Compounds pane displays a caution flag if the compound in any of the samples is not in compliance with the method criteria.

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.

Hold your cursor over the flag icon, , to display the details for the selected compound in the sample.

Flags in the Sample Results pane are displayed in these situations:

Flag	Description
	A green flag for compounds that are over the LOR amount specified in the method.
	A red flag for compounds that have violated (or are activated by) any of the values set in the method. See "Editing the QAQC Page" on page 190.
	A red flag for compounds that are outside the specified ion ratio range. See Ion ratio failure flag.
	An orange flag for compounds that are not found in Calibrator or QC sample types. "Not found" compounds are below the LOQ, below the LOD, or between the LOD and LOQ values specified in the method. The Sample Results pane does not flag compounds that are not found in Specimen sample types.
	No flag for compounds that have no errors or where no report options are selected.

Note These criteria for flag states do not apply to Negative sample types when the compound is an internal standard.

Error Indicators in the Sample Peaks Pane

In the Sample Peaks pane, peak plots are outlined with the color of their associated error flag. In the following example, the peak plot is highlighted in blue to indicate that Benzo_25557 is the selected sample and outlined in red to indicate that the FENTHION compound in the selected sample is outside the specified ion ratio range.

Figure 112. Ion ratio failure flag

Red flag indicating ion ratio failure

Selected peak

Peak with ion ratio failure
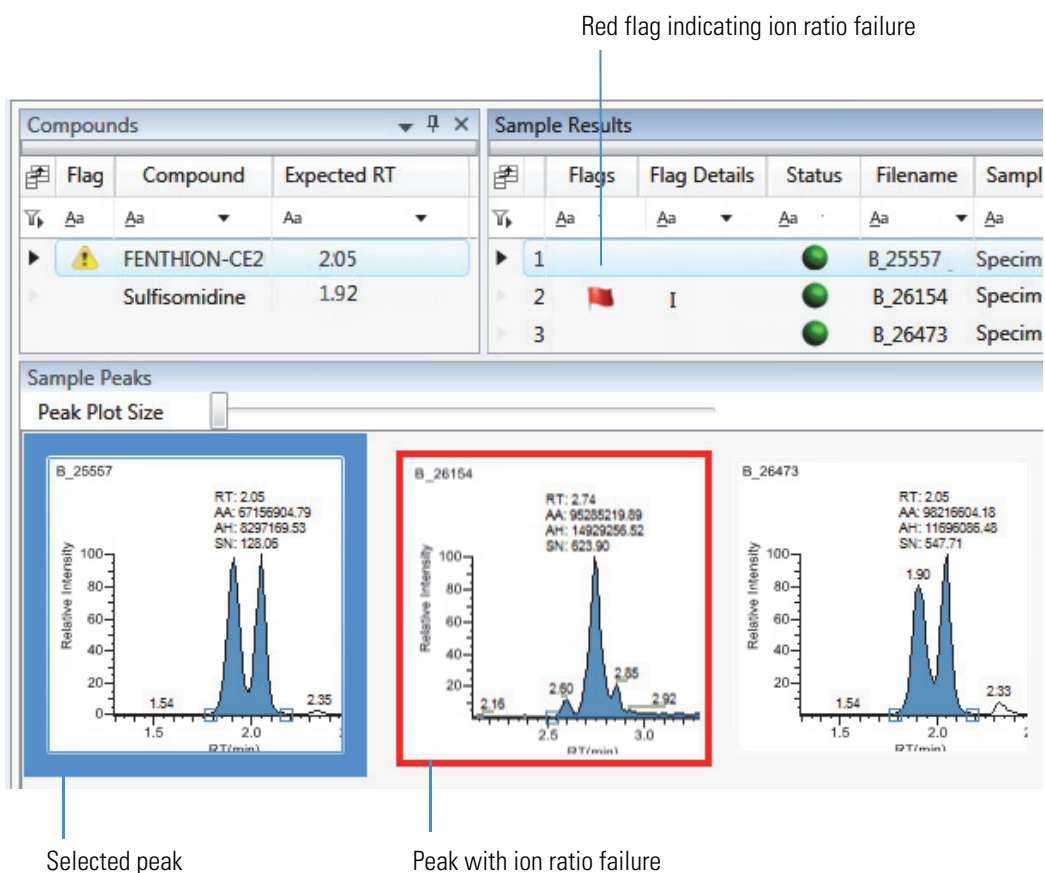
Viewing Compound View Panes

The Compound View display uses multiple panes to display data: Compounds, Sample Results, Sample Peaks, and Compound Details. You can display, hide, or move any of these panes.

❖ **To display or hide a Compound View pane**

From the View menu, choose from the following:

- **Samples with Data**: Displays or hides the Sample Results pane.

- **Compound View Peaks**: Displays or hides the Sample Peaks pane.

- **Compound Details**: Displays or hides the Compound Details pane.

> **Note** The Compounds pane is required for the Compound View display. You cannot hide the Compounds pane.

Displayed panes are indicated with a check mark.
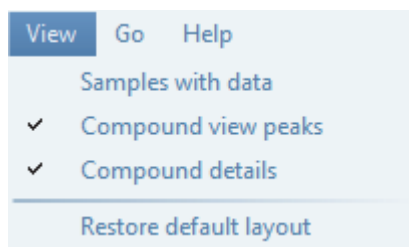
For procedures about creating docked, floating, or tabbed panes, see "Data Review Pane Display Features" on page 462.

Comparative View

The Comparative View uses three panes to display a list of all compounds available in the method, all samples in the current batch, and the sample peak plots for all compounds found in the samples with the horizontal threshold guide.

These are the default panes and their locations:

The panes in the Comparative View are identical to the Compound View with the addition of the Group column. This column identifies any groups that a sample belongs to, as specified in the Batch View.

The following factors define the threshold guide that the Comparative View displays on the sample peak plots:

- The threshold method and amount that you specified in the method

- The group that you created on the Sample page

- The threshold sample that you selected on the Threshold Samples page

Horizontal guide indicates the threshold value as specified in the method.
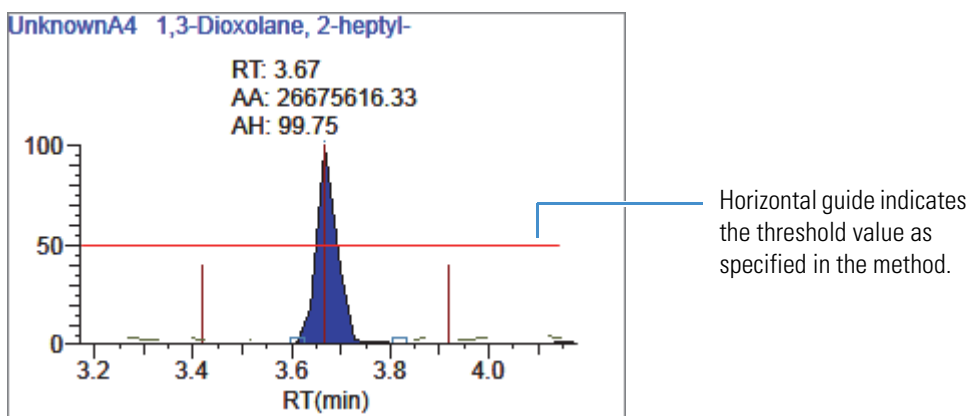
This section includes the following topics:

- Configuring Sample Peaks Display Settings

- Manually Integrating Peaks

For information about specifying the method to use for creating a threshold guide, see "Threshold" on page 197.

For information about creating groups, see "Groups" on page 396.

For information about specifying a threshold sample, see "Threshold Samples Page" on page 434.

Configuring Sample Peaks Display Settings

The Sample Peaks pane in the Comparative View displays one row per compound and one column per sample. The Sample Peaks pane displays all samples in a group when you select any of the samples belonging to that group.

For information about creating groups, see "Groups" on page 396.

❖ **To change the Sample Peaks pane display**

1. From the View menu, choose **Chromatogram Pane Settings**.

   The Chromatogram Plot Settings dialog box opens. See "Chromatogram Plot Settings Dialog Box" on page 479.

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 113. Number of Rows equals 1 and Number of Columns equals 1
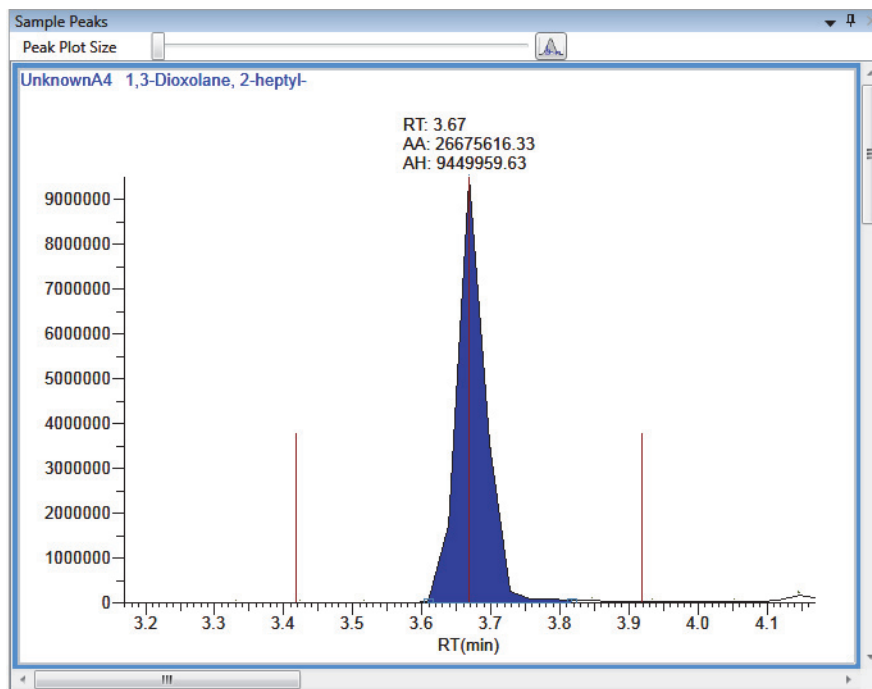
Figure 114. Number of Rows equals 4 and Number of Columns equals 4
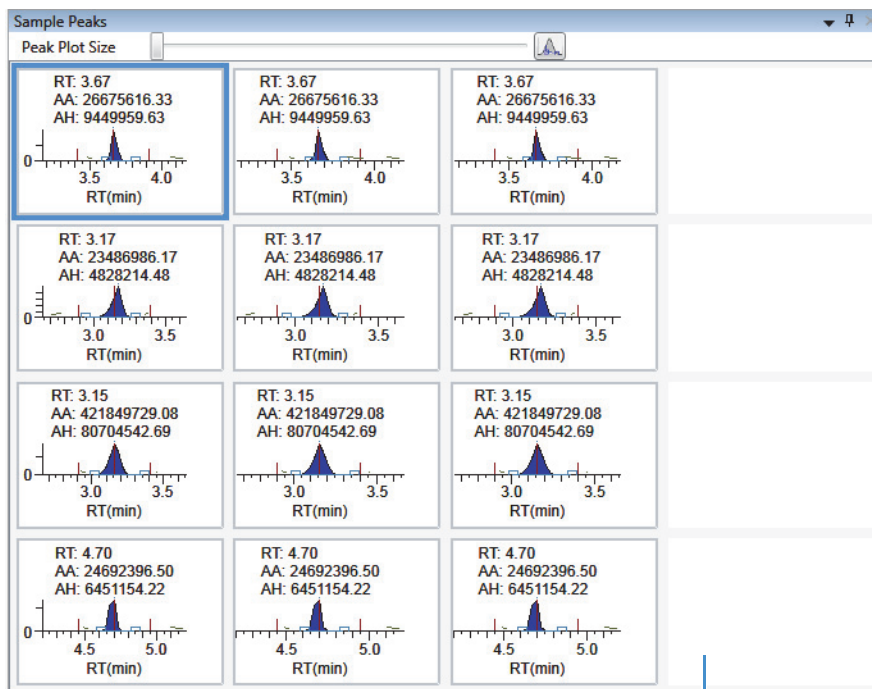
Because there are only three samples, this column is empty.

3. To change the display type for the *y*-axis scale, select one of the following:

- **Relative**: Displays the *y*-axis scale from 0 to 100.
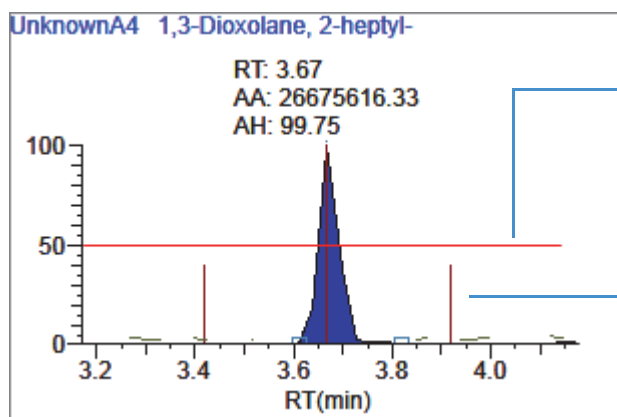
Horizontal bar indicates the threshold value as specified in the method.

Vertical bars indicate the expected retention time and window, as specified in the method.

- **Absolute**: Displays the *y*-axis scale from 0 to the actual value of the most intense peak in the group.
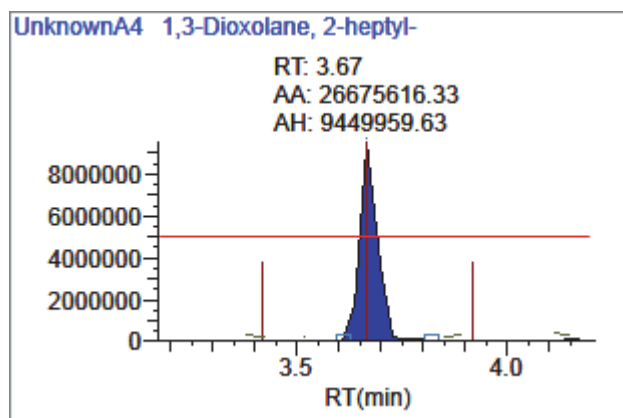
- **Label in Scientific Notation**: Displays the *y*-axis scale in scientific notation.
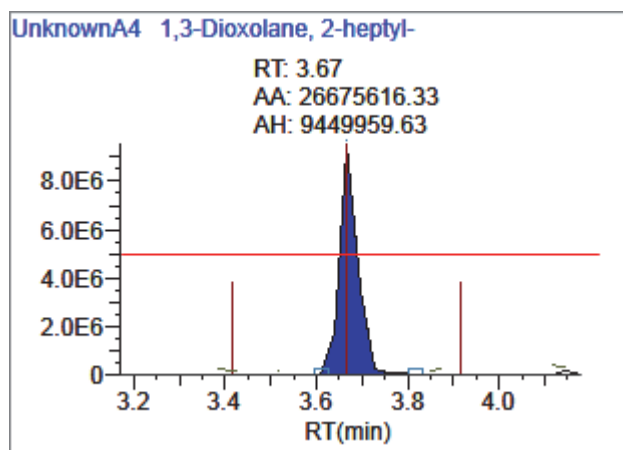
> **Note** The Sample Peaks pane displays a *y* axis only on the first chromatogram in each row. The limits of the scale are determined by the most intense peak in the group.

4. Specify which labels you want to display in the sample peak plots.

   For an example of all available peak plot labels, see Peak Plot Labels.

Chromatogram Plot Settings Dialog Box

Use the Chromatogram Plot Settings dialog box to change the Sample Peaks pane display.
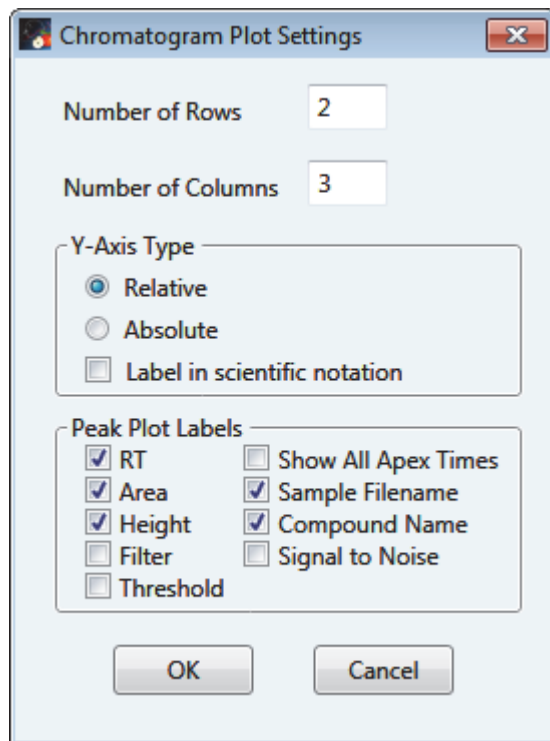
Table 86. Chromatogram Plot Settings dialog box parameters (Sheet 1 of 2)

Parameter	Description
Number of Rows	Specifies the number of rows visible in the Sample Peaks pane. When Number of Rows equals 1, the application scales the height of all chromatograms to fill the Y dimension of the Sample Peaks pane. Default: 3
Number of Columns	Specifies the number of columns visible in the Sample Peaks pane. When Number of Columns equals 1, the application scales the width of all chromatograms to fill the X dimension of the Sample Peaks pane. Default: 3

Table 86. Chromatogram Plot Settings dialog box parameters (Sheet 2 of 2)

Parameter	Description
Y-Axis Type	Displays the *y*-axis scale as Relative (to the most intense peak), Absolute, or in scientific notation.
Peak Plot Labels	Displays or hides the following peak labels: • RT • Area • Height • Filter • Threshold • Show All Apex Times • Sample Filename • Compound Name • Signal to Noise Example with all peak labels displayed:
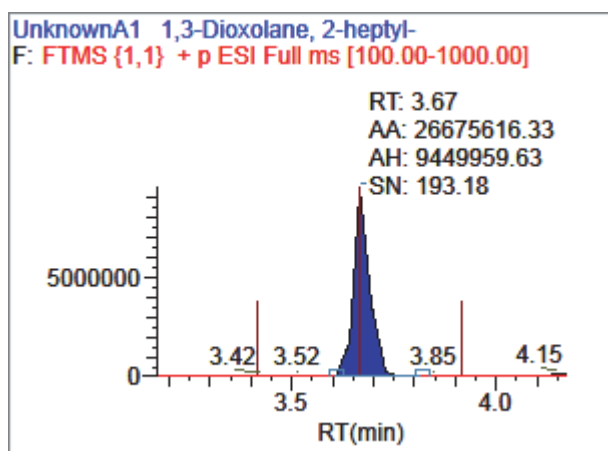
Manually Integrating Peaks

Use the manual integration feature to manually add a peak. You can manually add a peak in a chromatogram plot only when the application fails to identify a peak.

❖ **To manually integrate a peak**

1. In the Sample Peaks plot, click the **Manual Integration** icon.

Manual integration icon
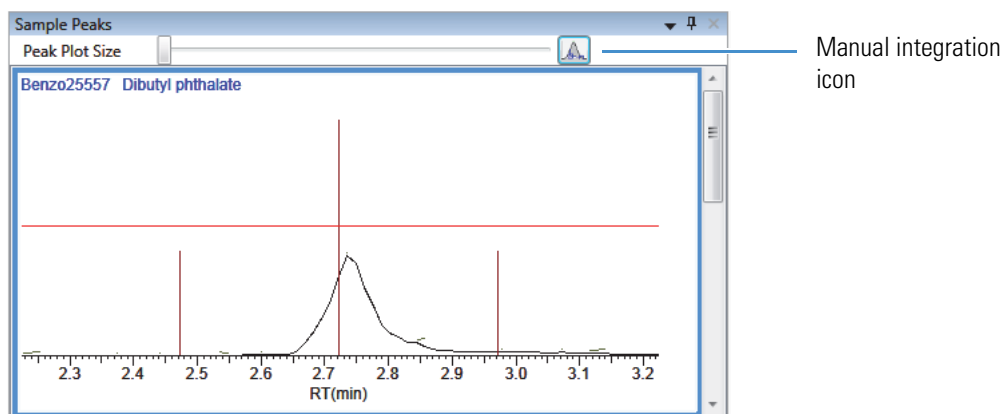
The cursor changes to look like this:

2. To integrate a peak, do the following:

a. Drag the cursor to describe the beginning and ending base points for the new peak.

> **Note** You must drag the cursor inside the *x*-axis and *y*-axis.

b. Click outside the plot to refresh the display.
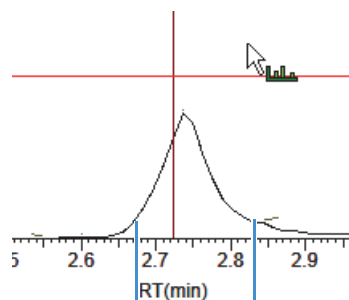
Click the first base point, and then drag to the second base point.
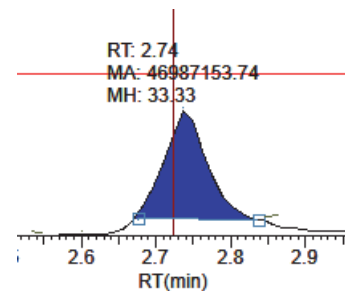
Click outside the plot to refresh the view.

The application identifies the peak and indicates the manual integration in the labels.

3. To zoom in on an area, do the following:

    a.   Drag the cursor below the *x*-axis or to the left of the *y*-axis.

        The plot zooms to fit the described X or Y dimension into the entire pane. The application zooms all compounds in the row to the same scale.

    b.   To return to the original view, right-click and choose **Reset Scaling** from the shortcut menu.

Qualitative View

The Qualitative View uses several different panes to display qualitative information for the selected sample. See Displaying Qualitative View Panes.

If the application finds no detected peaks for the selected sample, you can manually add peaks.

To see processed data for a sample in the Qualitative View, you must select the Qual Processing parameter for that sample in the Batch View before you process the batch. See "Batch View Sample List" on page 402.

These are the default panes and their locations:

Samples pane   Peaks pane

Sample   Peak Details pane   Spectrum pane   Library Hits pane
chromatogram pane

The Qualitative View displays data in the following panes:

- Samples Pane

- Peaks Pane

- Sample Chromatogram Pane

- Peak Details Pane

- Spectrum Pane (Library and Data)

- Library Hits Pane

Displaying Qualitative View Panes

The Qualitative View display uses multiple panes to display data: Samples, Peaks, Sample Chromatogram, Peak Details, Spectrum, and Library Hits. You can display, hide, or move any of these panes.

❖ **To display or hide a Qualitative View pane**

From the View menu, choose to display or hide the following:

- **Peaks**
- **Sample Chromatogram**
- **Peak Chromatogram**: Displays or hides the Peak Details pane.
- **Spectrum**
- **Library Hits**

Note The Samples pane is required for the Qualitative View display. You cannot hide the Samples pane.

Displayed panes are indicated with a check mark.
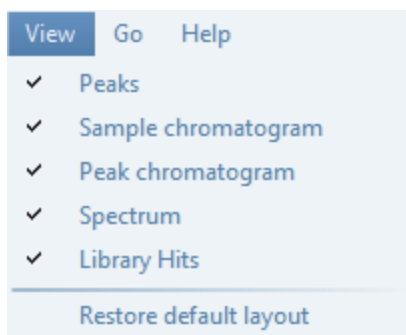
For procedures about creating docked, floating, or tabbed panes, see "Data Review Pane Display Features" on page 462.

Samples Pane

Use the Samples pane in the Qualitative View to select a specific sample. The associated Peaks Pane displays all peaks found in the selected sample.

❖ **To hide or display columns in the Samples pane**

1. Click the **Field Chooser** icon, , in the upper left corner of the pane.

   The Field Chooser displays all available columns of data for the Samples pane.
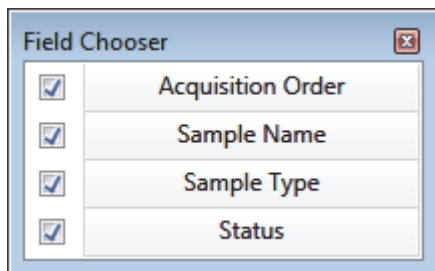
2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   The application immediately displays or hides the column in the Samples pane.

3. When you are finished modifying the column display, click to close the Field Chooser.

Figure 115. Samples pane

Table 87. Samples pane columns (Sheet 1 of 2)

Column	Description
Acquisition Order	Sequentially numbers the samples.
Flags	Caution flag displayed when a compound in the sample has an error. See "Caution Flags" on page 458.
Status	🔵 Sample is not acquired.
	🟡 Sample is acquired but not processed.
	🟢 Sample is acquired and processed.
	🟠 Sample is currently acquiring.

Table 87. Samples pane columns (Sheet 2 of 2)

Column	Description
Sample Name	A user-defined name that identifies a sample.
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative.

Peaks Pane

The Peaks pane in the Qualitative View works with the Samples pane to display graphical values for a unique sample and peak combination. For detailed descriptions of parameters in the Peaks pane, see "Peaks Pane" on page 491.

❖ **To display peaks for a specific compound**

1. From the Samples pane, select a sample.

   The Peaks pane displays the retention times for peaks identified in the selected sample, the values for the best match methods for each peak, and the library match.

   The method specifies which technique to use for identifying peaks: peaks within a specific retention time range, as a minimum percentage of the height or area of the largest peak, or as a minimum percentage of the nearest internal standard peak. You can change the method for identifying peaks in the Method Template Editor. See "Creating a Method Template" on page 254.

2. In the Peaks pane, select a peak in the sample.

Peak RT	SI	RSI	MP	Est Amt	Library Hit
9.82	124	732	0	0.000	Phenomorphan
1.05	274	793	59	0.000	Phosphoramidic acid, phenyl-, dipher
1.63	161	570	4	0.000	Sulfasomizole

Filter: + c ESI Full ms [200.00–800.00]

   The TraceFinder application displays the selected peak in the Peak Details pane, displays the Qual Data and Qual Library sections in the Spectrum pane, and locates the selected peak in the Sample Chromatogram pane.

   • The Qual Data section shows spectrum data for the peak in the raw data file.

   • The Qual Library section shows actual spectrum for the identified library compound.

Figure 116. Peak Details pane
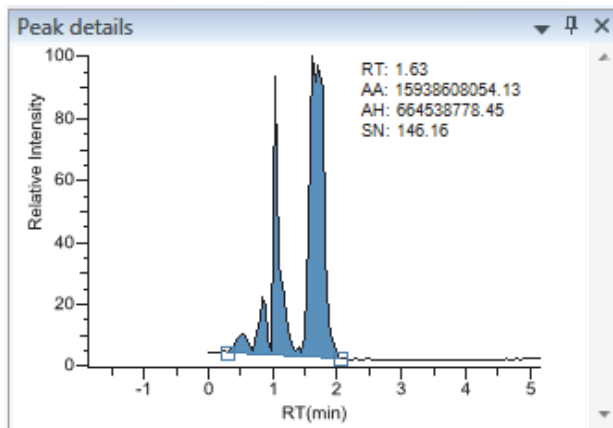
> **Note** When you select a data-dependent sample, the peak can be from either a full scan or a QED spectrum of an SRM-filtered chromatogram.

Figure 117. Spectrum pane

Reference spectrum from the library

Actual spectrum data for the compound
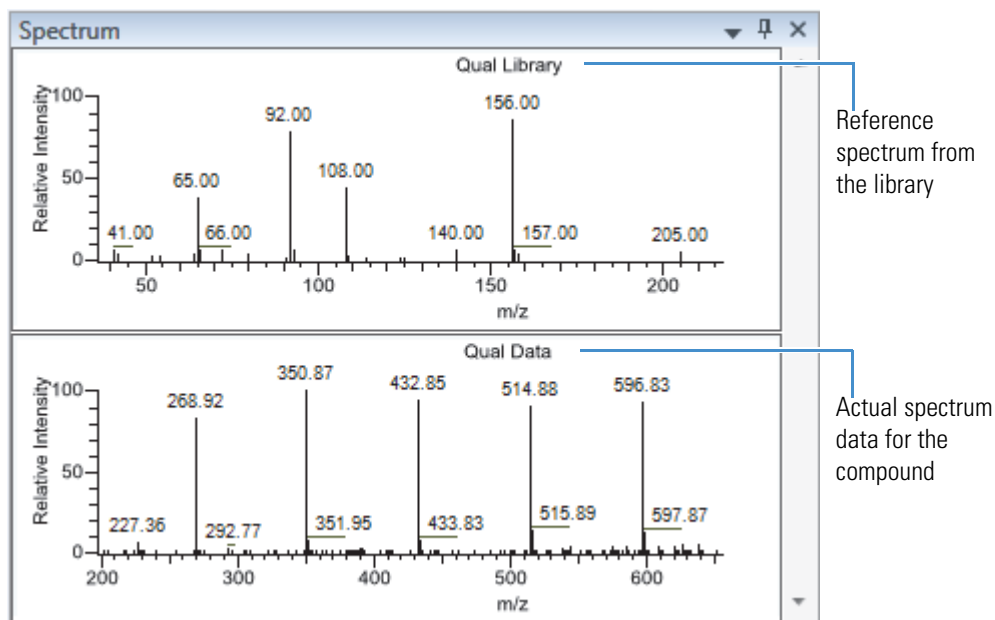
Figure 118. Selected peak in the Sample Chromatogram pane
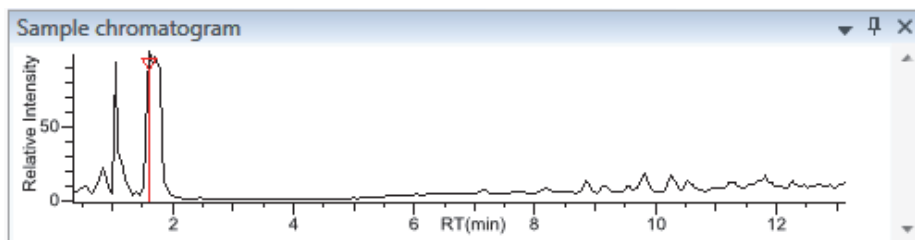
❖ **To remove a peak**

1. Select a peak in the Sample Chromatogram pane.

2. Right-click the Peak Details pane and choose **Remove Qual Peak** from the shortcut menu.

   The TraceFinder application removes the selected peak from all Qualitative View panes.

   > **Note** There is no undo for this action, but you can manually add a peak to redefine a removed peak. See "Sample Chromatogram Pane" on page 492.

❖ **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.
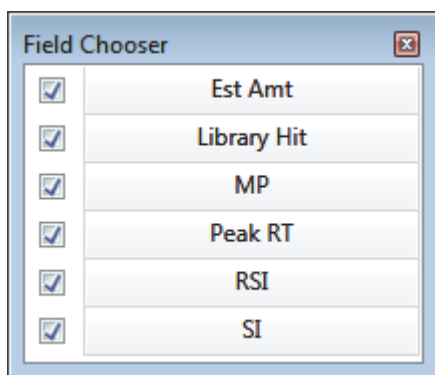
2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   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 on the Peaks pane to display graphical values for each sample and peak combination.

Figure 119. Peaks pane

Table 88. Peaks pane parameters

Parameter	Description
Filter	Filter used to identify the peaks. Specified in the raw data file or the master method.
	When your raw data file is data-dependent, the filter indicates this with a "d".
	Data-dependent filter
Peak RT	Peak retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
SI	Search index method used to search the NIST library.
RSI	(Reverse search index) A method used to search the NIST library. A reverse search compares a library entry to an unknown compound (a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
MP	Match probability.
Compound	Library compound that matches the identified peak.
Remove Selected Peak	Shortcut menu command that removes the selected peak from the peaks list.

Sample Chromatogram Pane

The Sample Chromatogram pane in the Qualitative View displays all peaks in the selected sample. The peak selected in the Peaks pane displays a red marker. See "Sample Chromatogram Pane" on page 493.

❖ **To zoom in on a peak**

1. In the Sample Chromatogram pane, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the Sample Chromatogram pane and choose **Reset Scaling** from the shortcut menu.

❖ **To manually add a peak**

1. Zoom in to better identify which peak to add to the results set.
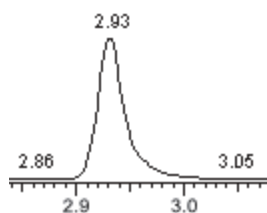
2. Right-click the Sample Chromatogram pane, and choose **Add Qual Peak** from the shortcut menu.

3. Click to indicate the left and right base points for the peak.

   The TraceFinder application marks the peak in the Sample Chromatogram pane.
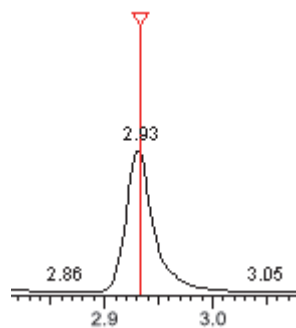
   The TraceFinder application places the peak delimiter tags at the base point locations and automatically updates the peak values in the Peaks pane and Peak Details pane. See Peak Details pane with a manually added peak.

Figure 120. Peak Details pane with a manually added peak

Manually added base points
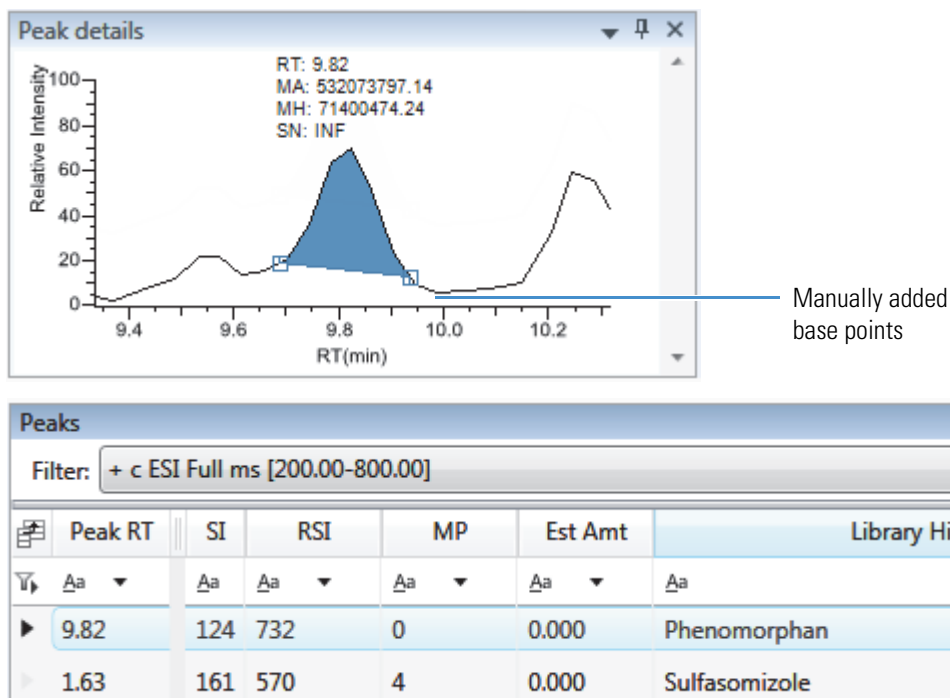
Sample Chromatogram Pane

Use the features on the Sample Chromatogram pane to display peaks in the selected sample.

Figure 121. Sample Chromatogram pane
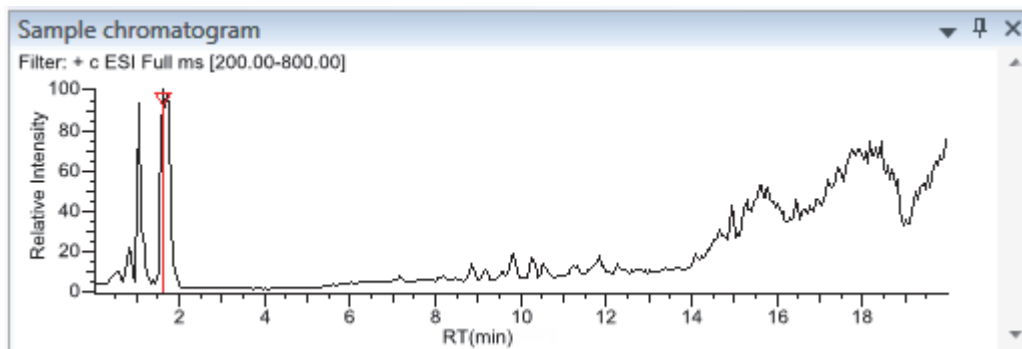
Table 89. Sample chromatogram pane shortcut menu commands

Command	Description
Add Qual Peak	Select the beginning and ending base points for a new qualitative peak. Available only when no peak is detected.
Reset Scaling	Resets the original scaling after a zoom operation.

Peak Details Pane

The Peak Details pane in the Qualitative View displays the selected peak. For a description of commands on the shortcut menu, see "Peak Details Pane" on .

Follow these procedures:

- To zoom in on a peak

- To manually add a peak

- To remove a peak

- To switch between method and manual integration modes

- To change the displayed information for detected peaks

❖ **To zoom in on a peak**

1. In the chromatogram plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

❖ **To manually add a peak**

1. Right-click anywhere in the Peak Details pane, and choose **Add Qual Peak** from the shortcut menu.

   If a peak is already detected, the Add Qual Peak command is not activated.

2. Click to indicate the left and right base points for the peak.

   The TraceFinder application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.

Manually added base points
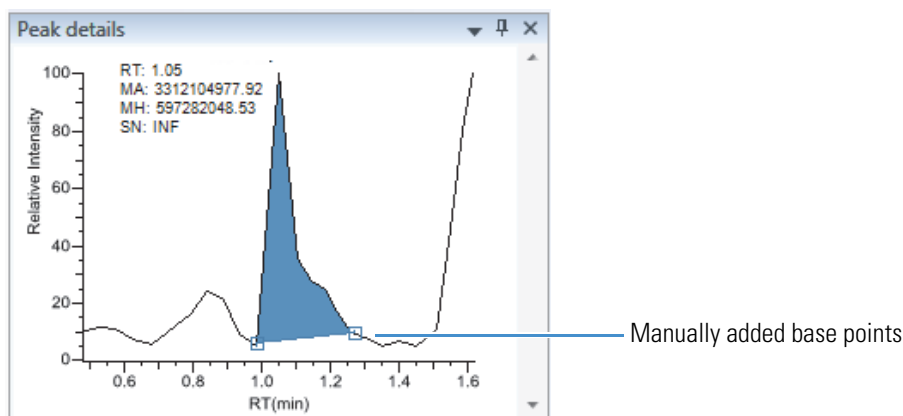
❖ **To remove a peak**

Right-click the Peak Details pane, and choose **Remove Qual Peak** from the shortcut menu.

The TraceFinder application removes the peak displayed in the Peak Details pane. All data for this peak are removed from the Qualitative View panes.

❖ **To switch between method and manual integration modes**

Right-click the Peak Details pane and choose **Method Integration** or **Manual Integration** from the shortcut menu.

Initially, the method and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the Peak Details plots and the result set update as you switch between method and manual modes.

As you switch between modes, each pane reflects the changes. The generated reports for these data identify the manual modifications.

❖ **To change the displayed information for detected peaks**

1. Right-click the Peak Details pane and hold the cursor over **Peak Labels**.

2. Choose to display labels for the peak retention time (RT), peak height (AH), peak area (AA), or signal-to-noise (SN).
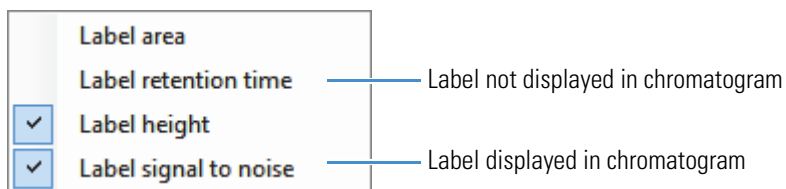
3. To remove a label, select the label type again to clear it.

Peak Details Pane

Use the features on the Peak Details pane to display the selected peak.

Figure 122. Peak Details pane
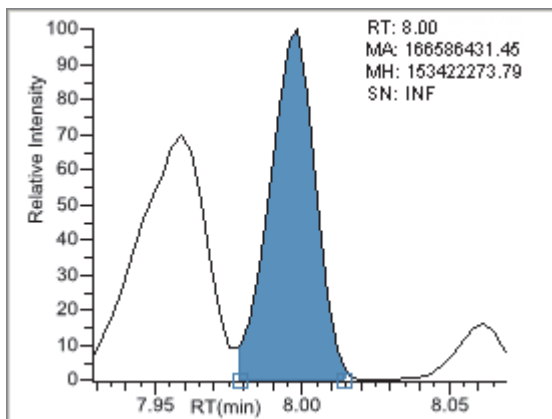
Table 90. Peak Details pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Method Integration	Displays method integration settings.
Manual Integration	Displays manual integration settings.
Peak Labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).
Remove Qual Peak	Available only for manually added peaks. Removes the peak displayed in the Peak Details pane.

Spectrum Pane (Library and Data)

The Spectrum pane in the Qualitative View displays the reference spectrum from the library and the spectrum data for the selected sample. The top pane displays the spectrum for the identified compound found in the reference library; the bottom pane displays the actual spectrum data for the selected peak.

Figure 123. Spectrum pane
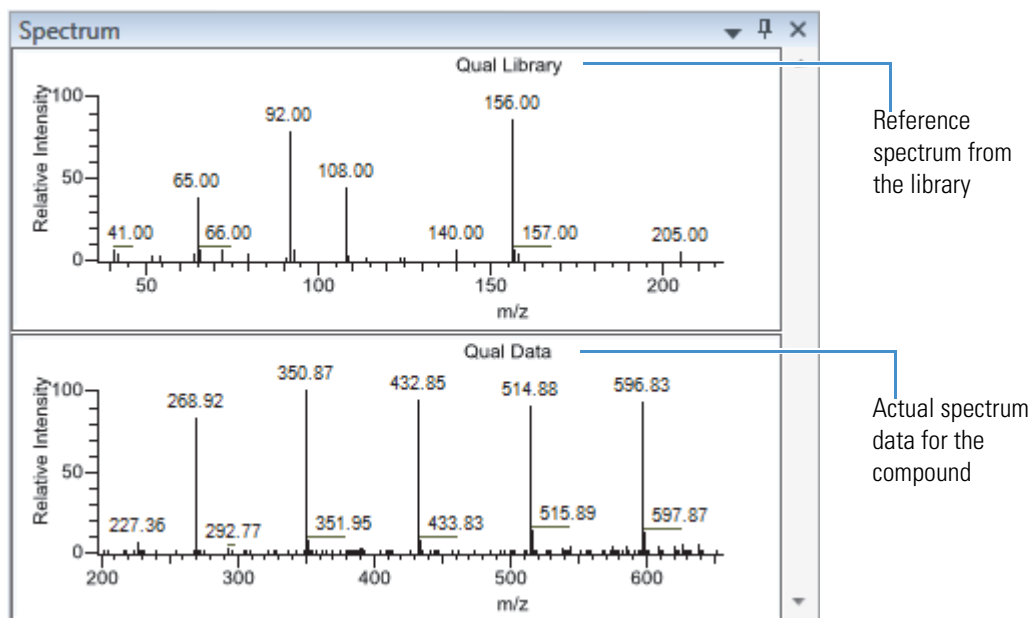
❖ **To zoom in on a peak**

1. In either spectrum plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the spectrum plot and choose **Reset Scaling** from the shortcut menu.

Library Hits Pane

The Library Hits pane in the Qualitative View displays the best library matches for the selected peak. Use this pane to select a different library entry for the peak. For detailed descriptions of the Library Hits pane parameters, see Library Hits pane.

When you select a library entry other than the original entry, the TIC Report and TIC Summary Report indicate this with a "P" flag:

Peak:	Retention Time	Area	Height	Inj Estimate	In-sample Est	Flag
Naphthalene	7.95	13829174	10605061	0.000	0.000	P

P flag

❖ **To change the library entry for a selected peak**

In the Library Hits pane, select the check box for the library entry that you want to use to identify the selected peak.

- In the Spectrum pane, the reference spectra change to show the spectra for the selected library entry.

- In the Peaks pane, the SI, RSI, MP, and Compound values update to reflect the selected library entry.

Selected library entry in the Library Hits pane
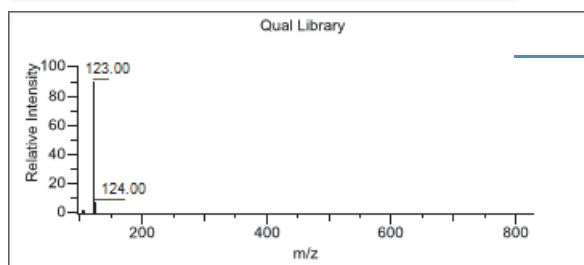
Reference spectra for Hexanone

Peak list for Hexanone

Figure 124. Library Hits pane

Table 91. Library Hits pane parameters

Parameter	Description
<Check box column>	Indicates selected library entries for the selected peak.
Rank	Indicates the order of best matches between the selected peak and library entries.
SI	(Search index) A method used to search the NIST library.
RSI	(Reverse search index) A method used to search the NIST library. A reverse search compares a library entry to an unknown compound (a forward search compares the mass spectrum of an unknown compound to a mass spectral library entry).
MP	Match probability.
Library Entry	Library compound that matches the identified peak.

Features Common to All Data Review Pages

The following features are common to all quantitative batch data review pages.

- Common Column Parameters

- Status Indicators

- Inactive and Excluded Compounds

- Compound Details

- Exporting Compounds

Common Column Parameters

Table 92. Common parameters for Compound Results and Sample Results tables (Sheet 1 of 3)

Column	Description
Height	The distance from the peak maximum to the peak base, measured perpendicular to the ordinate. When the Response Ratio is specified as Height, this column displays an asterisk (*Height).
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).
Expected RT	Expected retention time for the compound.
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.
Calculated Amt	The amount present in the sample, as determined using the calibration curve and the response ratio.
Theoretical Amt	Theoretical amount of the compound expected in the sample.
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.

Table 92. Common parameters for Compound Results and Sample Results tables (Sheet 2 of 3)

Column	Description
m/z (Expected)	Mass-to-charge ratio from the compound database. The charge is presumed to be 1.
	• When an adduct is found, the application displays the neutral mass value for the compound (calculated from the neutral formula) ± the mass of the most intense adduct ion found for the compound.
	• When no adduct is found, the application displays the neutral mass value for the compound ± the mass of the first adduct entered in the compound database.
	For details about defining adducts for the compound database, see "Specifying Adducts" on page 61.
	For details about adding adducts to compounds, see "Editing Compounds in the Database" on page 285
	Note When the adduct is a gain, the adduct mass is a positive number. When the adduct is a loss, the adduct mass is a negative number. The resulting mass value after adding or subtracting the adduct mass is always a positive number.
m/z (Apex)	Mass-to-charge ratio found in the spectra for the peak. The charge is presumed to be 1.
	When the application successfully integrates the peak, this column displays the charged *m/z* value for the compound, which is the highest intensity in the apex scan.
	When the application cannot successfully integrate the peak, this column displays N/F.
m/z (Delta)	Difference between the *m/z* (Expected) and *m/z* (Apex). The charge is presumed to be 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) = $1\,000\,000 \times ([m/z$ (Apex) $- m/z$ (Expected)$] \times m/z$ (Expected)).
	• When the mass tolerance is specified in mmu in the master method, then m/z (Delta) = $1000 \times m/z$ (Apex) $- m/z$ (Expected)).
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.
ISTD Amt	Amount of internal standard.
ISTD Response	Response of the internal standard.
Integration Mode	Integration mode specified in the method. See "Quan Peak" on page 508.

Table 92. Common parameters for Compound Results and Sample Results tables (Sheet 3 of 3)
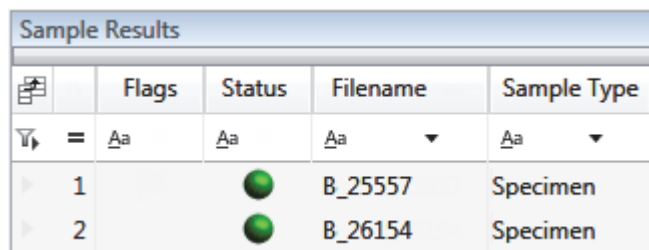
Column	Description
Active	Displays or hides a compound for a particular sample.
	• When a compound is marked inactive, the application does not remove its data and calculated values from the result set. Instead, the TraceFinder application masks the appearance of that compound for that particular sample and grays the compound in the compounds list.
	• When a calibration standard is marked inactive, the application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Compound Details pane. It is no longer part of the result set.
	In a Sample View, the Active parameter is in the Compound Results pane.
	In a Compound View, the Active parameter is in the Sample Results pane.
Excluded	Turns a compound on or off in the calibration curve in the Compound Details pane.
%Diff	The calculated amount minus the expected amount, divided by the expected amount, and then multiplied by 100.
%RSD	Standard deviation of the multiple samples of one level, multiplied by 100, and divided by the average of the multiple samples of that level. This calculation is based on the calculated amounts.
	Note This RSD value is not the same as the RSD value used with the Average RF curve type in the method. See "Calibration Page" on page 177. The application uses this %RSD value in Data Review and in the Compound Calibration Report when you acquire multiple samples for the same QC or Calibrator samples.
%CV	Coefficient of Variance. Standard deviation of the multiple samples of one level, multiplied by 100, and divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. The Channel column is available only when you have activated multiplexing in the Configuration console. See "Multiplexing" on page 70.
Final Units	Specifies the calculated amount. Default: 1
Comment	A user-defined comment for the sample.

Status Indicators

Status indicators for each sample indicate if the sample is currently acquiring, not acquired, acquired, or processed.

🔵 Sample is not acquired.

🟡 Sample is acquired but not processed.

🟢 Sample is acquired and processed.

🟠 Sample is currently acquiring.

Figure 125. Sample Results

Status indicators

Inactive and Excluded Compounds

Use the Active and Excluded columns to control which compounds are used for calculating the calibration curve and for reporting.

Follow these procedures:

- To make a sample active or inactive

- To exclude a calibration point

❖ **To make a sample active or inactive**

1. Select the sample in the Samples pane.

   All compounds in the selected sample are displayed in the Compounds pane. Inactive compounds are grayed out.

2. In the Compounds pane, select the compound whose active/inactive status you want to change.

   - When a compound it marked inactive, the application does not remove its data and calculated values from the result set. Instead, the TraceFinder application masks the appearance of that compound for that particular sample and grays the compound name in the compounds list.

   - When a calibration standard is marked inactive, the application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. The calibration point is no longer part of the result set.

3. In the Samples pane, select or clear the **Active** check box.

   Use the horizontal scroll bar at the bottom of the table to scroll to the Active column.

❖ **To exclude a calibration point**

In the sample list, select the **Excluded** check box for the sample.

Note Only calibration samples have the Excluded check box available.

Use the horizontal scroll bar at the bottom of the table to scroll to the Excluded column.

The application displays a value that is no longer used for calibration as an empty box in the graphical view of the calibration curve.
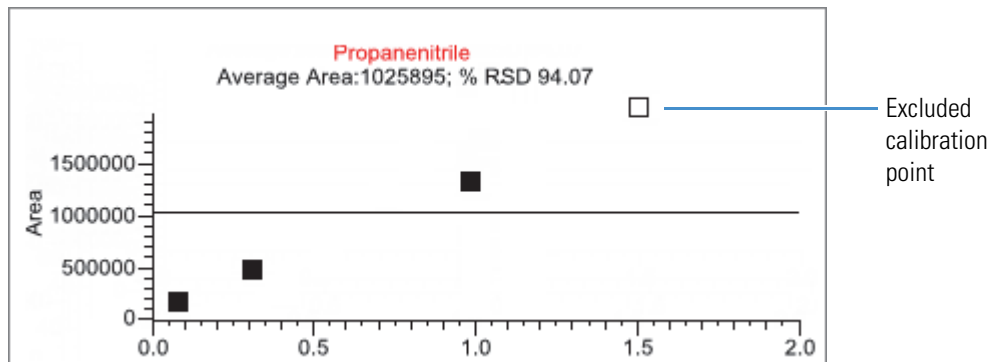
Compound Details

Use the Compounds Details pane to display any of the following types of data:

- Quan Peak
- Confirming Ions
- Calibration Curve
- Ion Overlay
- ISTD
- Reference Peak
- Spectra

❖ **To open the Compound Details dialog box**

1. Double-click the chromatogram in the Sample Peaks pane.

   The Compound Details pane opens.
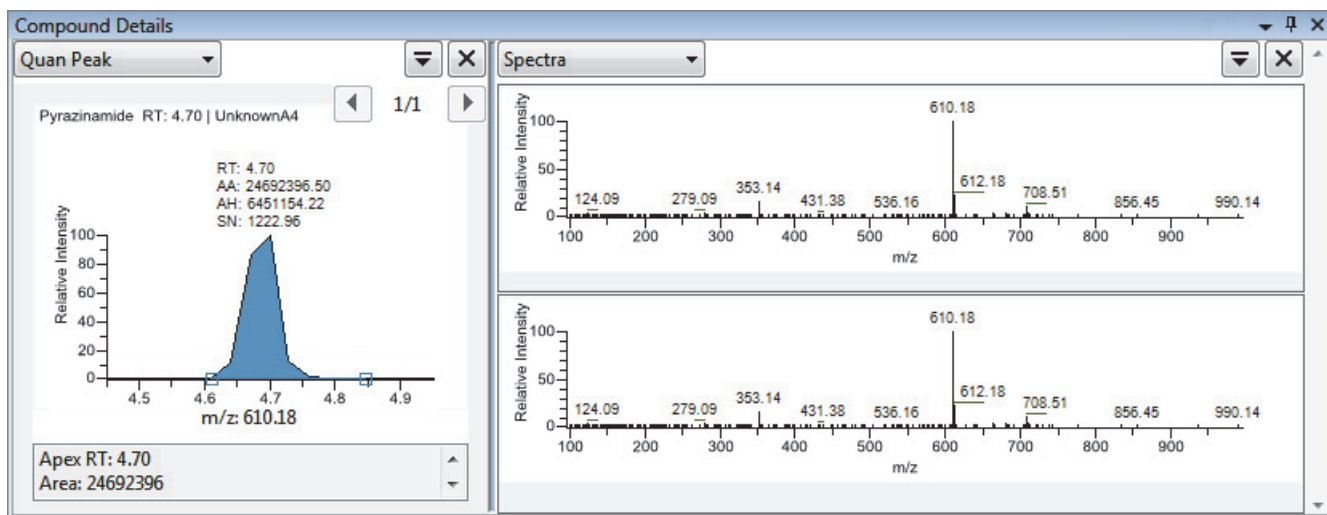
By default, the first display pane shows the quantitative peak for the selected compound.

2. In the second pane, select the additional type of data that you want to display.

Follow these procedures to change the display of the peak data in either of the panes:

- To change the peak panes
- To zoom in on a peak

❖ **To change the peak panes**

In any of the peak panes, click ▼ to view a list of commands.
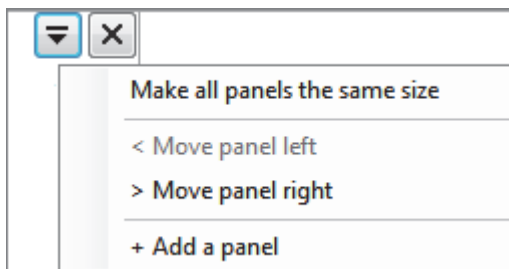
Command	Description
Make All Panels the Same Size	Evenly divides the area to make all panes the same width. This command does not change the pane height.
Move Panel Left	Moves the current panel one space to the left. This command is not available when the current pane is the leftmost pane.
Move Panel Right	Moves the current panel one space to the right. This command is not available when the current pane is the rightmost pane.
Add a Panel	Adds an empty peak pane to the display. You can display a maximum of four peak panes.

❖ **To zoom in on a peak**

1. In any of the views, drag your cursor to delineate a rectangle around the peak or spectra.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

Quan Peak

A compound can have multiple quantitative peaks. You can switch between quantitative peaks, but you cannot view multiple quantitative peaks at the same time. The indicator in the upper right corner of the Quan Peak pane displays which of the multiple quantitative peaks you are viewing. The Quan Peak pane uses a unique shortcut menu. See "Quan Peak pane shortcut menu commands" on page 512.

Figure 126. Quantitative peak pane with multiple quantitative peaks

Peak 1 of 2

Peak 2 of 2
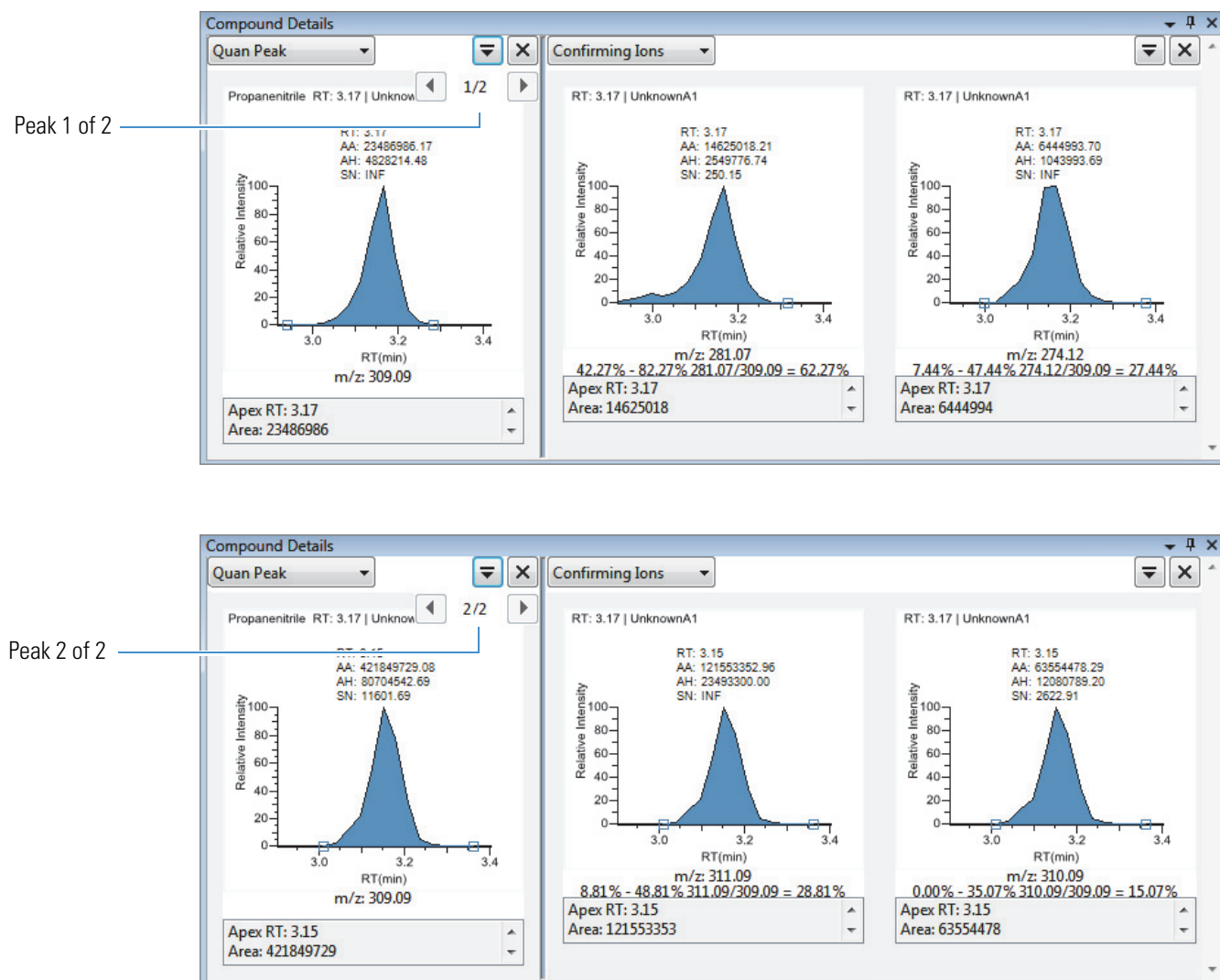
Follow these procedures to modify the quantitative or confirming ion peak data:

- To manually add a peak
- To remove a manually created peak
- To switch between method and manual integration modes
- To change the displayed information for detected peaks
- To modify the peak detection settings

❖ **To manually add a peak**

1. Right-click anywhere in the quantitative peak pane, and choose **Add Quan Peak** from the shortcut menu.

2. Click the left base of the peak you want to identify.

3. Drag to the right base and release the mouse.

   The application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.

Manually added right and left base points
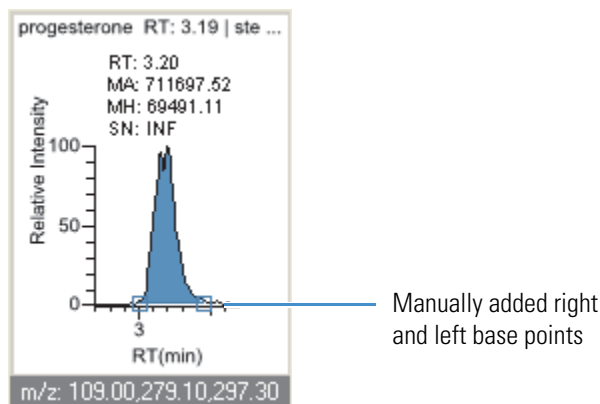
❖ **To remove a manually created peak**

Right-click the pane, and choose **Cancel Add Peak** from the shortcut menu.

The application cancels the Add Peak operation. If you have already completed adding the peak, select the peak and then choose **Remove Quan Peak** from the shortcut menu.

❖ **To manually integrate a quantitative peak**

1. Hold your cursor over one of the two peak delimiter tags in the peak pane.

   When the tag can be selected, the cursor changes to a crosshair-style cursor. You can zoom in on the baseline to make it easier to select the tag.

Crosshair cursor

2. Drag the peak delimiter tag to another location and automatically update the peak values (area, height, and so forth) into the result set.

   The generated reports for these data identify the manual modifications.

   You can store two peak value sets (method and manual integration settings) with each compound in each file. These settings can result in a different set of stored values. The application originally calculates the method values based on the processing method parameters. The manual values are a result of what you have edited.

❖ **To switch between method and manual integration modes**

Right-click the chromatogram view and choose **Method Integration Settings** or **Manual Integration Settings** from the shortcut menu.

Initially, the method and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the chromatogram plots and the result set update as you switch between method and manual modes.

As you switch between modes, each pane reflects the changes. The generated reports for these data identify the manual modifications.

❖ **To change the displayed information for detected peaks**

1. Right-click the peak pane and hold the cursor over **Peak Labels**.

2. Choose to display labels for the peak retention time, peak height, peak area, or signal to noise.

   The label types in the list are selected for displayed labels and are cleared for labels that are not displayed.

3. To remove a label, select the label type again and clear it.

   Label settings are globally applied to quantitative peaks, confirming ion peaks, and internal standard peaks.

> **Tip** The labels do not always update on all peak displays. To update all labels, select a different compound, and then reselect the compound whose labels you changed.

❖ **To modify the peak detection settings**

1. Right-click the chromatogram view and choose one of the following from the shortcut menu:

   • **Peak Detection Settings > Edit Local Method Peak Detection Settings**: Makes changes to the selected compound for all samples in this batch.

   • **Peak Detection Settings > Edit User Defined Peak Detection Settings**: Makes changes to the selected compound for only the selected sample. The TraceFinder application saves these changes with the batch and stops applying the local method detection settings to the compound for this sample only.

   The Peak Detection Settings dialog box opens where you can adjust detection settings that were specified in the method. The title bar of the dialog box lists the selected compound and indicates whether you are making changes to only the selected sample or to the local method.

Figure 127. Peak Detection Settings dialog box

Editing all samples in the batch

Editing only the selected sample

2. Edit any of the detection settings.

   For detailed descriptions of all detection settings, see "Detection" on page 125.

3. To save your changes to this compound, click **Apply**.

   • When you are editing a single sample, the application makes changes to the selected compound for this sample. If the sample is a calibration sample type, this update changes the calibration curve which, in turn, affects all calculated amounts.

   • When you are editing the local method, the application makes changes to the selected compound for all samples in this batch.

   Note The Peak Detection Settings commands are also available on the Confirming Ions pane.

Table 93. Quan Peak pane shortcut menu commands (Sheet 1 of 2)

Command	Description
Method Integration Settings	**Use Local Method Peak Detection Settings**: Applies the local method integration settings to the selected compound.
	To edit these peak detection settings, use the Peak Detection Settings > Edit Local Method Peak Detection Settings command.
	Use User Peak Detection Settings: Applies the user-customized method integration settings to the selected compound.
	To edit these user-customized settings, use the Peak Detection Settings > Edit User Defined Peak Detection Settings command.
Manual Integration Settings	Displays manual integration settings.
Add Quan Peak –or– Remove Quan Peak –or– Cancel Add Peak	Adds a peak, removes a peak, or cancels an add peak operation in progress.
Confirming Ion List	Select the confirming ions to be viewed. Not available for analog compounds.
Send RT to Method	Sets the current retention time as the expected retention time for the compound in the local method.
Peak Labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).

Table 93. Quan Peak pane shortcut menu commands (Sheet 2 of 2)

Command	Description
Show Peak Info	Displays peak information for the selected compound. For example
	Propanenitrile
	Quan ion m/z: 309.09
	Integration mode: Method
	Left RT: 2.94　Area: 23486986
	Apex RT: 3.17　Height: 4828214
	Right RT: 3.28　Noise: 0.00
	Data file: UnknownA3
	Filter: FTMS {1,2} + p ESI Full ms2
	Detector: MS
	Trace: Mass range
Reset Scaling	Resets the original scaling after a zoom operation.
Peak Detection Settings	**Edit User Defined Peak Detection Settings**: Opens the Peak Detection Settings dialog box where you can make changes to the selected compound for this sample.
	Edit Local Method Peak Detection Settings: Opens the Peak Detection Settings dialog box where you can make changes to the selected compound for all samples in this batch.
	After you apply either of these updates, the application does not retain manual integration settings.

Confirming Ions

The Confirming Ions pane displays a graphical view of all qualifying/confirming ions for the selected compound and displays calculated ion ratios and ion ratio acceptance windows. A red border indicates that an ion ratio is outside of its window. The Confirming Ions pane uses a unique shortcut menu. See Confirming Ions pane shortcut menu commands.

> **Note** For compounds with an analog detection type, the application displays "No Confirming Ions are Enabled" in the Confirming Ions pane.

Figure 128. Quantitative peak with multiple confirming ions
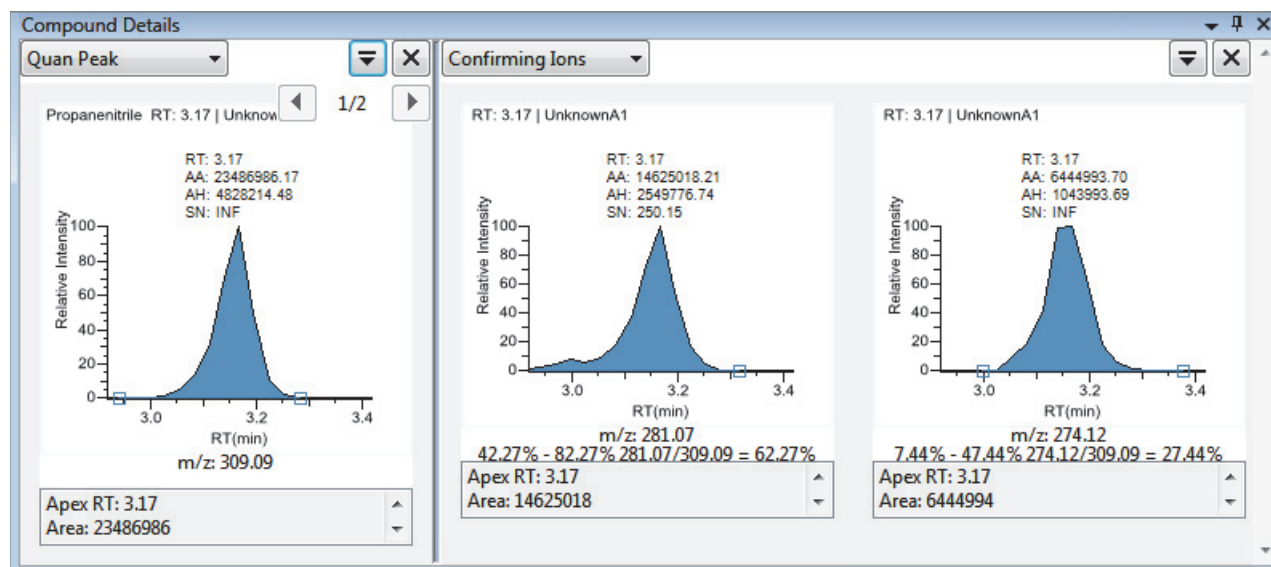
Figure 129. Confirming ion with coelution failure
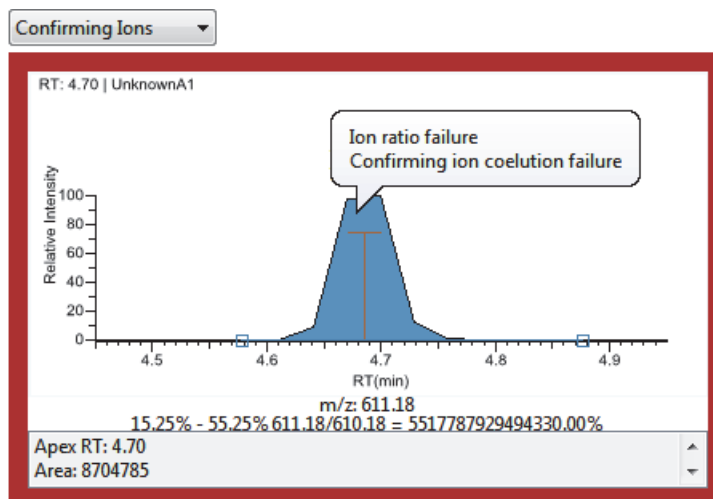
❖ **To manually integrate a confirming ion peak**

1. Hold your cursor over one of the two peak delimiter tags in the peak pane.

   When the tag can be selected, the cursor changes to a crosshair-style cursor. You can zoom in on the baseline to make it easier to select the tag.

2. Drag the peak delimiter tag to another location and automatically update the peak values (area, height, and so forth) into the result set.

   The generated reports for these data identify the manual modifications.

   You can store two peak value sets (method and manual integration settings) with each compound in each file. These settings can result in a different set of stored values. The application originally calculates the method values based on the processing method parameters. The manual values are a result of what you have edited.

   Note Because a Blank Report displays only the quantitation mass, when you manually integrate a confirming ion, the manual integration flag in the report is displayed on the quantitation mass.

Table 94. Confirming Ions pane shortcut menu commands

Command	Description
Method Integration Settings	Displays the method integration settings.
Manual Integration Settings	Displays the manual integration settings.
Add/Remove/Cancel Quan Peak	Adds a quantitation peak, removes a peak, or cancels an add peak operation in progress.
Range Calc Method: Manual	Selects the method used to calculate the ion ratio range windows: Manual, Average, Weighted Average, or Level.
Range Calc Level	Displays the range based on the calibration level.
Target Ratio	Specifies the theoretical ratio of the confirming ion's response to the quantification ion's response.
Window Type	Specifies the Absolute or Relative calculation approach for determining the acceptable ion ratio range.
Window	Specifies the acceptable ion ratio range as a percentage.
Peak Labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).
Show Peak Info	Displays peak information for the selected compound.
Reset Scaling	Resets the original scaling after a zoom operation.
Peak Detection Settings	Opens the Peak Detection Settings dialog box for the selected compound.

Calibration Curve

The Calibration Curve pane displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration. The Calibration Curve pane uses a unique shortcut menu. See Calibration Curve pane shortcut menu commands.

Figure 130. Quantitative peak with a calibration curve plot
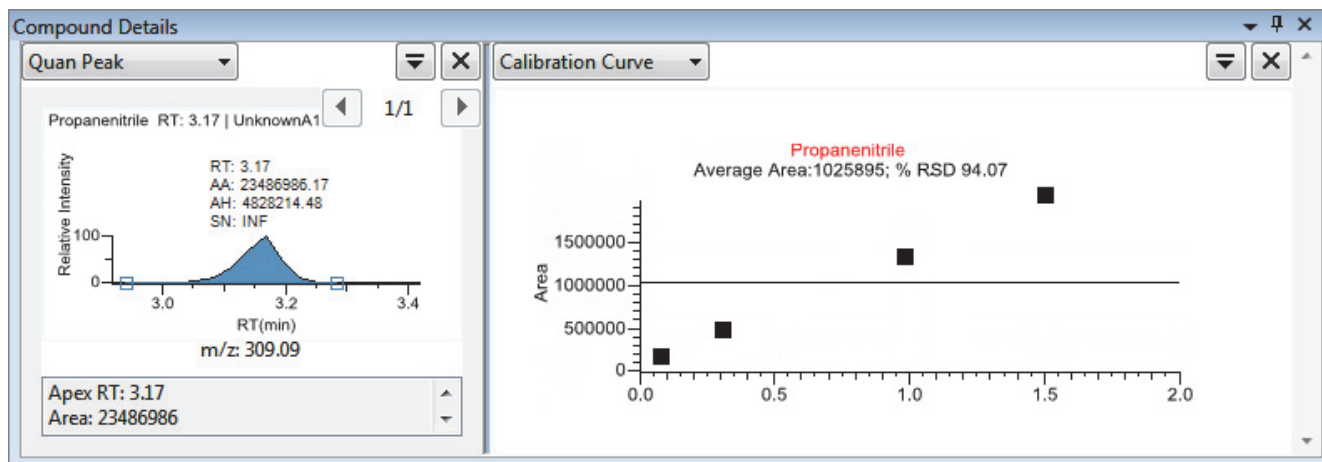
❖ **To manually exclude a calibration point**

In the sample list, select the **Excluded** check box for the sample.

Use the horizontal scroll bar at the bottom of the table to scroll to the Excluded column.

When a value is no longer used for calibration, it is displayed as an empty box in the graphical view of the calibration curve.
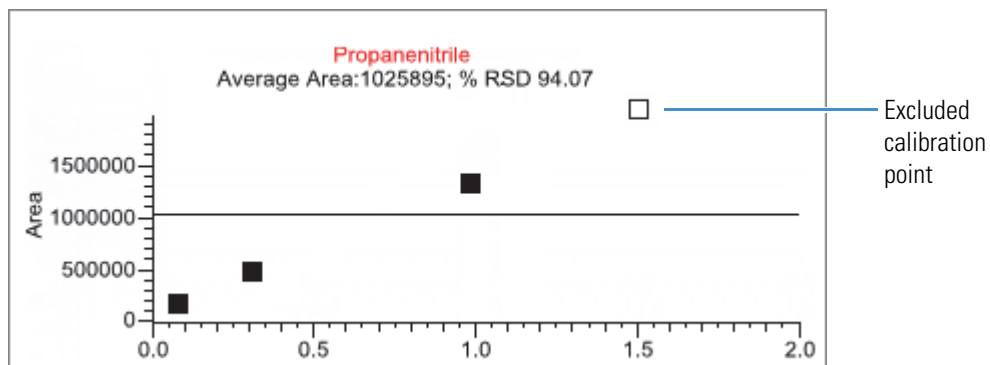
Table 95. Calibration Curve pane shortcut menu commands

Command	Description
Standard Type	Sets the standard type to External or Internal.
Calibration Curve Type	Sets the calibration curve type to one of the following: • Linear: Allows all settings with this exception: When Origin is set to Include, all Weighting values are grayed out and Weighting is set to Equal. • Quadratic: Allows all settings with this exception: When Origin is set to Include, all Weighting values are grayed out and Weighting is set to Equal. • Average RF: Allows no Weighting or Origin selections. All Weighting and Origin values are grayed out. Weighting is set to Equal, and Origin is set to Ignore.
Response Via	Sets the response to Area or to Height.
Weighting	Sets the weighting to equal, 1/X, 1/X^2, 1/Y, or 1/Y^2.
Origin	Sets the origin to Ignore, Force, or Include.
Units	Sets the units.
Done with Settings	Saves the calibration curve settings.
Reset Scaling	Resets the original scale in the calibration curve pane.

Ion Overlay

The Ion Overlay pane represents an overlay of the entire ion set—quantification and qualifying/confirming—for the selected compound. Use this pane to graphically review the peak apex alignment and coeluting peak profiles.

> **Note** For compounds with an analog detection type, the application displays "No Data" in the Ion Overlay pane.

Figure 131. Quantitative peak with confirming ion overlay
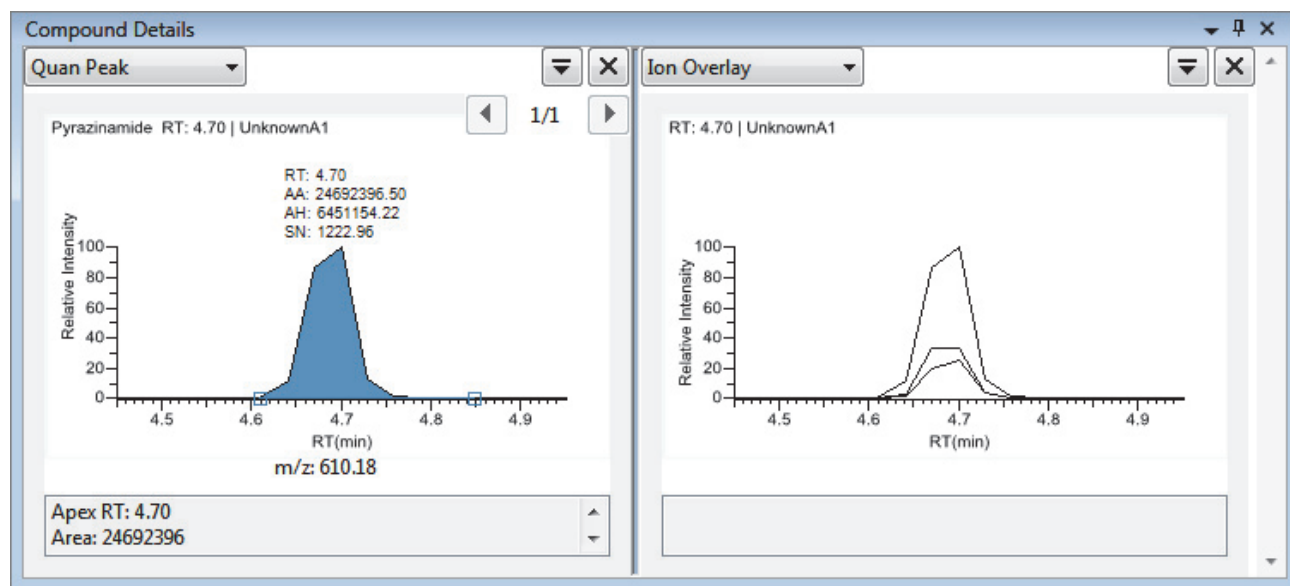
ISTD

The ISTD pane displays the internal standard specified for the compound in the method. See "To specify an internal standard type for a compound" on page 175.

Figure 132. Quantitative peak with an internal standard
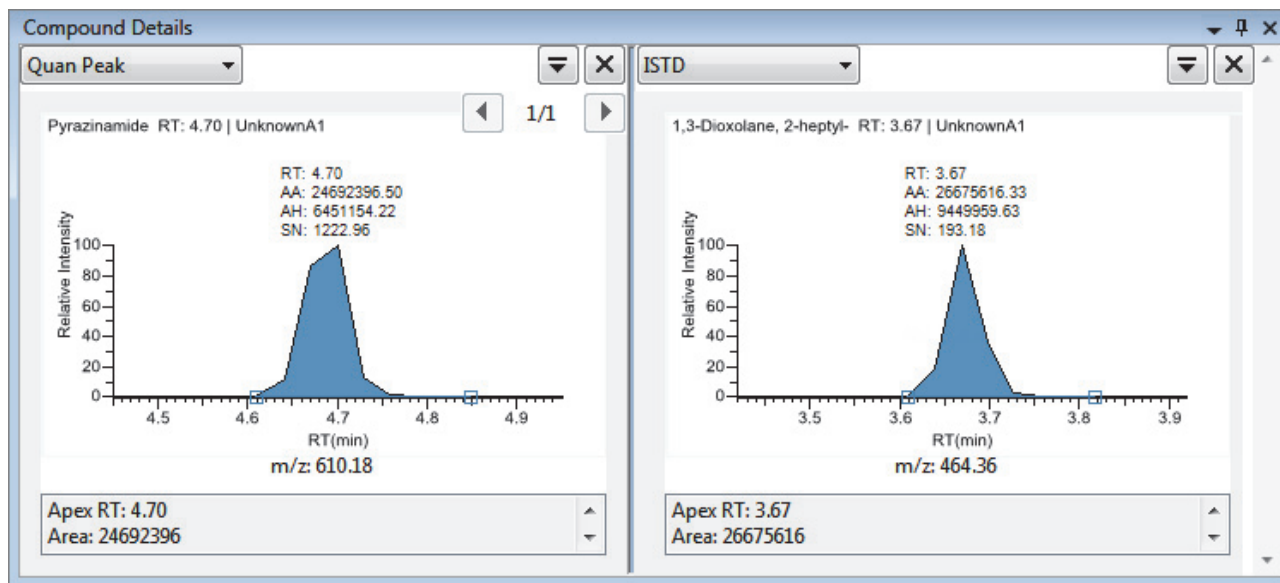
Reference Peak

The Reference Peak pane displays the reference peak as specified in the method.

Figure 133. Quantitative peak with a reference peak
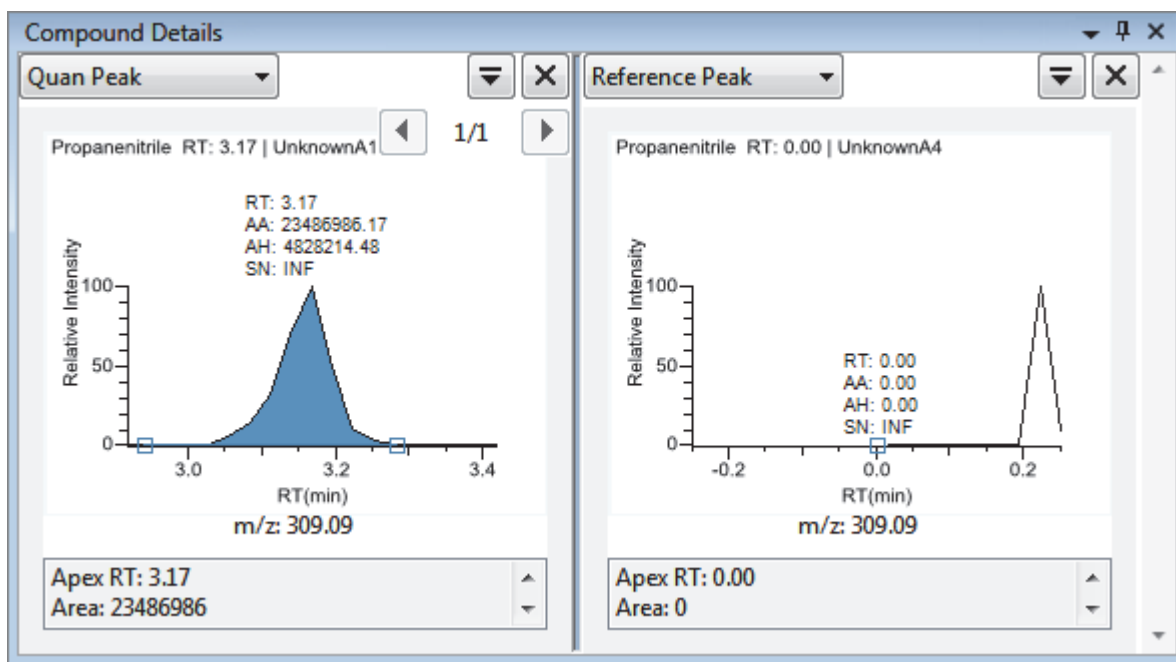
❖ **To specify a chromatogram reference peak**

1. In the Batch View task pane, click **Reference Sample**.

   An empty reference sample table opens.
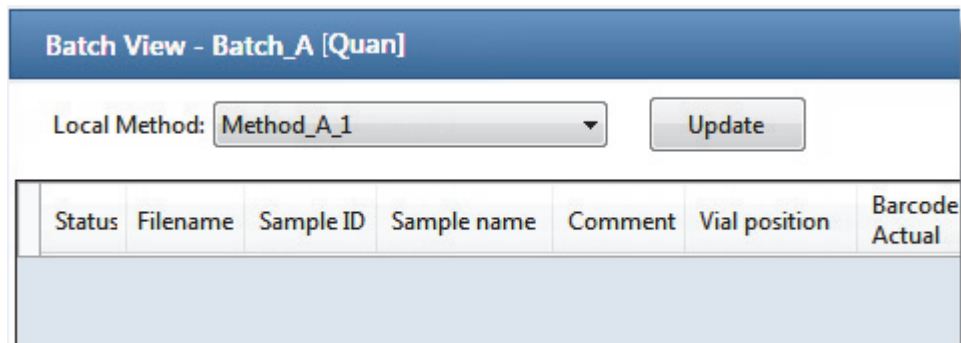
2. Click the **Add Reference Sample** icon, [1 ⬍ ⊞] , or right-click and choose **Add Reference Sample** from the shortcut menu.

   The Open Chromatograph Reference Sample dialog box opens.
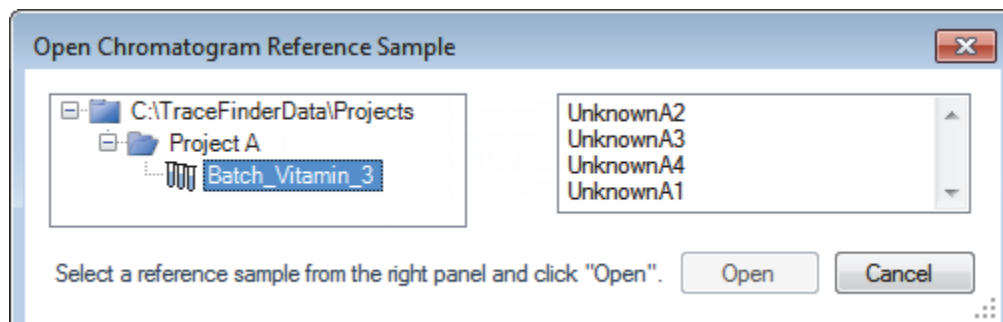
   > **Note** If you are creating a new method, you will not see any reference samples here. You must create and save a batch using the current method to see the reference samples in this list.

3. Select a project from the list of projects.

4. Select a subproject from the list of subprojects.

5. Select a batch from the list of batches.

   The TraceFinder application displays only batches that were created using the current master method.

6. Select a sample from the list of processed samples.

   The TraceFinder application displays all the processed samples in the selected batch. To use a sample as a reference sample, the sample must have been processed with the current master method.

7. Click **Open**.

The selected sample is displayed as the chromatogram reference sample in the Method View in the Method Development mode.

> **Tip** To clear the reference sample from the master method, select **None** in the Set Chromatogram Reference Samples pane.

Spectra

The Spectra pane displays a comparison of the spectra found in the data and the method reference.

> **Note** For compounds with an analog detection type, the application displays "Not Available" in the Spectra pane.

Figure 134. Quantitative peak with data and reference spectra
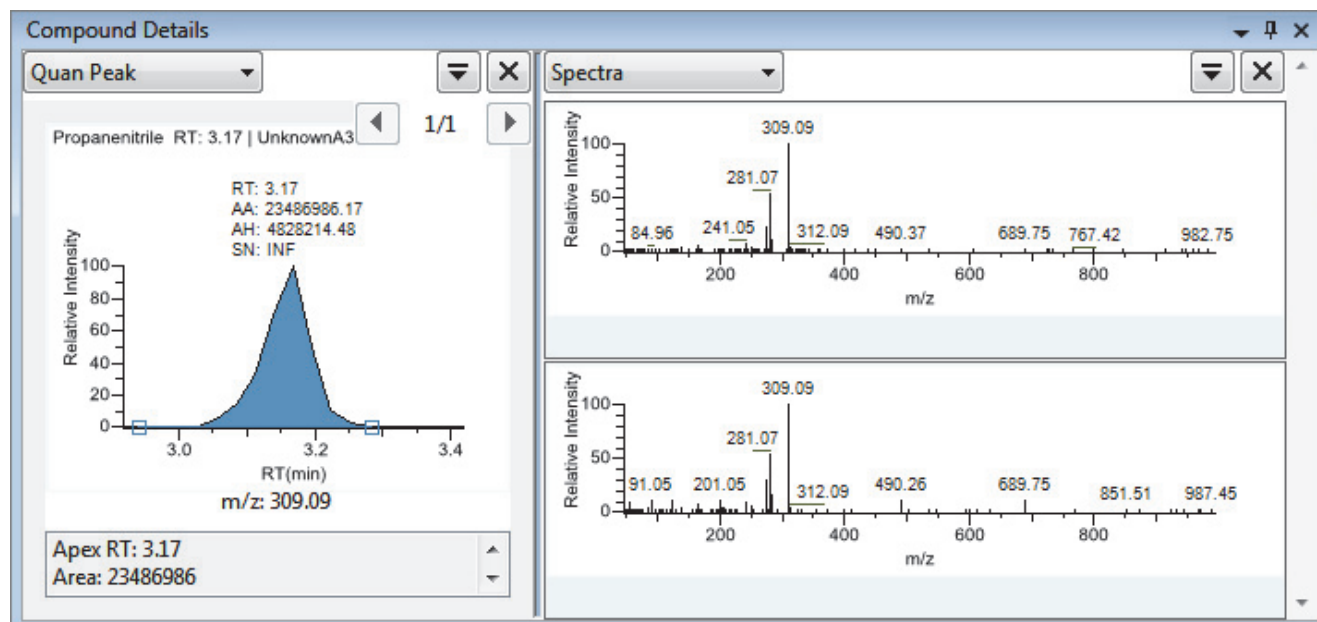
Exporting Compounds

You can export compound data to an Excel spreadsheet, to a CSV file, to a compound database, or to a new quantitation method. These export functions are available from the File menu in the Sample View, Compound View, and Comparative View.

Follow these procedures:

- To export compounds to an Excel spreadsheet
- To export compounds to a CSV file

❖ **To export compounds to an Excel spreadsheet**

1. Choose **File > Export Data To > CSV or Excel** from the main menu.

   The Data Review Export dialog box opens.

2. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.

3. Type a file name for the XLSX file and click **Save**.

4. In the File Format area, in the Data Review Export dialog box, select the **Excel** option.

5. In the Sheet Layout area, select one of the following file formats for the spreadsheet.

   - **Multiple Worksheets**: Writes one sample to each Excel worksheet tab.

   - **Single Worksheet**: Writes all samples to a single Excel worksheet tab.

6. In the Data to Export area, select one of the following sets of data to export.

   - **Export Visible Columns Only**: Writes data from only the displayed columns to the specified worksheet format.

   - **Export All Batch Data**: Writes data from all columns (displayed or hidden) of all samples to the specified worksheet format.

7. Click **Export**.

   The application saves the specified compound data to an Excel spreadsheet and opens the folder where you saved the file. The application names the file *Batch*.xlsx.

❖ **To export compounds to a CSV file**

1. Choose **File > Export Data To > CSV or Excel** from the main menu.

   The Data Review Export dialog box opens.

2. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.

3. Type a file name for the CSV file and click **Save**.

4. In the File Format area, in the Data Review Export dialog box, select the **CSV** option.

5. In the Sheet Layout area, select one of the following file formats for the spreadsheet.

   • **Multiple Files**: Writes one sample to each CSV file.

   • **Single File**: Writes all samples to a single CSV file.

6. In the Data to Export area, select one of the following sets of data to export.

   • **Export Visible Columns Only**: Writes data from only the displayed columns to the specified worksheet format.

   • **Export All Batch Data**: Writes all data from all samples in the batch to the specified worksheet format.

7. Click **Export**.

   The application saves the specified compound data to a CSV spreadsheet.

   When you selected to create multiple files, the application opens the folder where you saved the files. The application names each file *Batch_Compound*.csv.

   When you selected to create a single file, the Excel application opens, displaying the exported data for all samples. The application names the file *Batch*.csv.

Working in Data Review for Target Screening Methods

The Data Review view displays the data generated by the target screening master method. Use Data Review to verify the data for a compound before you generate reports.

❖ **To open the Data Review view**

1. Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.

2. Click **Data Review**.
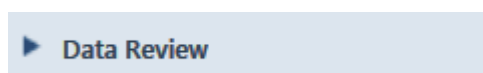
The Data Review navigation pane opens.
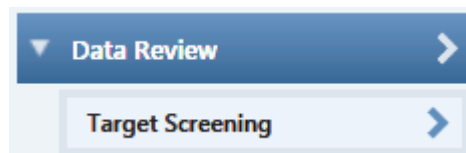
In the target screening display, the panes show a list of all samples in the current batch, the compound results for all compounds in the method, and chromatogram and spectrum plots for all compounds found in the currently selected sample.

❖ **To display or hide a pane on the Target Screening page**

From the View menu, choose to display or hide the following:

- **Samples**

- **Target Screening Results**: Displays or hides the Compounds pane.

- **Chromatogram**

- **Spectrum**

Displayed panes are indicated with a check mark.
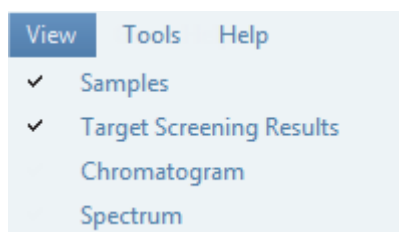
Figure 135. Target Screening panes

Chromatogram pane

Samples pane   Compounds pane   Spectrum pane
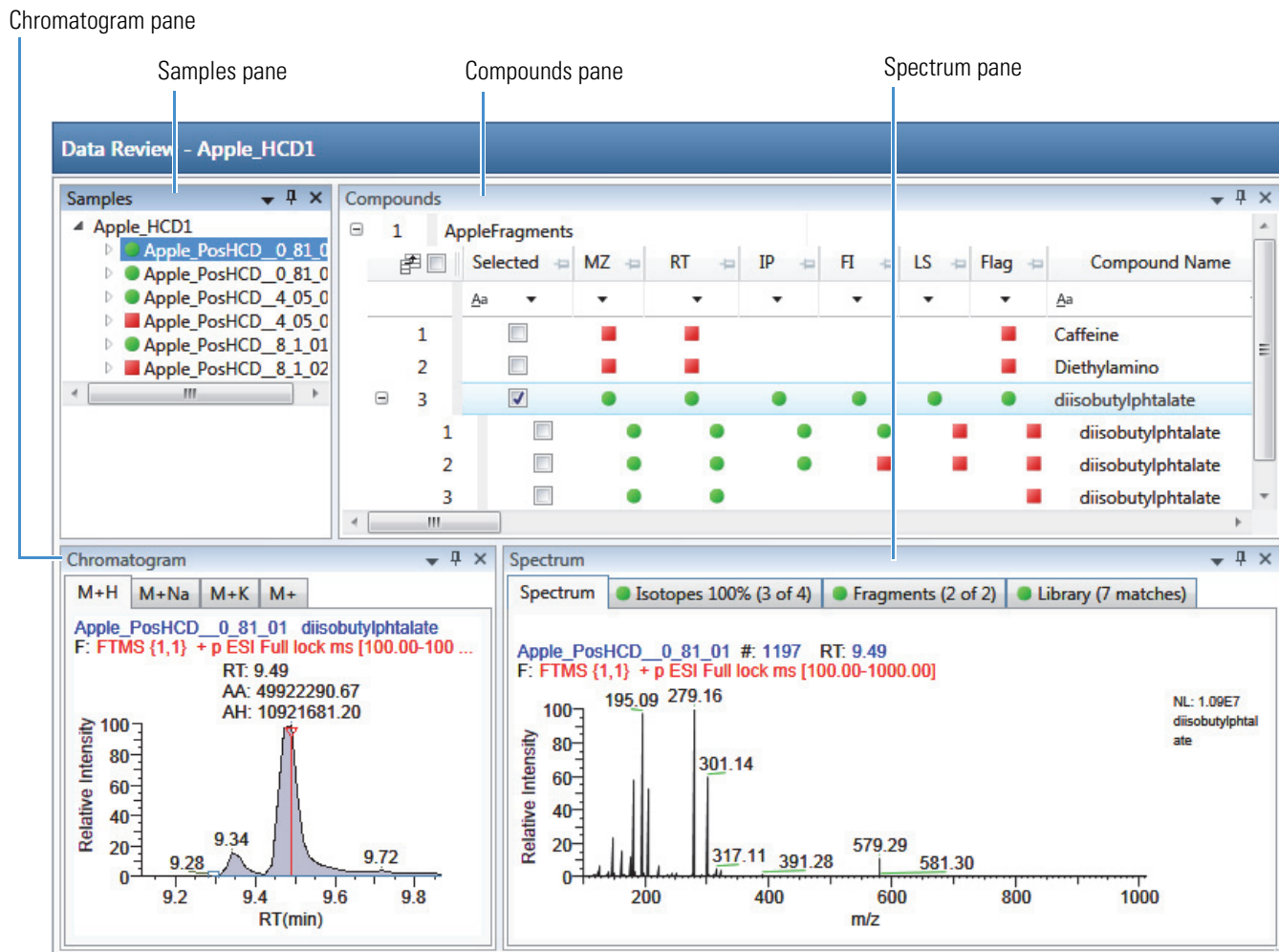
When you select a sample in the Samples pane, the associated Compounds pane flags any compound with errors in the selected sample. The associated Chromatogram pane displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the selected sample. The Spectrum pane highlights the compound selected in the Compounds pane. You can display, hide, or move any of these panes.

For procedures about creating docked, floating, or tabbed panes, see "Data Review Pane Display Features" on page 462.

The target screening display includes the following features:

- Samples Pane
- Compounds Pane
- Chromatogram Pane
- Spectrum Pane

Samples Pane

Use the Samples pane to select a specific sample in the batch. The associated Compounds Pane displays all compounds in the method and flags any compound with errors in the selected sample.

Flags in the Samples pane indicate one of the following:

● A green circle when the sample/compound/peak combination is identified and fully confirmed.

▲ A yellow triangle when the sample/compound/peak combination is identified but not fully confirmed.

■ A red square when the sample/compound/peak combination is not identified.

Figure 136. Samples pane
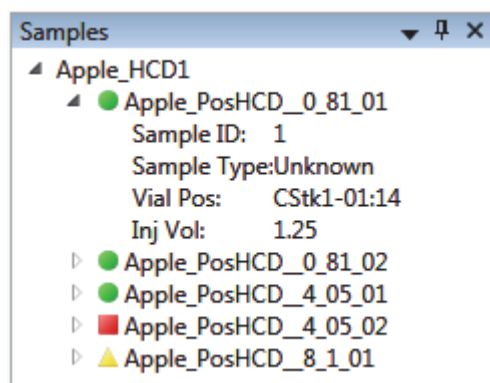
Table 96. Samples pane shortcut menu commands

Command	Description
Sort by Alphabetical	Sorts the samples alphabetically by sample name.
Sort by Import Order	Sorts the samples in the order they were processed.

Compounds Pane

The Compounds pane displays all found peaks in the selected sample and flags any compound with errors. The compounds table reflects the identified compounds found in the compound database and the results of the method processing criteria. See "Compounds Pane Columns" on page 534.

Color Coding for Measured or Calculated Values

The Compounds pane uses color-coded text to indicate the following:

- Green—Indicates that the measured value of scoring and confirmations pass the criteria specified in the method.

- Red—Indicates that the measured or calculated value does not pass the criteria specified in the method.

Measured Area
3.1312E04
1.9131E05
6.7147E04
1.4341E05

Library Score (%)
12
10
10
11

Displaying Multiple Adducts

When the TraceFinder application finds multiple adducts at the same retention time in a sample, the Compounds pane displays the adducts on separate rows in the table.

Exporting Compounds

Use the functions on the File menu to export data to an Excel spreadsheet, to a CSV file, to a compound database, or to a new quantitation method.

Follow these procedures:

- To export compounds to an Excel spreadsheet
- To export compounds to a CSV file
- To export compounds to a compound database
- To create a new quantitation method with the selected compounds
- To create a new quantitation method and update the compound database

❖ **To export compounds to an Excel spreadsheet**

1. For each compound that you want to export to an Excel spreadsheet, select the check box in the Selected column.

2. Choose **File > Export Data To > CSV or Excel** from the main menu

   The Data Review Export dialog box opens.
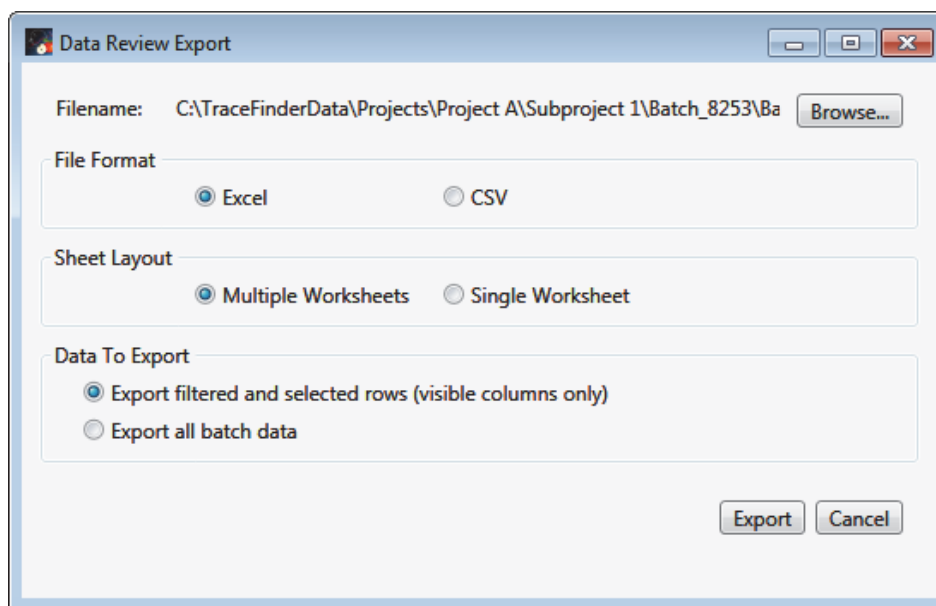
3. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.

4. Type a file name for the XLSX file and click **Save**.

5. In the File Format area, select the **Excel** option.

6. In the Sheet Layout area, select one of the following file formats for the spreadsheet.

   • **Multiple Worksheets**: Writes one sample to each Excel worksheet tab.

   • **Single Worksheet**: Writes all samples to a single Excel worksheet tab.

7. In the Data to Export area, select one of the following sets of data to export.

   • **Export Filtered and Selected Rows (Visible Columns Only)**: Writes data from the displayed columns of selected samples to the specified worksheet format.

   • **Export All Batch Data**: Writes data from all columns (displayed or hidden) of all samples to the specified worksheet format.

8. Click **Export**.

   The application saves the specified compound data to an Excel spreadsheet and opens the folder where you saved the file.

❖ **To export compounds to a CSV file**

1. For each compound that you want to export to a CSV file, select the check box in the Selected column.

2. Choose **File > Export Data > To CSV or Excel** from the main menu.

   The Data Review Export dialog box opens.
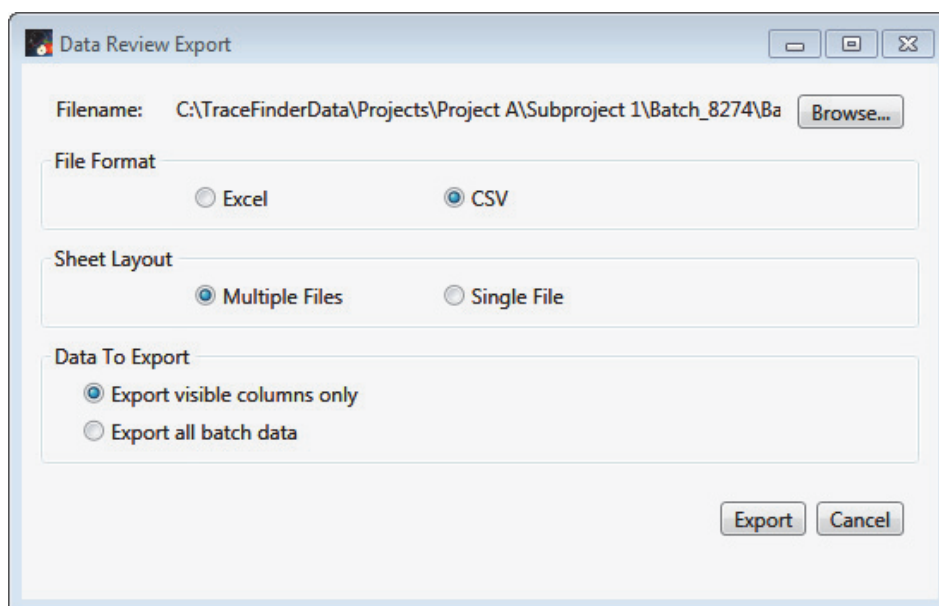
3. Click **Browse** and, in the Export Data to Excel dialog box, locate the folder where you want to save the file.

4. Type a file name for the CSV file and click **Save**.

5. In the File Format area, select the **CSV** option.

6. In the Sheet Layout area, select one of the following file formats for the spreadsheet.

   • **Multiple Files**: Writes one sample to each CSV file.

   • **Single File**: Writes all samples to a single CSV file.

7. In the Data to Export area, select one of the following sets of data to export.

   • **Export Filtered and Selected Data Only**: Writes data from the selected compounds to the specified worksheet format.

   • **Export All Batch Data**: Writes all data from all samples in the batch to the specified worksheet format.

8. Click **Export**.

   The application saves the specified compound data to an CSV spreadsheet and opens the folder where you saved the file.

❖ **To export compounds to a compound database**

1. For each compound that you want to export to a compound database, select the check box in the Selected column, including any adducts that you want to export.

2. Choose **File > Export Data To > Compound Database** from the main menu.

   The Export Compounds to CDB dialog box opens.
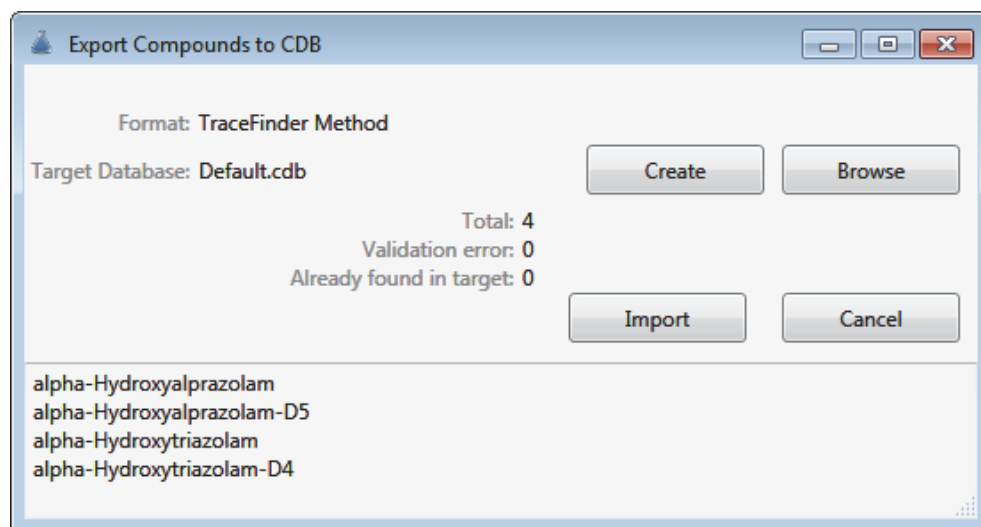
3. Do one of the following:

   - Accept the default target database.

   - Click **Create** and type the name for a new compound database.

   - Click **Browse** and select from the list of compound databases.

4. Click **Import**.

   - When you export compounds to a database that already contains these compounds, the application updates the retention times in the database.

   - When you add compounds to a database that does not contain these compounds, the application adds all the compound data to the database.

   When you export only one adduct for a compound, the application uses the selected adduct as the peak in the updated or new compound database. When you export multiple adducts for export, the application uses the adducts in the order of intensity.

   The application uses the measured retention time value for the compound in the updated or new compound database.

   The application uses the expected *m/z* value for the compound in the updated or new compound database.

   The application exports all found fragments to the updated or new compound database.

❖ **To create a new quantitation method with the selected compounds**

1. For each compound that you want to export to a new quantitation method, select the check box in the Selected column including any adducts that you want to export.

2. Choose **File > Export Data To > New Quantitation Method** from the main menu.

   The General 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 and observe that the application exported the selected compounds from the screening method to the new quantitation method.

   The application uses data from the selected compounds as follows:

   • Exports quantitation peaks in the order of intensity.

   • Exports measured retention time value for the compounds in the new method.

   • Exports expected *m/z* value for the compounds in the new method.

   • Exports all found fragments to the new method.

   • Adds a filter for both quantitative peaks and confirming ions.

❖ **To create a new quantitation method and update the compound database**

1. For each compound that you want to export, select the check box in the Selected column, including any adducts that you want to export.

2. Choose **File > Export Data > Update Compound Database and Create New Quantitation Method** from the main menu.

   The Import Compounds to CDB dialog box opens.
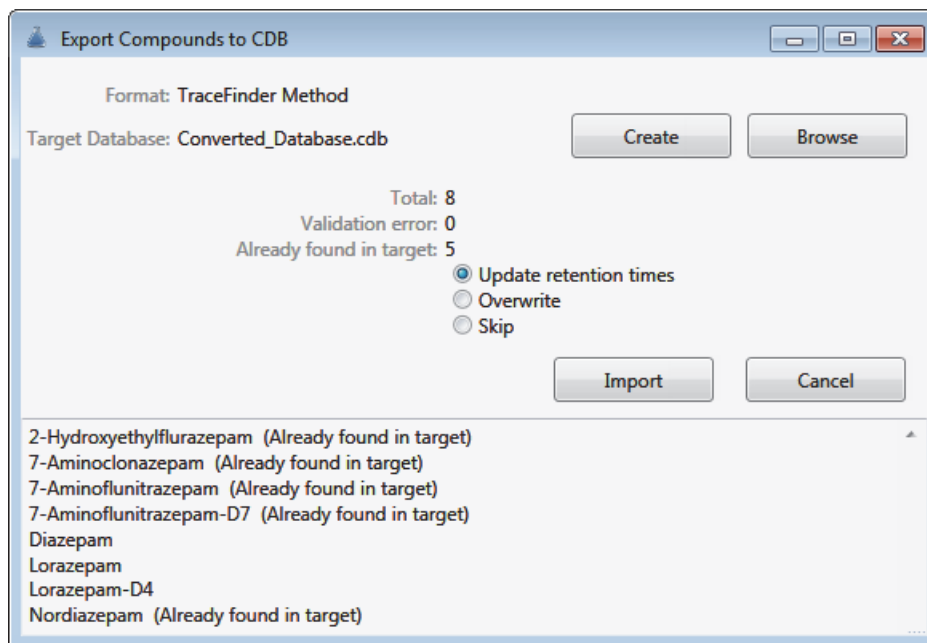
   The dialog box lists all compounds selected in the screening batch.

3. Do one of the following:

   • Accept the default target database.

   • Click **Create** and type the name for a new target database.

   • Click **Browse** and select from the list of compound databases.

   The compounds list indicates which compounds already exist in the target compound database and which do not.

4. When any of the compounds already exist in the target database, choose one of the following options:

   • **Update Retention Times**: Updates only the retention times for the duplicate compounds in the target database.

   • **Overwrite**: Overwrites all compound data for the duplicate compounds in the target database.

   • **Skip**: Does not write any data from the duplicate compounds to the target database.

5. Click **Import**.

   The General page of a new quantitation method opens.

6. From the Instrument Method list, select a method (.meth) file to use for acquiring the data.

7. Choose **File > Save** from the main menu.

8. In the Save Master Method dialog box, type a name for the method and click **OK**.

9. Click **Compounds** in the Method View navigation pane and observe that the new method uses the specified compound database and that the application exported the selected compounds (with the specified options) from the screening method to the new quantitation method.

Compounds Pane Columns

The columns of data in the Compounds pane display all parameter values associated with each compound in the selected sample. See Compounds Pane Parameters.

❖ **To hide or display columns in the Compounds pane**

1. Click the **Field Chooser** icon, ⊞ , in the upper left corner of the pane.

   The Field Chooser displays all available columns of data for the Compounds pane.

Field Chooser	
☑	Selected
☑	MZ
☑	RT
☑	IP
☑	FI
☑	LS
☑	Flag
☑	Compound Name
☑	Match Result Name
☑	Formula
☑	Adduct
☑	Confirmed
☑	m/z (Expected)
☑	m/z (Apex)
☑	m/z (Delta (ppm))
☑	RT (Expected)
☑	RT (Measured)
☑	RT (Delta)

☑	Measured Area
☑	Isotopic Pattern Score (%)
☑	Num Isotopes Matched
☑	Lib Match Name
☑	Library Score (%)
☑	Library Match Rank
☑	Fragment 1
☑	Fragment 1 (Delta (ppm))
☑	Fragment 2
☑	Fragment 2 (Delta (ppm))
☑	Fragment 3
☑	Fragment 3 (Delta (ppm))
☑	Fragment 4
☑	Fragment 4 (Delta (ppm))
☑	Fragment 5
☑	Fragment 5 (Delta (ppm))
☑	S/N
☑	Left RT
☑	Right RT
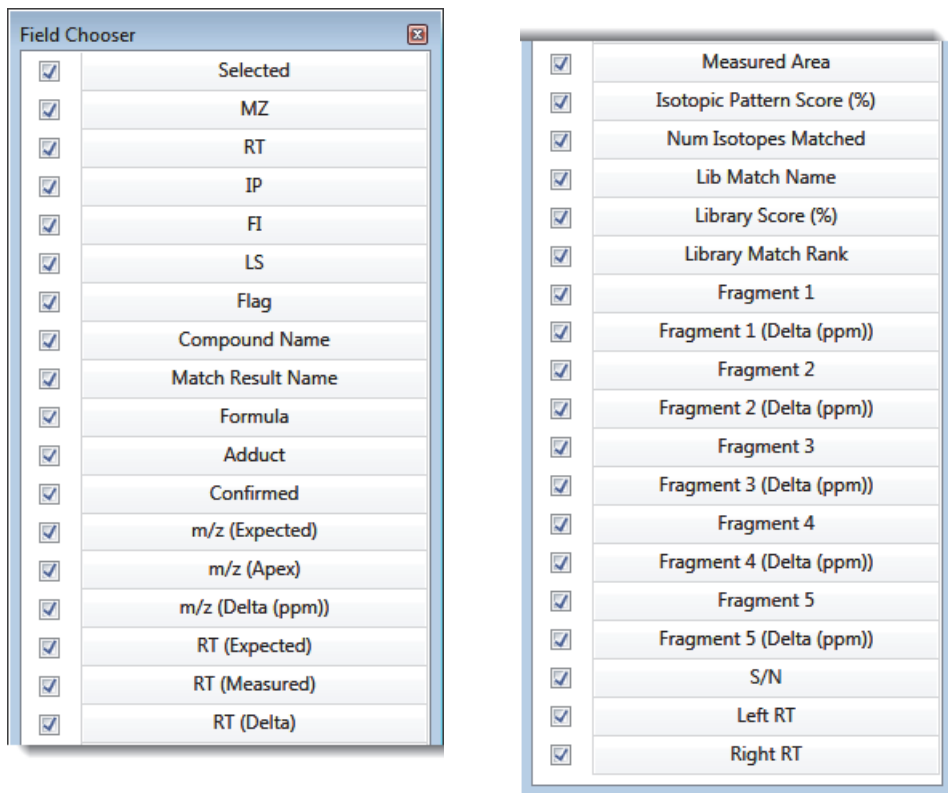
2. Select the check box for each column that you want to display, or clear the check box for each column that you want to hide.

   The application immediately displays or hides the column in the Compounds pane.

3. When you are finished modifying the column display, click ⊠ to close the Field Chooser.

Compounds Pane Parameters

The Compounds pane displays all parameter values associated with each compound in the selected sample.

Figure 137. Compounds pane

Table 97. Compounds pane parameters (Sheet 1 of 6)

Column	Description
Database	Displays the current compound database. When you have multiple screening databases, the application lists the results for each database separately. Expand the list of found compounds in the screening database.
Selected	Identifies individual compounds for export. To select all compounds for export, select the check box in the first column. Selects all compounds in the Compounds pane. Selects the compound for export.
MZ	Mass-to-charge ratio flag. The application displays one of these indicators: • A green circle (pass) when the measured *m/z* value is within the specified threshold. • A red square (fail) when the measured *m/z* value is not within the specified threshold. • A blank when the mass-to-charge value is unavailable. To display the expected, measured, and delta *m/z*, hold your cursor over the indicator. m/z Expected: 285.08000 Apex m/z Measured: 285.08000 Apex m/z Delta: 0.06

Table 97. Compounds pane parameters (Sheet 2 of 6)

Column	Description
RT	Retention Time flag. The application displays one of these indicators: • A green circle (pass) when the measured retention time value is within the RT Window value specified in the compound database. • A red square (fail) when the measured retention time value is not within the RT Window value specified in the compound database. In turn, this results in a failure flag for the *m/z* value because the application cannot identify an *m/z* value that meets the retention time. • A blank when the retention time value is unavailable. When the retention time is selected as "confirm" and the *m/z* is not detected, there is no flag. Or, you can set a different retention time window in the method. See "Specifying Identification and Confirmation Settings" on page 235. To display the expected, measured, and delta retention times, hold your cursor over the indicator.
IP	Isotopic Pattern flag. The application displays one of these indicators: • A green circle (pass) when the score percentage is higher than the specified fit threshold percentage. • A red square (fail) when the score percentage is lower than the specified fit threshold percentage. • A blank when the parameter is not scored. To display the score of matched isotopes, hold your cursor over the indicator.
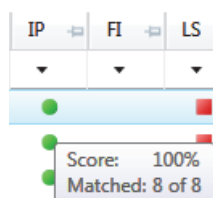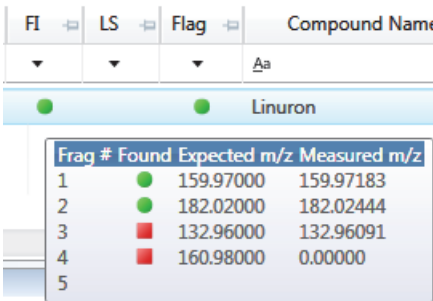
Table 97. Compounds pane parameters (Sheet 3 of 6)

Column	Description
FI	Fragment Ions flag. The application displays one of these indicators: • A green circle (pass) when the measured *m/z* value of any of the fragments is within the mass tolerance specified in the method. On the Isotopes page in the Spectrum pane, the All Isotopes and Multi-Isotopes flags are also green. • A red square (fail) when the measured *m/z* value of none of the fragments is within the mass tolerance specified in the method. On the Isotopes page in the Spectrum pane, the All Isotopes and Multi-Isotopes flags are also red. • A blank when there are no fragments detected. To display a list of fragments and their pass/fail status, hold your cursor over the indicator.
LS	Library Search flag. The application displays one of these flags: • A green circle when the library search is successful. • A red square when the library search is not successful.
Flag	Indicates the status of the identification and confirmation criteria. • A green circle when the sample/compound/peak combination is identified and fully confirmed. • A yellow triangle when the sample/compound/peak combination is identified but not fully confirmed. • A red square when the sample/compound/peak combination is not identified.
Compound Name	The compound name match in the compound database.
Match Result Name	The compound name match in the compound database and the retention time.
Formula	The formula for the peak as specified in the compound database.
Adduct	The most intense adduct for the retention time for a compound.
Confirmed	The number of criteria confirmed out of the total number specified in the method.

Table 97. Compounds pane parameters (Sheet 4 of 6)

Column	Description
m/z (Expected)	Mass-to-charge ratio from the compound database. The charge is presumed to be 1.
	• When an adduct is found, the application displays the neutral mass value for the compound (calculated from the neutral formula) ± the mass of the most intense adduct ion found for the compound.
	• When no adduct is found, the application displays the neutral mass value for the compound ± the mass of the first adduct entered in the compound database.
	For details about defining adducts for the compound database, see "Specifying Adducts" on page 61.
	For details about adding adducts to compounds, see "Editing Compounds in the Database" on page 285
	Note When the adduct is a gain, the adduct mass is a positive number. When the adduct is a loss, the adduct mass is a negative number. The resulting mass value after adding or subtracting the adduct mass is always a positive number.
m/z (Apex)	Mass-to-charge ratio found in the spectra for the peak. The charge is presumed to be 1.
	When the application successfully integrates the peak, this column displays the charged *m/z* value for the compound, which is the highest intensity in the apex scan.
	When the application cannot successfully integrate the peak, this column displays N/F.
m/z (Delta)	Difference between the *m/z* (Expected) and *m/z* (Apex). The charge is presumed to be 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 $m/z \text{ (Delta)} = 1\,000\,000 \times ([m/z \text{ (Apex)} - m/z \text{ (Expected)}] \times m/z \text{ (Expected)})$.
	• When the mass tolerance is specified in mmu in the master method, then $m/z \text{ (Delta)} = 1000 \times m/z \text{ (Apex)} - m/z \text{ (Expected)})$.
RT (Expected)	The retention time for the peak as specified in the compound database.
RT (Measured)	The found retention time for the peak apex.
RT (Delta)	Difference between the expected and measured retention time for the peak.
Measured Area	The AA value from the chromatogram pane.
Isotopic Pattern Score (%)	The percentage of the number of total isotopes to the number of matched isotopes.

Table 97. Compounds pane parameters (Sheet 5 of 6)

Column	Description
Num Isotopes Matched	The number of isotopes matched in the expected calculated isotope spectra relative to the total number of isotopes used in the score calculation, in the format "x of y", where • x = the number of isotopes matching the elemental composition used for the Isotopic Pattern Score calculation. • y = the total number of isotopes considered in the Isotopic Pattern Score calculation. This is the number of isotope peaks expected to be above the spectral noise.
Lib Match Name	The name of the best matching compound in the library search. When the application finds a match in the library, this column displays the matching library entry with the highest score. • When the application does not perform a library search, this column displays "N/A" in black text. • When the application does not perform an MS/MS scan, this column displays "N/A" in red text.
Library Score (%)	The score from the library fit. When the application finds a match in the library, this column displays the highest score associated with the Lib Match Name parameter. When the application performs both a library search and an MS/MS scan and both the library entry and the formula match the target compound: • The criteria passes when the library score is higher than or equal to the score threshold. This column displays its values in green text. • The criteria fails when the library score is lower than the score threshold. This column displays its values in red text. When the application does not perform a library search, this column displays "N/A" in black text. When the application does not perform an MS/MS scan, this column displays "N/A" in red text. Range: 1 to 100%

Table 97. Compounds pane parameters (Sheet 6 of 6)

Column	Description
Library Match Rank	Displays the ranking of the library match. When the application finds a match in the library, this column displays the library entry's relative rank, in the format "x of y", where • x = the rank of the highest scoring library match. • y = the total number of library matches from the list of matches for a particular adduct that contains the highest scoring match. When the application performs both a library search and an MS/MS scan and both the library entry and the formula match the target compound: • The criteria passes when the library score is higher than or equal to the score threshold. This column display its values in green text. • The criteria fails when the library score is lower than the score threshold. This column display its values in red text. When the application does not perform a library search, this column displays "N/A" in black text. When the application does not perform an MS/MS scan, this column displays "N/A" in red text.
Fragment n	Displays the measured m/z for the fragment ion. The application displays a separate column for each found fragment. • For each fragment found in the compound database that passes the filter in the method, the Compounds table displays the m/z value in green text. • For each fragment found in the compound database that does not pass the filter in the method, the Compounds table displays the m/z value in red text. • For each fragment that is not found in the compound database, the Compounds table displays N/S (none specified). Fragment 1 Aa N/S ——— Fragment not found in the compound database 187.06 ——— Fragment found but does not meet method parameters 159.97 ——— Fragment found and meets method parameters **Note** Compounds can have a maximum of five fragments, and the Compounds table has a maximum of five Fragment columns. When a compound contains fewer than five fragments, all remaining Fragment columns display N/S.
Fragment n (Delta (ppm/mmu))	The difference between the expected fragment ion m/z from the compound database and the measured fragment ion m/z. The application displays a separate delta column for each identified fragment.
S/N	The signal-to-noise ratio calculated for the found peak.
Left RT	The time point of the left leading edge of the integrated peak.
Right RT	The time point of the right trailing edge of the integrated peak.

Chromatogram Pane

Use the Chromatogram pane to display all extracted chromatograms of all adducts of the selected compound.

The first tab displays the most intense target adduct for the peak result. Additional (optional) tabs display extracted ion chromatograms for other adducts for the target compound at the same retention time in order of intensity. If no signal exists for an adduct, it displays the XIC of the expected *m/z* within the specified retention and chromatogram windows. When you do not specify a retention time or window, the application displays the full time range.

For each adduct, the Spectrum pane displays the spectrum, isotopes, fragments, and library matches. See "Spectrum Pane" on page 542.

Figure 138. Chromatogram pane
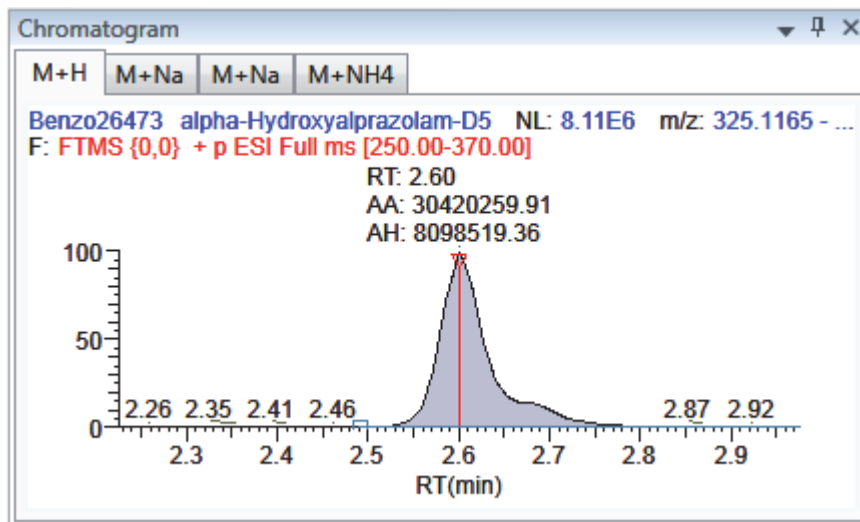
Table 98. Chromatogram pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Spectrum Pane

Use the Spectrum pane to display the spectrum, isotopes, fragments, and library search information for the selected adduct in the Chromatogram pane. The Spectrum pane displays only the identification and confirmation criteria specified in the method. The confirmations are based only on the most intense adduct. See "To specify identification and confirmation settings" on page 236.

The Spectrum pane includes the following pages of information (when available) for each selected sample/compound/peak combination:

- Spectrum
- Isotopes
- Fragments
- Library

Spectrum

The application displays the neutral loss (NL) and compound/peak name information on the right side of the Spectrum page. When data is available, the plot width is the full mass range in the raw data file. Otherwise, the application scales the width to the scan range.

Figure 139. Spectrum page
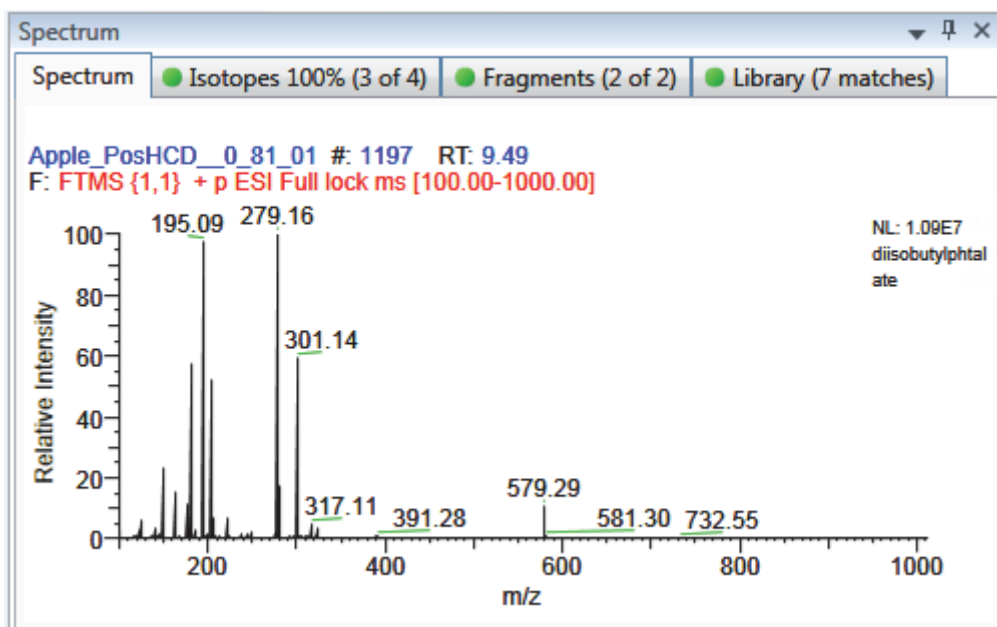
Table 99. Spectrum page shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.

Isotopes

The isotopes page displays isotopic pattern results for all adducts of a compound according to the threshold and deviation parameters defined in the screening method.

To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

- An isotope peak is not found if its intensity, relative to the monoisotopic ion's intensity, is more than the specified intensity deviation percentage away from the theoretical relative intensity of the isotope ion.

- An isotope peak is found if its measured *m/z* is less than the specified mass deviation amount away from its expected *m/z*.

To specify threshold and deviation parameters, see "To specify identification and confirmation settings" on page 236.

The Isotopes page displays the isotopes in one of three ways:

- All Isotopes

- Multi-Isotopes

- Individual Isotopes

All isotopes pages use a shortcut menu to specify how you want the data displayed. See " Isotopes page shortcut menu commands" on page 548.

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 dotted blue line.

The application displays these headers for the All Isotopes view:
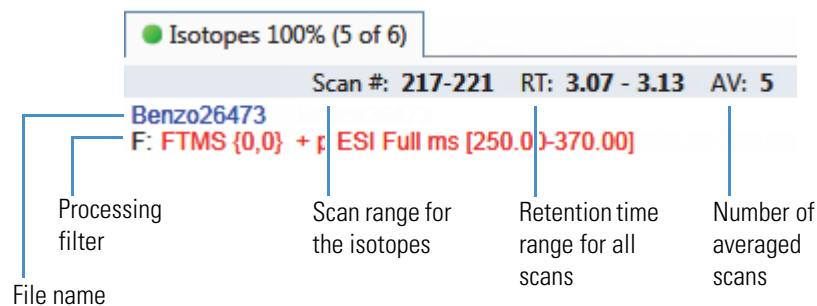
Figure 140. Isotopes page with stacked spectra for all isotopes

Expected *m/z* of the isotope   Measured spectrum   Expected spectrum
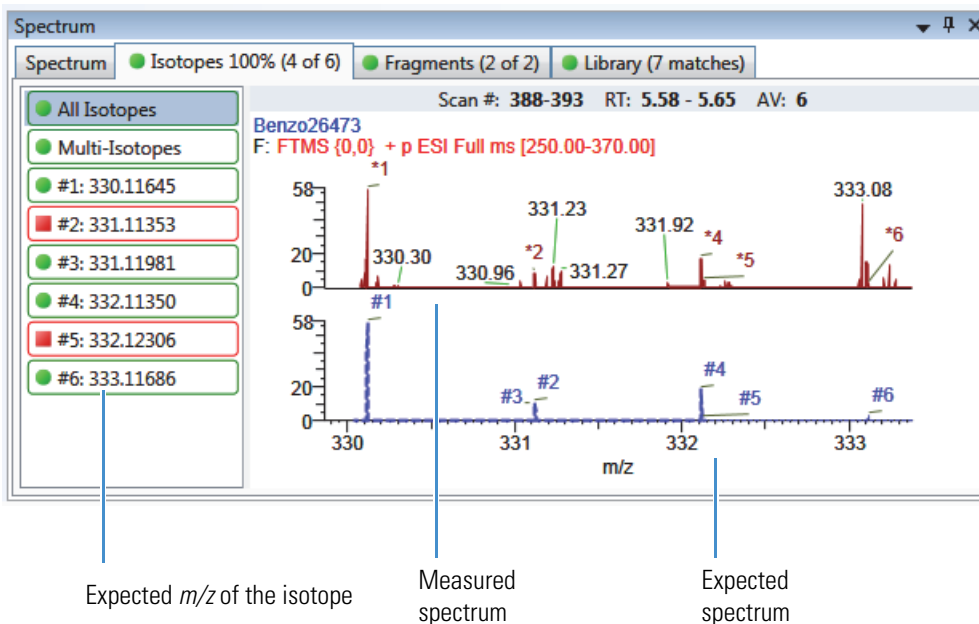
Figure 141. Isotopes page with overlaid spectra for all isotopes

Expected spectrum in blue   Measured spectrum in red
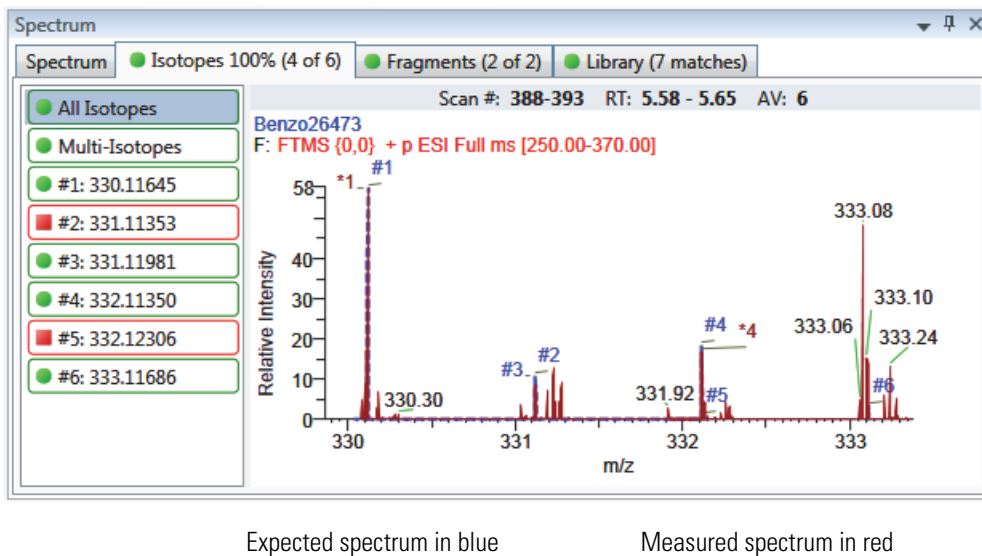
Multi-Isotopes

The Multi-Isotopes view displays individual plots for each isotope. You can individually stack or overlay the plots for each isotope.

The application displays these headers for the Multi-Isotopes view:

Scan range for the isotopes | Retention time range for all scans | Number of averaged scans
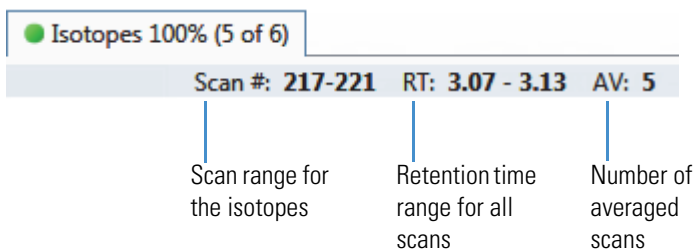
Figure 142. Isotopes page with overlaid spectra for multi-isotopes
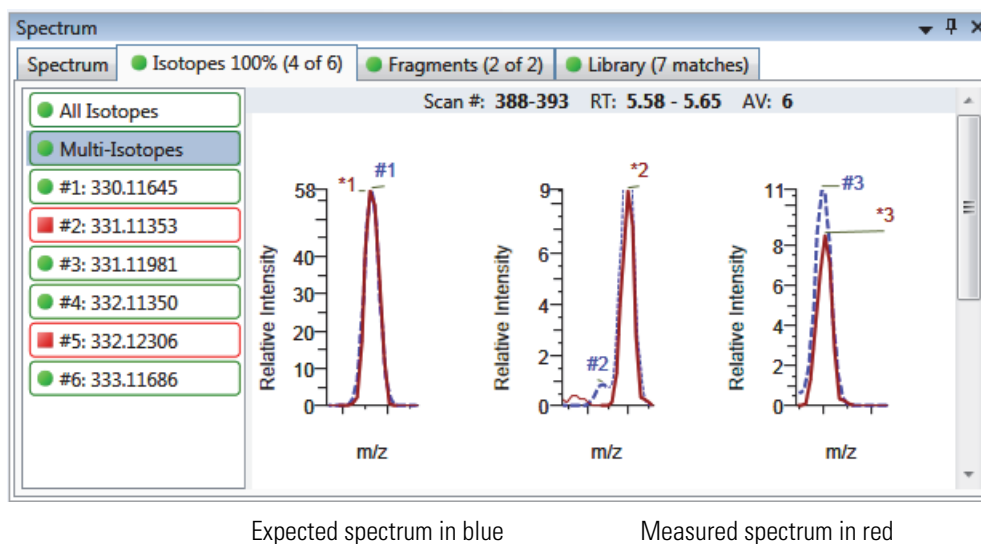
Figure 143. Isotopes page with stacked spectra for multi-isotopes
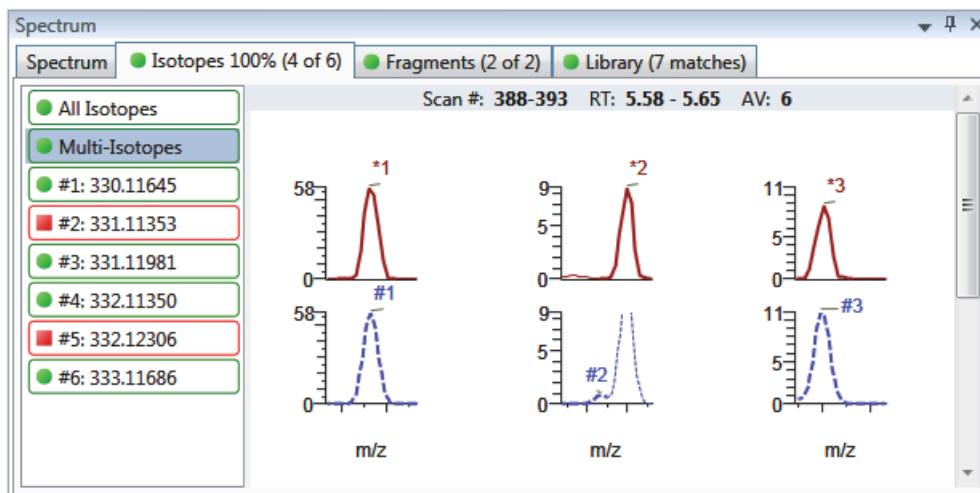
Expected spectrum in blue   Measured spectrum in red

Figure 144. Isotopes page with stacked and overlaid spectra for multi-isotopes
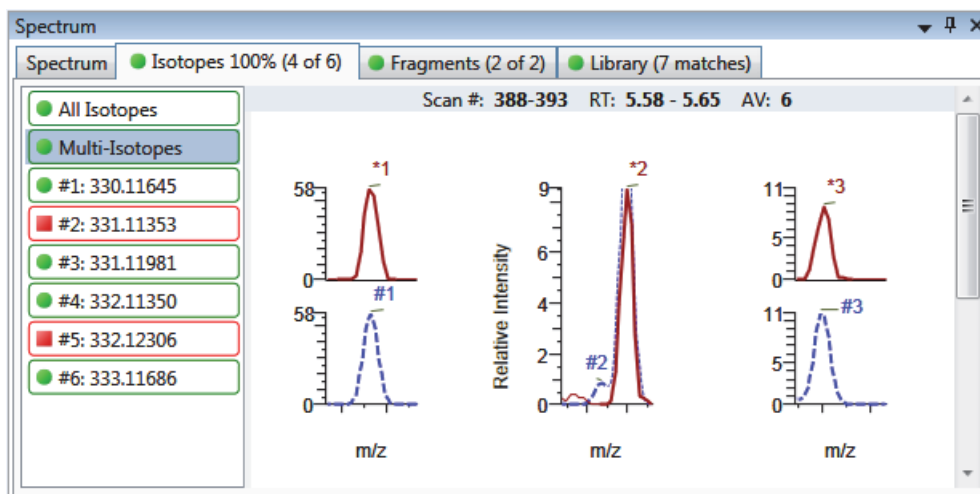
Expected spectrum in blue   Measured spectrum in red

Individual Isotopes

The individual isotopes view displays the expected and measured peaks for a single isotope.

The application displays these headers for the individual isotopes view:
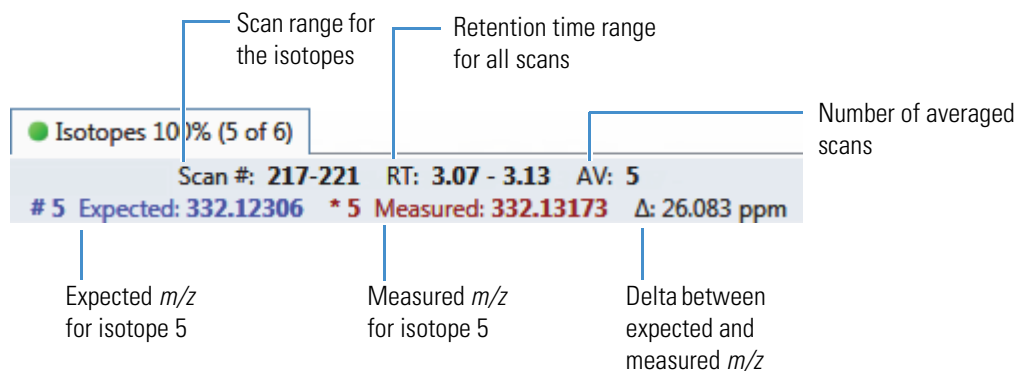
Figure 145. Isotopes page with overlaid spectra for a single isotope

Figure 146. Isotopes page with stacked spectra for a single isotope
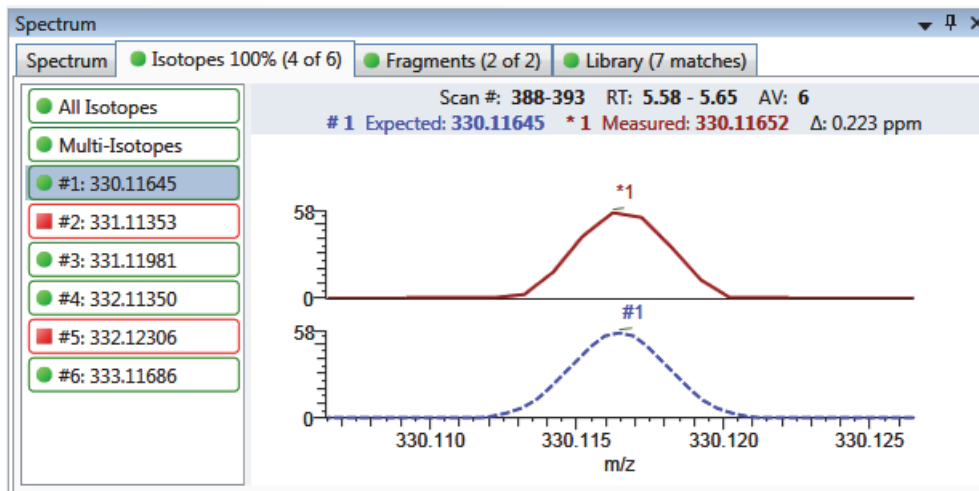
Expected spectrum in blue   Measured spectrum in red

Table 100. Isotopes page shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.
Show/Hide Noise Label	Adds a noise label to each peak. Expected isotope peaks (displayed in blue) do not display a noise label.
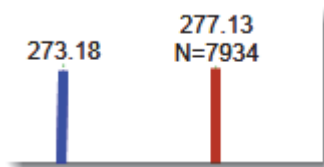
Show/Hide Resolution Label	Adds a resolution label to each peak. Expected isotope peaks (displayed in blue) do not display a resolution label.
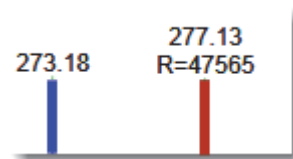
Fragments

The Fragments page displays the maximum number of fragments as specified in the screening method. See "To specify identification and confirmation settings" on page 236.

If there are no fragments defined in the screening library for the compound, you can add fragments to the screening library. See "To add a fragment to a target peak" on page 292.

The Fragments page displays the fragments in one of two ways:

- All Fragments

- Individual Fragments

All Fragments

The All Fragments view displays a composite of all fragments found in the compound. The application displays the measured peak as a solid red line; the application displays the expected peak as a dotted blue line.

The application displays these headers for the All Fragments view:

Figure 147. Fragments page with overlaid spectra for all fragments
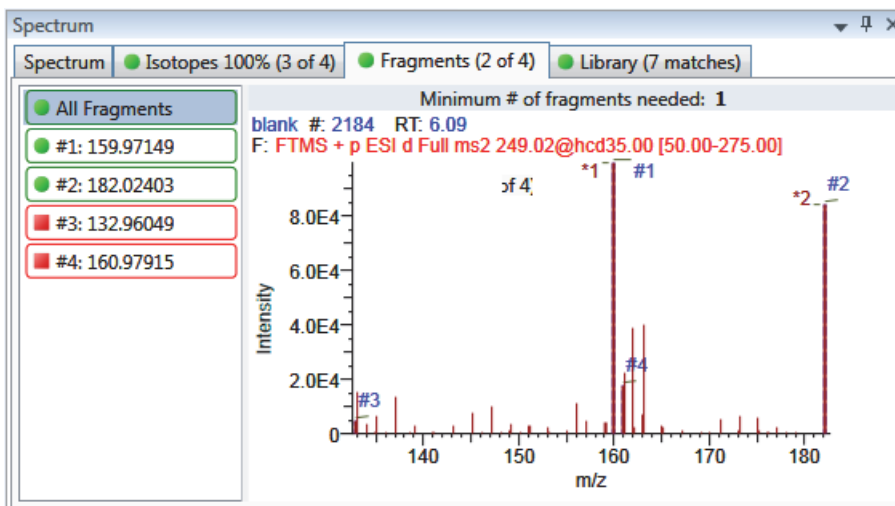
Figure 148. Fragments page with stacked spectra for all fragments
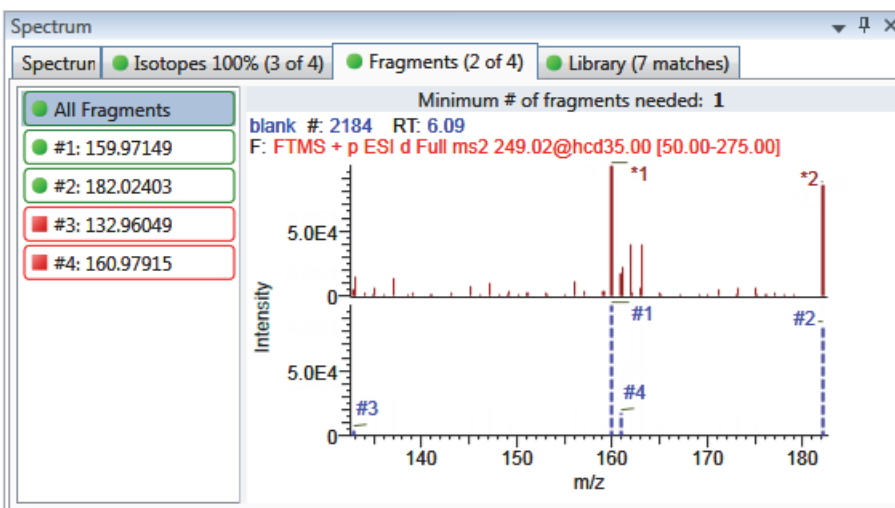
Individual Fragments

The individual fragments view displays the expected and measured peaks for a single fragment.

The application displays these headers for the individual fragments view:

Minimum number of fragments specified in the method

Fragments (2 of 4)

Minimum # of fragments needed: **1**
#1 Expected: **159.97149**   *1 Measured: **159.97183**   Δ: 2.140 ppm

Expected *m/z* for fragment 1

Measured *m/z* for fragment 1

Delta between expected and measured *m/z*
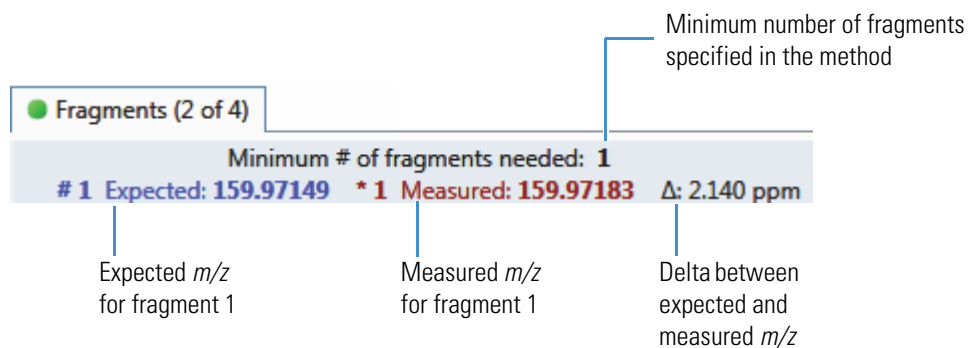
Figure 149. Fragments page with overlaid spectra for a single fragment

Intensity threshold specified in the method
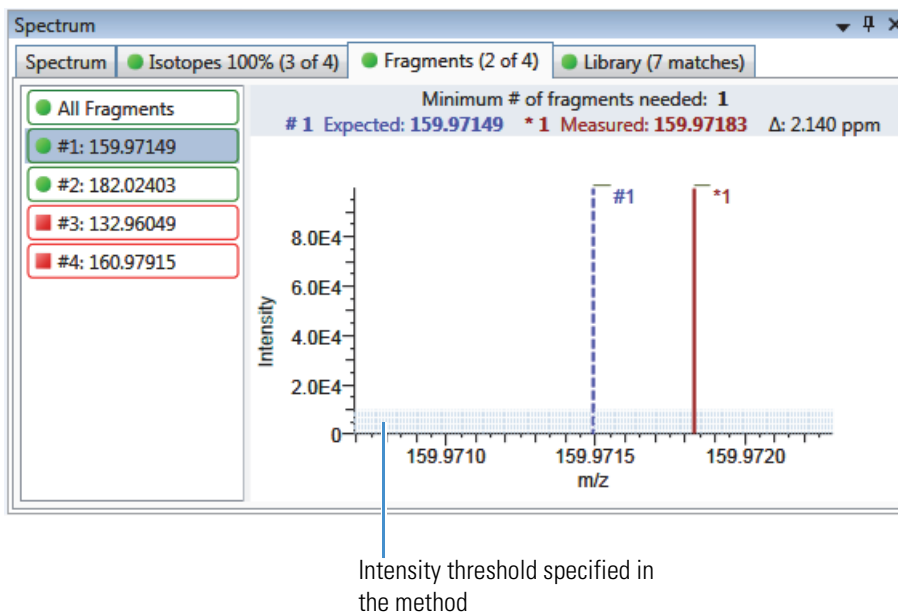
Figure 150. Fragments page with stacked spectra for a single fragment
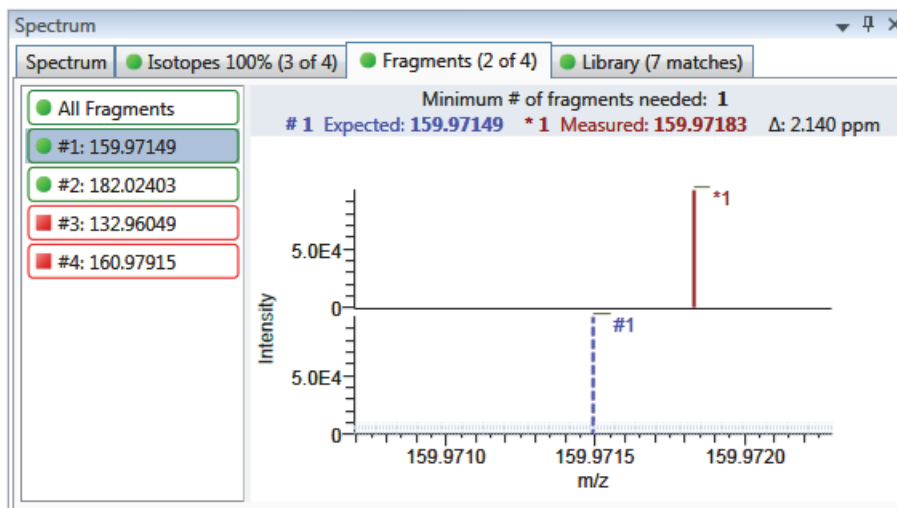
Table 101. Fragments page shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Copy to Clipboard	Copies the graphic display to the Clipboard.
Display Overlay Spectra Display Stack Spectra	Overlays the two spectrum displays, or stacks the simulated spectrum and the peak apex spectrum.

Library

The Library page displays the matching library spectrum (in blue) and the experimental spectrum (in black). The resulting score percentage from a library search match must be higher than your specified threshold value to identify or confirm the presence of a compound. See "To specify identification and confirmation settings" on page 236.

The application scales both the matched library spectrum and the highest peak in the experimental spectra at 100 percent intensity and displays the resulting neutral loss (NL) value for the matched library entry name on the right of the plot.

The application displays these headers for the individual adducts:

Library match name   Library score percentage

● Library (7 matches)

M+H #1: **Phthalic_acid_bis-iso-butyl_ester** C16H22O4 Score: 88 Rank: 1 of 7

Adduct   Formula   Library match rank
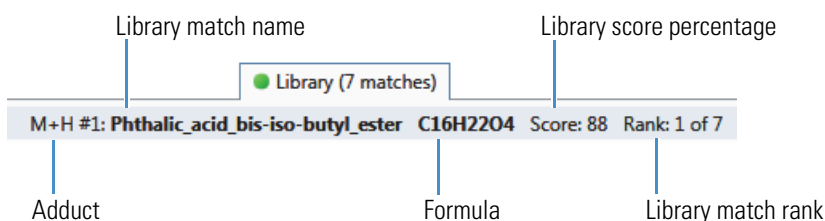
Figure 151. Library page with stacked spectra
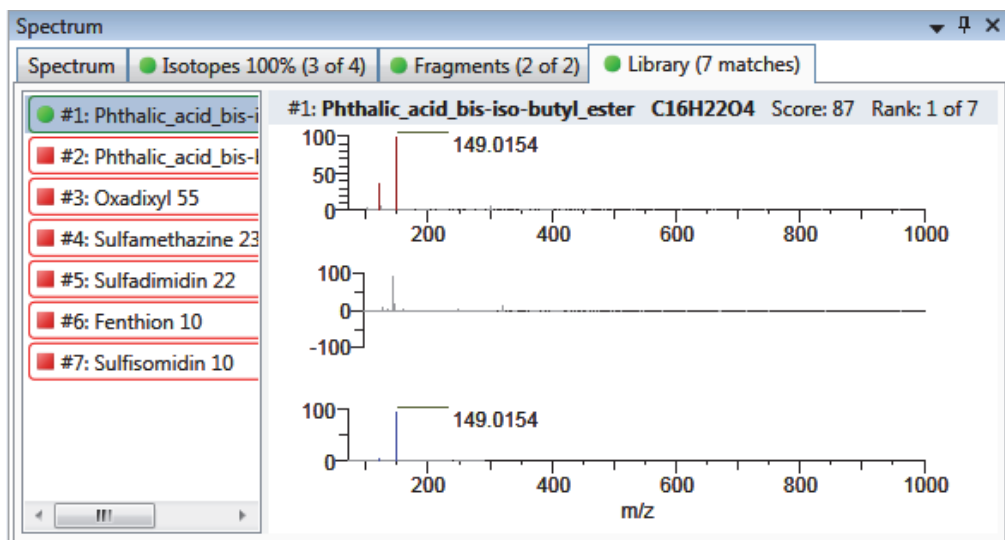
Figure 152. Library page with overlaid spectra
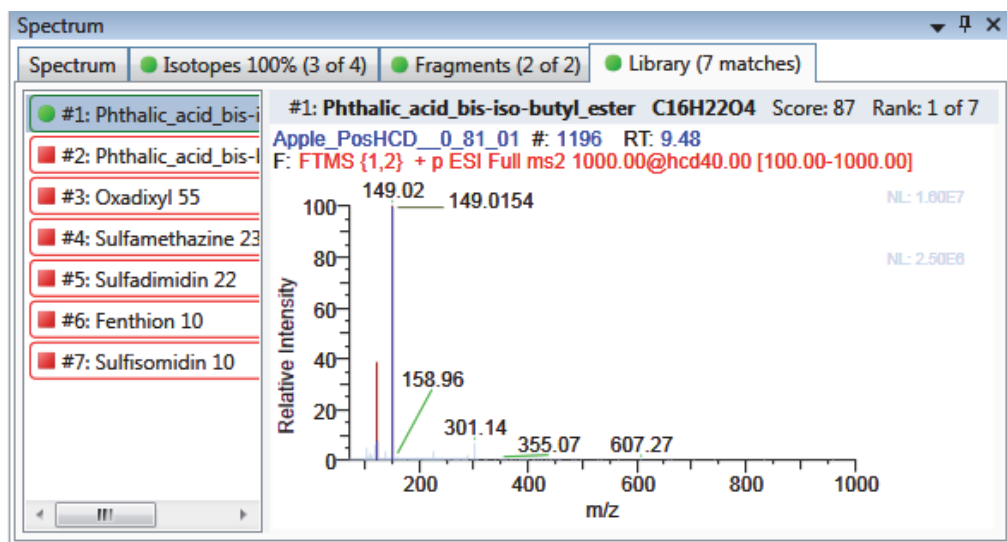
Table 102. Library page shortcut menu commands

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

Use the Report View to display or generate reports for the currently selected batch in the Analysis mode. See Report View in Analysis mode. You must process each sample in the batch before you can view or generate a sample-level report for that sample.

❖ **To open the Report View**

1. Click **Analysis** in the navigation pane from any mode.

2. In the Analysis navigation pane, click **Report View**.

Report View	>

The Report View for the currently selected batch opens.

❖ **To refresh the Report View**

If you make changes to your reports, click **New Data Available - Refresh**.

New data available - Refresh
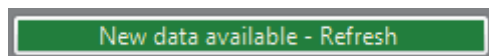
Figure 153. Report View in Analysis mode

Report View - Batch_A

Mode: ◉ View Only ○ Generate Only
Select a report: ▼

Report View
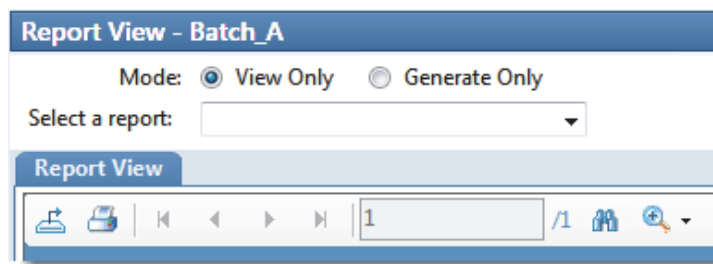
- **View Only**: Displays a PDF or Excel spreadsheet preview of the selected report type for the batch, sample, or compound. See "Viewing Reports."
  - For quantitative batches, preview reports for all Standard report types are always available.
  - For target screening batches, preview reports for all Standard and Target Screening report types are always available.
  - You must generate Custom and ToxID report types before they are available.

  The Report View page displays one of the following report outputs:
  - Standard reports as PDF files
  - Custom reports in XLSM format
  - ToxID reports as PDF files
  - Target Screening reports as PDF files (available only for target screening batches)

- **Generate Only**: Creates all specified report output formats for the selected sample-level or batch-level report. See "Generating Reports" on page 560.

This section includes the following topics:

- Viewing Reports
- Generating Reports
- Working with Reports
- Working with the Active View

Viewing Reports

Use the View Only features to view all configured standard or target screening reports and any custom or ToxID reports that you have generated. After you generate a report, the application displays the report in the View Only report list.

Follow these procedures:

- To select a report
- To select a sample
- To select a compound
- To select a sample and a compound

❖ **To select a report**

1. Select the **View Only** option.

2. Open the Select a Report list to display all configured report types.

Select a report:	Batch Report		
Report View	Report Name	Type	Requires
	Batch Report	Standard	
Batch Report	Batch Report Rev 1	Standard	
	Blank Report	Standard	Sample

Filter Reports
☐ Only show automated batch reports
☑ Standard reports ☑ Custom reports ☑ Tox ID reports ☑ Target Screening reports
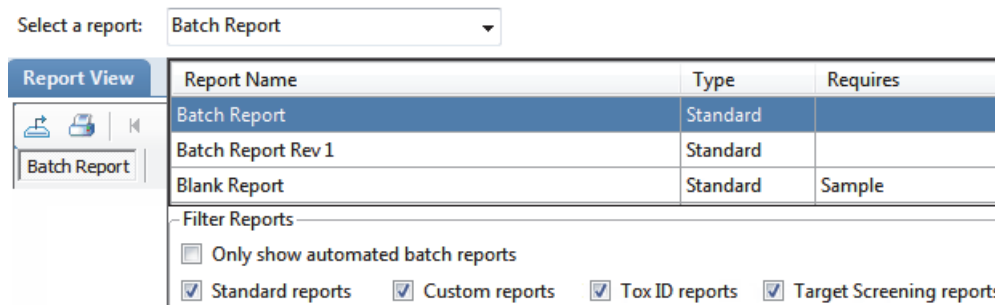
These reports reflect the Displayed Reports selections in the Configuration console. To change the configured reports that are available in this view, see "Specifying the Reports" on page 40.

To sort the reports, click the column headers. The application maintains this sort order each time you open the Report View for this batch. To help organize your reports, you can filter the list.

3. To limit the types of reports to display in the report list, select any combination of report filter options in the Filter Reports area.

Table 103. Filter Reports options

Option	Result
Only Show Automated Batch Reports	Displays only report types that have an output format specified in the Automated Batch Reports area in the Batch View. See "Automated Batch Reports Pane" on page 407.
Standard Reports	Displays Standard report types.
Custom Reports	Displays generated Custom report types. Custom reports are not available for viewing until you have generated the report.
ToxID Reports	Displays generated ToxID report types. ToxID reports are not available for viewing until you have generated the report.
Target Screening Reports	Displays Target Screening report types.

Note When you make changes to the method in the Local Method view, to the peaks in the Data Review view, or to the samples in the Batch View, you must regenerate the custom or ToxID reports before these changes take effect.

4. Double-click the name of the report.

The report list closes.

• When the selected report is a batch-level report, the application displays the report on the Report View page.

• When the selected report includes separate reports for each sample, you must select a sample file.

Select a report: Blank Report ▼   Sample file: ▼

Follow the procedure "To select a sample" on page 558.

• When the selected report includes separate reports for each compound, you must select a compound.

Select a report: Compound Calibration Report ▼   Compound: ▼

Follow the procedure "To select a compound" on page 558.

- When the selected report includes separate reports for each sample and each compound in the sample, you must select both a sample and a compound.

Select a report: Confirmation ▾   Sample file: ▾   Compound: ▾

Follow the procedure .

❖ **To select a sample**

1. Open the Sample File list to display all processed samples in the batch.

   Note Unprocessed samples are not listed. A message in the sample list reports the number of unprocessed samples in the batch.

   Filter Samples - [1 unprocessed sample(s) found but not displayed in list.]

2. To show only samples that would be included in the selected report, select the **Only Show Samples Relevant…** check box.

   For example, if you selected the Quality Control Report, the sample list displays only QC samples.

   Note Click the column headers to sort the samples. The application maintains this sort order each time you open the Report View for this batch.

3. Double-click the name of the sample.

   The Sample File list closes. The Report View page displays the sample-level report.

❖ **To select a compound**

1. Open the Compound list to display the names and retention times of all compounds in the sample.

RT	Compound Name
	All Compounds
3.14	Propanenitrile
3.15	Pyrazinamide

2. Double-click a single compound or **All Compounds**.

   The compound list closes. The Report View page displays the compound-level report.

❖ **To select a sample and a compound**

1. Open the Sample File list to display all samples in the batch.

Sample Name	Sample ID	Sample Type
UnknownA1	1	Specimen
UnknownA2	1	Specimen

Filter Samples

☐ Only show samples relevant to the selected report.

2. To show only samples that would be included in the selected report, select the **Only Show Samples Relevant…** check box.

   For example, if you selected the Quality Control Report, the sample list displays only QC samples.

   > **Tip** Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

3. Double-click the name of the sample.

   The Sample File list closes.

4. Open the Compound list to display the names and retention times of all compounds in the sample.

RT	Compound Name
	All Compounds
3.14	Propanenitrile
3.15	Pyrazinamide

5. Double-click a single compound or **All Compounds.**

   The Compound list closes.

   The Report View page displays the compound-level report for the selected sample and compound.

Generating Reports

Use the Generate Only features to create sample-level reports. You cannot use the View Only features to view custom, ToxID, or target screening reports until you generate the report. When you make changes to either the method in the Local Method view or the peaks in the Data Review view, you must regenerate the custom, ToxID, or target screening reports to see the effects of those changes.

Follow these procedures:

- To select a report

- To select a sample

❖ **To select a report**

1. Select the **Generate Only** option.

2. Open the Select a Report list to display the available reports.
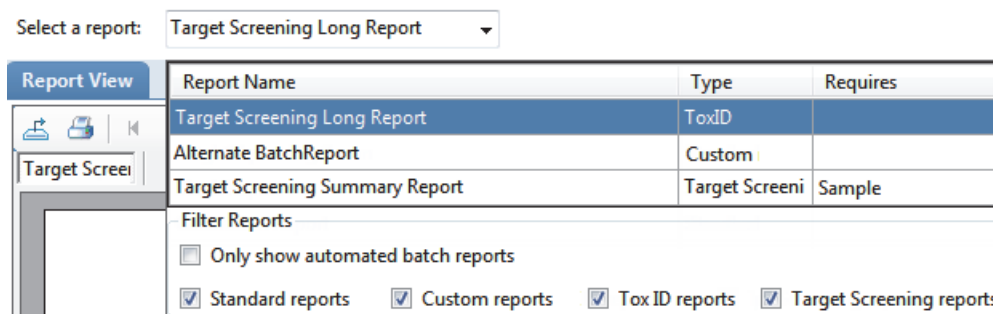
The application displays only configured sample-level report types in the list. You cannot generate batch-level or compound-level reports from this view. To change the configured reports that are available in this view, see "Specifying the Reports" on page 40.

If you have many reports, you can filter the list.

3. To limit the types of reports to display in the report list, select any combination of report filter check boxes in the Filter Reports area.

Option	Result
Only Show Automated Batch Reports	Displays only sample-level reports that have an output format specified in the Automated Batch Reports area in the Batch View. See "Automated Batch Reports Pane" on page 407. If you have only batch-level reports specified in the Batch View, selecting this option excludes all reports in the Report Name list.
Standard Reports	Displays sample-level Standard report types.
Custom Reports	Displays sample-level Custom report types.
ToxID Reports	Displays sample-level ToxID report types.
Target Screening Reports	Displays sample-level Target Screening report types.

Note Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

4. Double-click the name of the report.

The report list closes. You must select a sample file for the selected report.

❖ **To select a sample**

1. Open the Sample File list to display all samples in the batch.

Select	Sample Name	Sample ID	Sample Type
☐	UnknownA1	1	Specimen
☐	UnknownA2	1	Specimen
☐	UnknownA3	1	Specimen
☐	UnknownA5	1	Specimen

— Filter Samples —
☐ Only show samples relevant to the selected report.
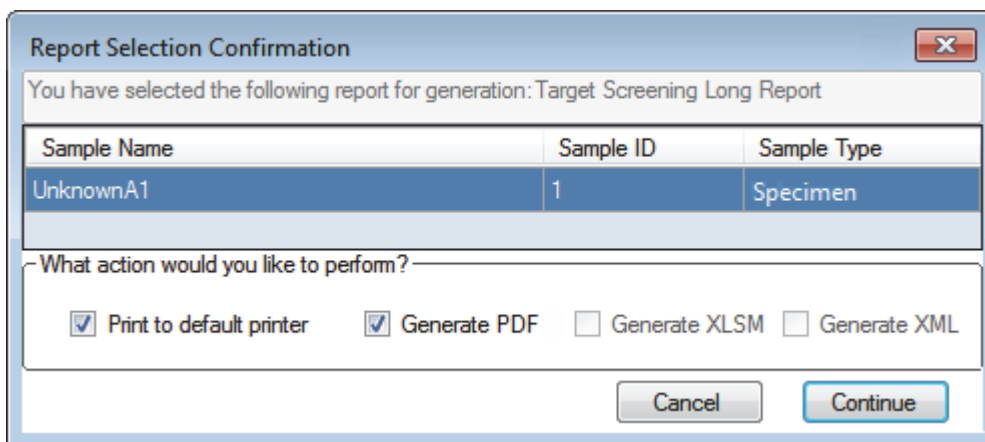
2. To show only samples that would be included in the selected report, select the **Only Show Samples Relevant…** check box.

   For example, if you selected the Quality Control Report, the sample list displays only QC samples.

   > **Note** Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

3. Select the check box for each sample that you want to include in the report.

4. Click **Generate**.

   The Report Selection Confirmation dialog box opens.

   Report Selection Confirmation

   You have selected the following report for generation: Target Screening Long Report

Sample Name	Sample ID	Sample Type
UnknownA1	1	Specimen

   — What action would you like to perform? —
   ☑ Print to default printer   ☑ Generate PDF   ☐ Generate XLSM   ☐ Generate XML

   [Cancel]   [Continue]

5. In the What Action Would You Like to Perform area, select the types of reports that you want to create.

   > **Note** The application automatically selects required output formats. These options are not editable.

6. Click **Continue**.

The application submits the selected samples to the report queue.
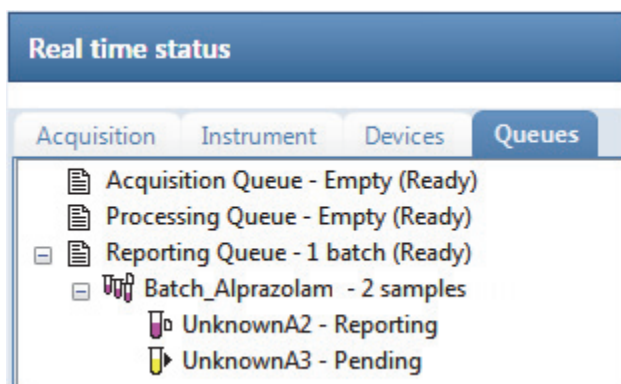
When you have already generated this report in the Batch View or Acquisition mode, the application time-stamps the new report to differentiate it from the original report.

7. To view the report you generated, follow the instructions in "Viewing Reports" on page 556.

Note When you make changes to the method in the Local Method view, the peaks in the Data Review view, or the samples in the Batch View, you must regenerate the custom or target screening reports before those changes take effect.

Working with Reports

Use the icons on the Report View page to view, print, or export a report.
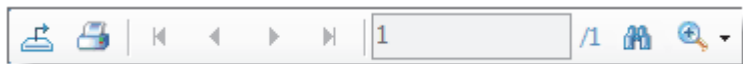
- For each standard report, you can create a hardcopy printout, a PDF file, or an XML file.

- For each custom report, you can create a hardcopy printout or an Excel Macro-Enabled Workbook (.xlsm) file.

- For each ToxID report, you can create a hardcopy printout or a PDF file.

- For each target screening report, you can create a hardcopy printout, a PDF file, or an XML file.

Follow these procedures:

- To print a report

- To export a standard report

- To search for text

- To enlarge the report text

❖ **To print a report**

1. Select the report to print from the Select a Report list.

2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.

3. Click the **Print Report** icon, 🖶 .

The Print dialog box for your default printer opens.

4. Follow the typical procedure to print from your printer.

Landscape reports automatically rotate to fit the paper.

❖ **To export a standard report**

1. Select the report that you want to print from the Select a Report list.

2. (Optional) Select a sample from the Sample File list.

The application displays the report on the Report View page.

3. Click the **Export Report** icon, 📤 .

The Export Report dialog box opens.

4. Locate the folder where you want to write the report file.

5. Type a file name for the exported report file.

6. Select a file type from the Save as Type list:

Save as type:	PDF (*.pdf)	▼
	PDF (*.pdf)	
	Character Separated Values (CSV) (*.csv)	
	Microsoft Excel (97-2003) (*.xls)	
	Microsoft Excel (97-2003) Data-Only (*.xls)	
	Microsoft Excel Workbook Data-Only (*.xlsx)	
	Microsoft Word (97-2003) (*.doc)	
	Microsoft Word (97-2003) - Editable (*.rtf)	
	Rich Text Format (RTF) (*.rtf)	
	XML (*.xml)	
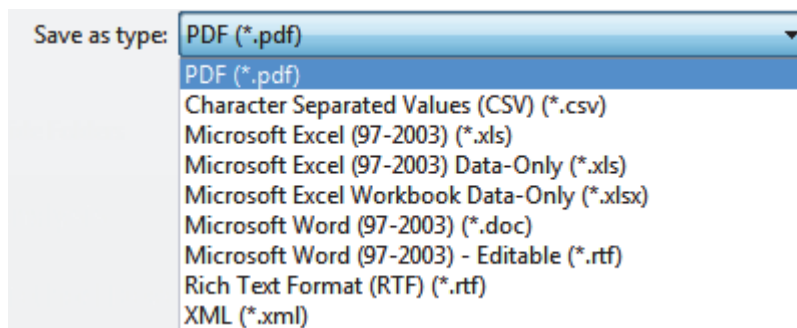
7. Click **Save**.

The TraceFinder application saves the file as the specified file type and writes the report file to the specified folder.

❖ **To search for text**

1. Select a report from the Select a Report list.

2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.

3. Click the **Find Text** icon, 🔍 .

   The Find Text dialog box opens.

4. Enter your text and click **Find Next**.

   When the TraceFinder application locates the text, it encloses the text in a red box.
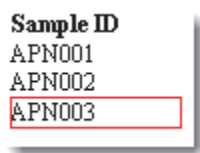
❖ **To enlarge the report text**

1. Select a report from the Select a Report list.

2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.

3. Click the **Zoom** icon, 🔍▾ , and select a zoom scale.
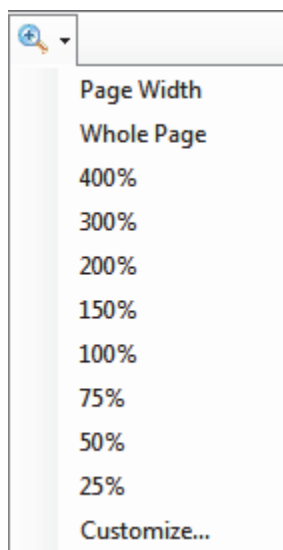
Working with the Active View

Use the Active View page to view quantitative data for each sample in a report. Data in the Active View are labeled with flag information. These flags are based on a comparison of the batch data to criteria defined in the master method.

❖ **To display the Active View page**

Click the **Active View** tab.

The Active View page displays quantitative data and QAQC error flags for each sample. For detailed descriptions of all active view parameters, see "Active View page."

❖ **To display a report**

1. Select a report type from the Select a Report list.

   Only the report types created for the current batch are displayed in the list.

2. (Optional) When the report type includes separate reports for each sample, select a sample file.

Each standard report that uses the Active View displays values that are both common to all reports and specific to that report. See "Active View Report Contents" on page 572.

❖ **To filter which compounds to display**

Click the Showing button to switch the display to either all compounds or only compounds that are flagged for failing a QAQC test.

Figure 154. Active View page
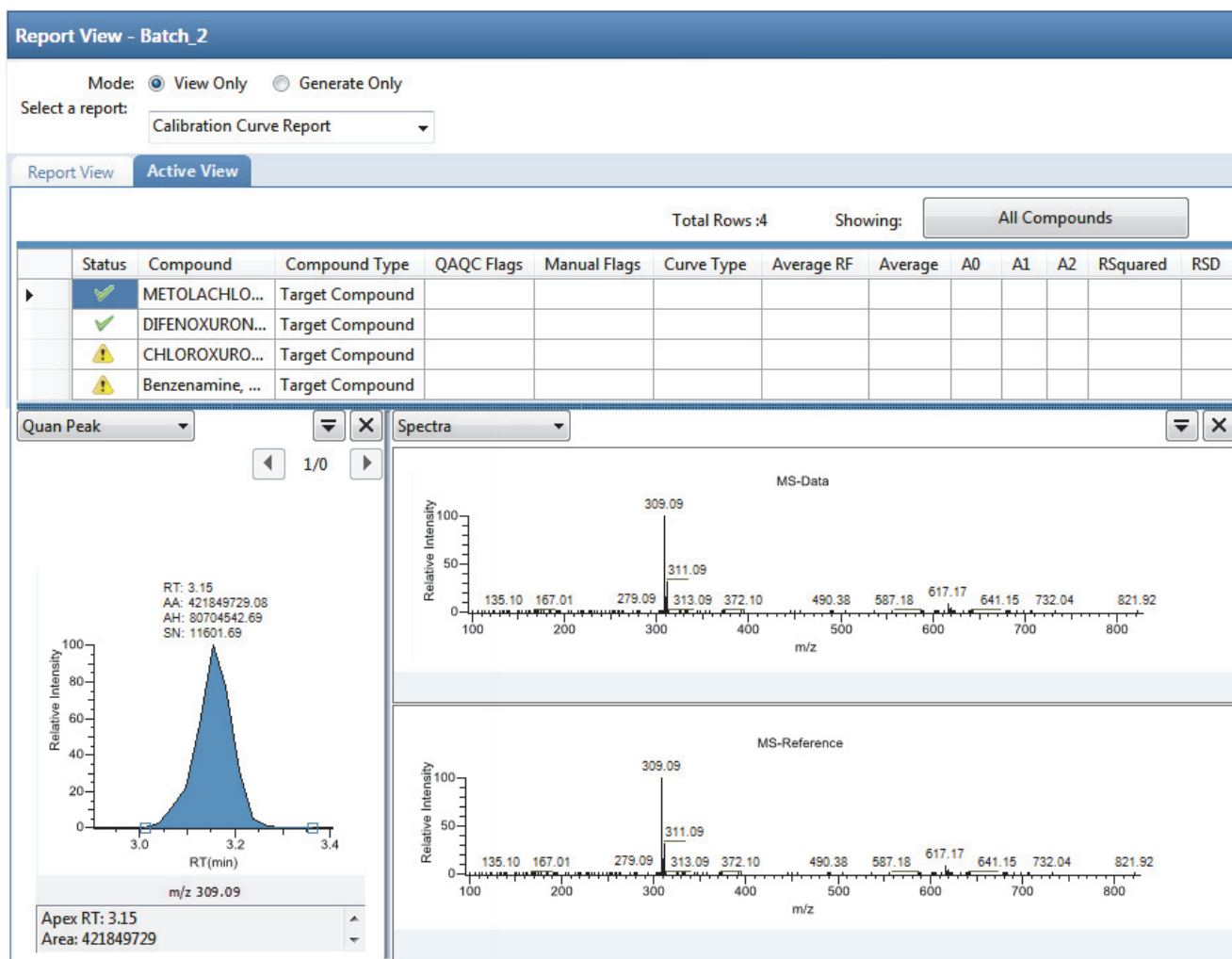
Table 104. Active View page parameters (Sheet 1 of 4)

Parameter	Description
View Only	Makes the Active View pane available for reports that support the active view.
Generate Only	Switches the pane to Report View and makes the Active View pane not available.
Select a Report	Displays the report types created for the current batch.
Sample File	Used when the report type includes separate reports for each sample.
Total Rows	The number of compound rows currently displayed in the pane.
Showing	Displays all compounds or only the flagged compounds.

Table 104. Active View page parameters (Sheet 2 of 4)

Parameter	Description
Column headings	Many column headings are specific to individual reports. See "Active View Report Contents" on page 572.
Status	Indicates the status of the reported compound. • A yellow caution sign indicates one of the following conditions: – The compound was manually integrated. – Any of the confirming peaks was manually integrated. – The compound has quantitation flags. – The compound has a QAQC failure. • A green check mark indicates that none of these conditions exists. When the compound is an internal standard, warning flags are displayed only on the internal standard report.
Compound Name	Alphanumeric name assigned to the compound.
Compound Type	Target Compound or Internal Standard.
QAQC Flags	Indicates that the QAQC check for the sample failed. Manual Integration reports do not use the QAQC column.
Quan Flags	• Limit of Detection (LOD) • Limit of Quantitation (LOQ) • Limit of Reporting (LOR) • Values between the limit of detection and the limit of quantitation, known as the J flag • Upper Limit of Linearity (ULOL) • Est indicating the estimated compound type for semi-quantitative compounds Quan flags do not apply to these sample types: Calibrator, QC, or Solvent. Manual Integration reports do not use the Quan Flag column.
Manual Flags	Indicates manually integrated peaks. **M:** Indicates a manually integrated quantitative peak. **m:** Indicates a manually integrated confirming peak.
Depending on the selected report, the Active View page contains any or all of the following parameters:	
Quan Peak *m/z*	Mass-to-charge ratio for the selected quantitative peak.
Total Response	The sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quantitative peak.
Quan Peak RT	Retention time for the quantitative peak.
Theoretical Amount	Theoretical amount of the compound. Reports N/A when not applicable.

Table 104. Active View page parameters (Sheet 3 of 4)

Parameter	Description
Concentration	The injected concentration.
Confirming *n* Mass	Mass of the confirming peak.
Confirming *n* Response	Response of the confirming peak.
Confirming *n* Manual Flag	Indicates a manually integrated confirming peak.
Confirming *n* Ion Ratio Flag	Indicates that the ion ratio is out of range. Not available for analog compounds.
Confirming *n* Ion Ratio	Actual ratio of the confirming ion response to the quantitation ion response.
Confirming *n* Range	Acceptable range for the confirming ion.
Retention Time	The time after injection when the compound elutes. The total time that the compound is retained on the column.
Quan Mass	The mass-to-charge ratio used to determine the peak area and peak height of the compound.
Response	Sum of all Quan Peak Response values for the compound.
Injection Concentration	Calculated amount as the sample was injected, with no conversion applied.
Injection Units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 175.
Sample Concentration	The injected concentration multiplied by the conversion factor.
Sample Units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 175.
QIon	Mass range for the quantitative peak. When you select the analog detector in the signal parameters for the master method, the application displays this value as Analog and reports with spectra displays show the spectra as Not Available. See "Signal" on page 141.
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Manual Integration reports	
m/z	Mass-to-charge ratio for the quantitative peak.
Method RT	Apex retention time for the method-integrated peak.
Method Peak Height	Height of the method-integrated peak.
Method Peak Area	Area of the method-integrated peak.
Manual RT	Apex retention time for the manually integrated peak.
Manual Peak Height	Height of the manually integrated peak.

Table 104. Active View page parameters (Sheet 4 of 4)

Parameter	Description
Manual Peak Area	Area of the manually integrated peak.
Internal Standard reports	
Std Response	Average of the internal standard's response as found in the calibration file.
Minimum Response	Minimum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 195.
Maximum Response	Maximum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 195.
Sample Response	Area found in the sample.
Std RT	Average retention time as found in the calibration file.
Min RT	Minimum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 195.
Max RT	Maximum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 195.
Sample RT	Retention time found in the sample.
Graphical data	
Quan Peak	Displays a graphical view of the quantitative peak for the selected sample and compound.
ISTD	Displays a graphical view of the internal standard specified for the compound in the method
Calibration Curve	Displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration. For semi-quantitative compounds, the displayed curve is a linked calibration curve and is indicated with a blue-green background.
Confirming Ions	Displays a graphical view of all qualifying/confirming ions for the selected sample and compound, and displays calculated ion ratios and ion ratio acceptance windows.
Reference Peak	Displays a graphical view of the reference peak as specified in the method.
Ion Overlay	Displays a graphical view of an overlay of the entire ion set—quantification and qualifying/confirming—for the selected compound. Use this pane to graphically review the peak apex alignment and coeluting peak profiles.
Library Match	Displays a graphical view of the matching library spectrum (in blue) and the experimental spectrum (in black).

Active View Report Contents

Each standard report that uses the Active View displays values that are common to all reports. See "Common Active View report columns" on page 573.

In addition to the common values, the following reports display additional active view features:

- Blank Report Active View columns

- Calibration Report Active View columns

- High Density Sample reports (Report 1 and Report 1 Long) Active View columns

- High Density Sample reports (Report 2 and Report 2 Long) Active View columns

- High Density Sample reports (Report 3 and Report 3 Long) Active View columns

- Internal Standard Summary Report Active View columns

- Ion Ratio Failure Report Active View columns

- Manual Integration Report Active View columns

- Quality Control Report Active View columns

- Quantitation Report Active View columns

- Solvent Blank Report Active View columns

Table 105. Common Active View report columns

Column	Description

Status	Indicates the status of the reported compound.
	
	• A yellow caution sign indicates one of the following conditions:
	
	    – The compound was manually integrated.
	
	    – Any of the confirming peaks was manually integrated.
	
	    – The compound has quantitation flags.
	
	    – The compound has a QAQC failure.
	
	• A green check mark indicates that none of these conditions exists.
	
	When the compound is an internal standard, warning flags are displayed only on the internal standard report.

Compound Name	Alphanumeric name assigned to the compound.
Compound Type	Target Compound or Internal Standard.
QAQC Flags	Indicates that the QAQC check for the sample failed. The Method Validation and MDL reports do not use the QAQC column.
Quan Flags	• Limit of Detection (LOD) • Limit of Quantitation (LOQ) • Limit of Reporting (LOR) • Values between the limit of detection and the limit of quantitation, known as the J flag • Upper Limit of Linearity (ULOL) • Est indicating the estimated compound type for semi-quantitative compounds (Blank, Quantitation, and High Density reports only) Quan flags do not apply to these sample types: Calibrator, QC, or Solvent. The Calibration report does not use the Quan Flags column. The Calibration Curve report does not use the Quan Flags column.
Manual Flags	Indicates manually integrated peaks. • **M** indicates a manually integrated quantitative peak. • **m** indicates a manually integrated confirming peak.

Table 106. Blank Report Active View columns (Sheet 1 of 2)

Column	Description
Retention Time	Retention time for the quantitation mass. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Quan Mass	Mass range for the quantitative peak.
Response	Sum of all Quan Peak Response values for the compound.

Table 106. Blank Report Active View columns (Sheet 2 of 2)

Column	Description
Inj Conc	Calculated amount as the sample was injected, with no conversion applied.
Inj Units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 175.
Sample Conc	Calculated amount multiplied by the conversion factor.
Sample Units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 175.

Table 107. Calibration Report Active View columns

Column	Description
Curve Type	The type of curve used when calibrating the compound (linear, quadratic, or average response factor).
Average RF	The average response factor. Applicable if curve type is Average RF.
Average Response	The average response for the internal standard across all calibration points. Applies only to Internal Standard sample types.
A0	The value with no X. Applies only to linear and quadratic curves.
A1	The X value. Applies only to linear and quadratic curves.
A2	The X^2 value. Applies only to quadratic curves.
R^2	The minimum correlation coefficient (r^2) for an acceptable calibration (when in linear or quadratic mode).
RSD	Relative standard deviation. Applies only to internal standards and targets calibrated with an average RF curve.
Level	The column specifies the level name; the field value specifies the data point used in calibration. This field can be Response Factor for external calibration, Response Ratio for internal linear or quadratic, or Relative Response Factor for Internal Average RF. There is one column for each level in the curve. If the batch uses an extended calibration, there might be more columns than calibration standards in the current batch.

Note The Calibration Report does not report semi-quantitative compounds.

Table 108. High Density Sample reports (Report 1 and Report 1 Long) Active View columns (Sheet 1 of 2)

Column	Description
m/z	Mass-to-charge ratio for the quantitative peak.
Total Response	The sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quantitative peak.
Quan Peak RT	Retention time for the quantitative peak.

Table 108. High Density Sample reports (Report 1 and Report 1 Long) Active View columns (Sheet 2 of 2)

Column	Description
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.

Table 109. High Density Sample reports (Report 2 and Report 2 Long) Active View columns

Column	Description
m/z	Mass-to-charge ratio for the quantitative peak.
Total Response	Sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quantitative peak.
Quan Peak RT	Retention time for the quantitative peak.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.
Confirming 1 Mass	Mass of the confirming peak.
Confirming 1 Response	Response of the confirming peak.
Confirming 1 Manual Flag	Indicates a manually integrated confirming peak.
Confirming 1 Ion Ratio Flag	Indicates that the ion ratio is out of range. Not available for analog compounds.
Confirming 1 Ion Ratio	Actual ratio of the confirming ion response to the quantitation ion response.
Confirming 1 Range	Acceptable range for the confirming ion.

Table 110. High Density Sample reports (Report 3 and Report 3 Long) Active View columns (Sheet 1 of 2)

Column	Description
m/z	Mass-to-charge ratio for the quantitative peak.
Total Response	Sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quantitative peak.
Quan Peak RT	Retention time for the quantitative peak.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.
Confirming 1 Mass	Mass of the confirming peak.
Confirming 1 Response	Response of the confirming peak.
Confirming 1 Manual Flag	Indicates a manually integrated confirming peak.
Confirming 1 Ion Ratio Flag	Indicates that the ion ratio is out of range. Not available for analog compounds.
Confirming 1 Ion Ratio	Actual ratio of the confirming ion response to the quantitation ion response.

Table 110. High Density Sample reports (Report 3 and Report 3 Long) Active View columns (Sheet 2 of 2)

Column	Description
Confirming 1 Range	Acceptable range for the confirming ion.
Confirming 2 Mass	Mass of the confirming peak.
Confirming 2 Response	Response of the confirming peak.
Confirming 2 Manual Flag	Indicates a manually integrated confirming peak.
Confirming 2 Ion Ratio Flag	Indicates that the ion ratio is out of range. Not available for analog compounds.
Confirming 2 Ion Ratio	Actual ratio of the confirming ion response to the quantitation ion response.
Confirming 2 Range	Acceptable range for the confirming ion.

Table 111. Internal Standard Summary Report Active View columns

Column	Description
Std Response	Average of the internal standard's response as found in the calibration file.
Minimum Response	Minimum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 195.
Maximum Response	Maximum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 195.
Sample Response	Area found in the sample.
Std RT	Average retention time as found in the calibration file.
Min RT	Minimum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 195.
Max RT	Maximum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 195.
Sample RT	Retention time found in the sample.

Table 112. Ion Ratio Failure Report Active View columns

Column	Description
Quan Ion	The ion for quantitative peak.
Qual Ion	The ion for the confirming peak.
Quan Ion Response	Response of the quantitation ion.
Qual Ion Response	Response of the qualitative ion.
Ratio	The ratio of the confirming ion response to the quantitation ion response.
Range	The acceptable range.

Table 113. Manual Integration Report Active View columns

Column	Description
m/z	Mass-to-charge ratio for the quantitative peak.
Method RT	Apex retention time for the method-integrated peak.
Method Peak Height	Height for the method-integrated peak.
Method Peak Area	Area for the method-integrated peak.
Manual RT	Apex retention time for the manually integrated peak.
Manual Peak Height	Height of the manually integrated peak.
Manual Peak Area	Area of the manually integrated peak.

Table 114. Quality Control Report Active View columns

Column	Description
Curve Type	L - Linear A - Average RF Q - Quadratic
Daily RF	The response factor value for Average RF curve types. For all other curve types, this column is blank.
Mean RF	The average response factor as found in the calibration file. Displayed for Average RF curve types. For all other curve types, this column is blank.
Min RF	Minimum QC response factor as found on the QC Check page in the method.
RF % D	Percent difference between daily and average response factor.
Max RF Diff (%)	Maximum QC response factor as found on the QC Check page in the method.
QC Amount	The amount defined by the level for the compound.
Calculated Amount	Reportable amount of concentration.
Amount % Difference	Percentage difference between the calculated amount and the QC amount. Use the injected concentration to calculate this value.
Max Amount % Difference	Maximum allowed percentage difference between the calculated amount and the QC amount.

Table 115. Quantitation Report Active View columns

Column	Description
RT	Retention time for the peak. The time after injection when the compound elutes. The total time that the compound is retained on the column.
QIon	Mass range for the quantitative peak. When you select the analog detector in the signal parameters for the master method, the application displays this value as Analog and reports with spectra displays show the spectra as Not Available. See "Signal" on page 141.
Response	Sum of all quantitative peak response values for the compound.
Injected Concentration	Calculated amount as the sample was injected, with no conversion applied. As each additional sample is processed, calibration data change; therefore, except for the final sample in a batch, a report in active view or report view shows different values from a physical (PDF, XML, or printed) report created at the end of processing. To avoid this discrepancy, do one of the following: • For the standard Quantitation Report or Quantitation Report - 2, observe the active or report view for only the last sample in the batch. • For the custom Quantitation Report, make the report a batch-level report.
Injected Units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 175.
Sample Conc	Calculated injection amount multiplied by the conversion factor. See the Injected Concentration description.
Sample Units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 175.

Table 116. Solvent Blank Report Active View columns

Column	Description
RT	Retention time for the quantitative peak. The time after injection when the compound elutes. The total time that the compound is retained on the column.
QIon	Mass range for the quantitative peak. When you select the analog detector in the signal parameters for the master method, the application displays this value as Analog and reports that display spectra report the spectra as Not Available. See "Signal" on page 141.
Response	Sum of all Quan Peak Response values for the compound.
Method	Method of evaluation defined in the method.
Upper Limit	Defined in the method.

Working in the Local Method View

A local method is a copy of a master method associated with a batch. You can edit only the local copy of the method, or you can edit the master method and overwrite the local copy with the edited master method.

In the Local Method view, you can edit the local method parameters. A local method is a copy of a master method associated with a batch. Local methods are named *Batch_MasterMethod*.

❖ **To open the Local Method View**

1. Click **Analysis** in the navigation pane.

2. In the Analysis navigation pane, click **Local Method**.

The Local Method view for the currently selected batch opens.

You can edit many of the method parameters in a local method. Editing the local method does not affect parameters in the master method.

For detailed descriptions of method parameters, see "Working with Master Methods" on page 85.

3. Enter any local changes to the method.

4. When you have finished editing the local method, choose **File > Save**.

5. To process the batch or create new reports with the edited local method, return to the Batch View and submit the batch.

❖ **To overwrite the local method with the master method in the Batch View**

In the Batch View, click **Update**.

The application overwrites the local method with the master method of the same name. You can use this feature to overwrite an edited local method with the original master method or to overwrite the local method with an updated master method.

Figure 155. Local Method View of a quantitation method

Figure 156. Local Method View of a screening method

Working in the Batch Template Editor

In the Batch Template Editor, you can create a batch template that contains the basic settings for your batches. See "Batch Template Editor" on page 587. Batches are created as a routine operation and, because the nature and types of batches are often similar (in some cases specified by laboratory operating procedure), you can define a batch template that supplies the basic structure of a batch.

To create a batch using a batch template, choose **File > New > Batch Using Wizard** from the application menu. See "Creating a Batch Using the Batch Wizard" on page 435.

Follow these procedures:

- To create a new batch template

- To open a batch template

- To specify method information for the template

- To add a sample to the batch

- To insert a sample into the list

- To copy a sample

- To remove samples from the list

- To edit sample values

- To add multiple samples of the same type

- To specify auto samples

- To specify active compounds

- To specify report options

❖ **To create a new batch template**

1. Choose **File > New > Batch Template** from the application menu.

   The Open Method dialog box opens where you can select a master method to use for your template.
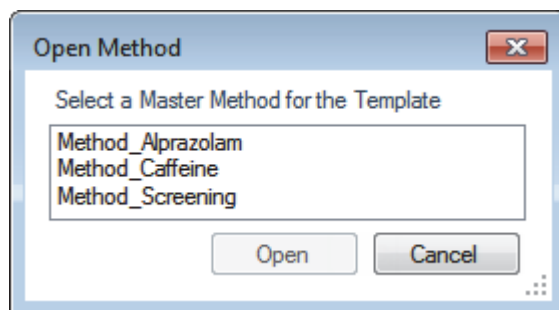
2. Select a master method and click **Open**.

The Batch Template Editor opens. For detailed descriptions of all parameters, see "Batch Template Editor" on page 587.

The editor uses the selected master method for the template.

❖ **To open a batch template**

1. Choose **File > Open > Batch Template** from the application menu.

The Open Batch Template dialog box opens.
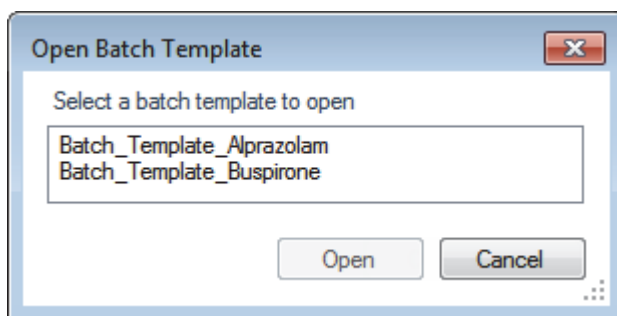
2. Select a batch template and click **Open**.

The Batch Template Editor opens with the settings from the selected template. To view the editor and for detailed descriptions of the parameters, see "Batch Template Editor" on page 587.

❖ **To specify method information for the template**

1. Click **Select Folder.**

The Select or Create Batch Folder dialog box opens. See "Select or Create Batch Folder" on page 589.

2. Expand the TraceFinderData\Projects folder and select a batch folder where you want to create the batch template.

3. Click **OK**.

4. To change the current method, click **Select Method** and select a method from the list of methods.
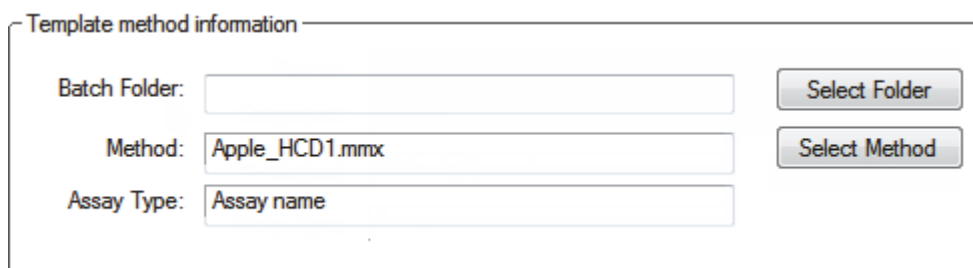
5. (Optional) Type an assay name in the Assay Type box.

❖ **To add a sample to the batch**

Right-click and choose **Add Sample** from the shortcut menu, or click the add sample icon, ▯⊞.

The application adds a new, Specimen sample to the end of the sample list.

❖ **To insert a sample into the list**

1. Select the sample above which you will insert a new, Specimen sample.

2. Right-click and choose **Insert Sample** from the shortcut menu.

   The application inserts a new, Specimen sample above the selected sample.

	Sample type		Qual Processing	Sample ID	Sample name	Repeat sample count
	Specimen	▼	☐			1
✎	Negative	▼	☐			1

Inserted
sample

❖ **To copy a sample**

1. Select the sample that you want to copy.

2. Right-click and choose **Insert Copy Sample** from the shortcut menu.

   The application inserts the copy above the selected sample.

❖ **To remove samples from the list**

1. Select the sample that you want to remove.

   Use the SHIFT or CTRL keys to select multiple samples.

2. Right-click and choose **Remove Selected Samples** from the shortcut menu, or click the **Remove Sample** icon, ▯⊟ .

   The application removes the selected samples from the list.

❖ **To edit sample values**

1. For each sample, click the Sample Type column and select a sample type from the list.

Available sample types		
Specimen	QC	Hydrolysis
Solvent	Calibrator	
Unextracted	Negative	

2. For each QC or Calibrator sample, click the Level cell and select a level from the list.

   The calibration and QC levels were defined in the master method. If there is nothing to select in the Level list, do the following:

   a. Close the Batch Template Editor.

   b. Return to the Method Development mode.

   c. Open the master method.

   d. Click the **Compounds** tab.

   e. Click the **Calibration Levels** tab.

   f. Add the levels.

   g. Save the method.

   h. Return to the Analysis mode, and begin this batch template again.

   You must close your original batch template without saving it and start a new template. For detailed instructions, see "Editing a Quantitation Master Method" on page 109.

3. (Optional) Type a sample ID, sample name, or comment.

   These values can be any text string.

❖ **To add multiple samples of the same type**

In the Repeat Sample Count column, type the number of samples that you want to create for each sample type.

When you use this template to create a batch, the batch will contain this number of individual samples of the specified type. In the batch, you can change any of the column values for the individual samples.

❖ **To specify auto samples**

1. Click the **Auto Samples** tab.

2. Right-click and choose **Add Auto Sample** from the shortcut menu, or click the **Add New Auto Sample** icon, 1 ⬆ ⬇ ⬛➕ .

   The application adds a Solvent sample to the sample list.

   You can add, insert, or remove samples from this list as you would any sample list. See "Samples Page" on page 390.

3. To change the sample type to a Negative, click the Sample Type column and select Negative from the list.

4. In the Injection Volume column for the sample, type a volume.

   The minimum injection volume value allowed is 0.1 μL; the maximum injection volume value allowed is 5000 μL.

5. In the Number of Injections column, type the number of injections available in the designated Solvent or Negative vial.

   After auto sample injections have occurred, you can return to this page to view the number of Injections Used in each vial.

6. In the Vial Position column, type the vial position for the Solvent or Negative sample.

❖ **To specify active compounds**

1. In the sample table, click anywhere in the sample row to select the sample for which you want to specify active compounds.

   Compound selections are specific to a sample. You can select different compounds for each of the samples even if they are the same sample type.

2. In the Compound Active Status area, select the Active check box for each compound that you want identified in the selected sample.

   If you created compound groups, you can make the entire group active or inactive. Right-click and choose the group from the list.
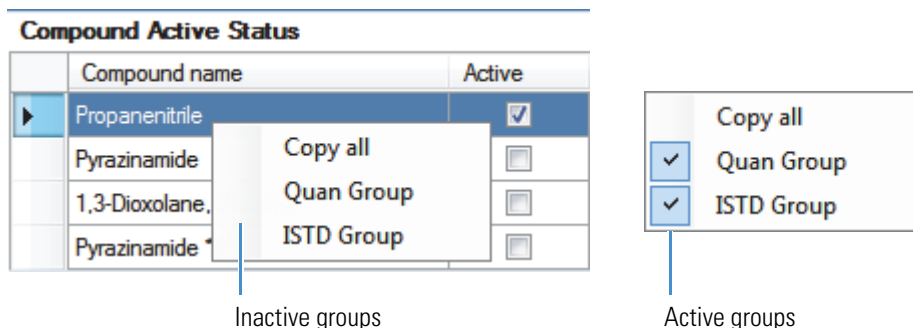
Inactive groups   Active groups

❖ **To specify report options**

1. To specify the type of report output to create for each report type, select the check box in the appropriate column.

   By default, all report output types are cleared.

2. To duplicate the output type for all reports below the selected report, click the cell to select it, and then right-click and choose **Copy Down** from the shortcut menu.
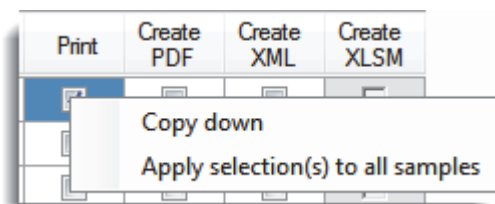
   All check boxes in the column below the selected cell duplicate the selected or cleared state of the selected cell.

   You can duplicate the output type only for reports that have this output format available.

3. To duplicate the selected report output formats for all samples in the batch, right-click the cell and choose **Apply Selection to All Samples** from the shortcut menu.

Here is an example:

Copying selected report output formats from the first sample

Duplicates the selected report output formats to all samples in the batch

Batch Template Editor

Use the Batch Template Editor features to create a batch template that contains the basic settings for your batches. The Auto Samples page is available only when you activate Intelligent Sequencing in the Configuration console. See "Intelligent Sequencing" on page 71.

Figure 157. Batch Template Editor
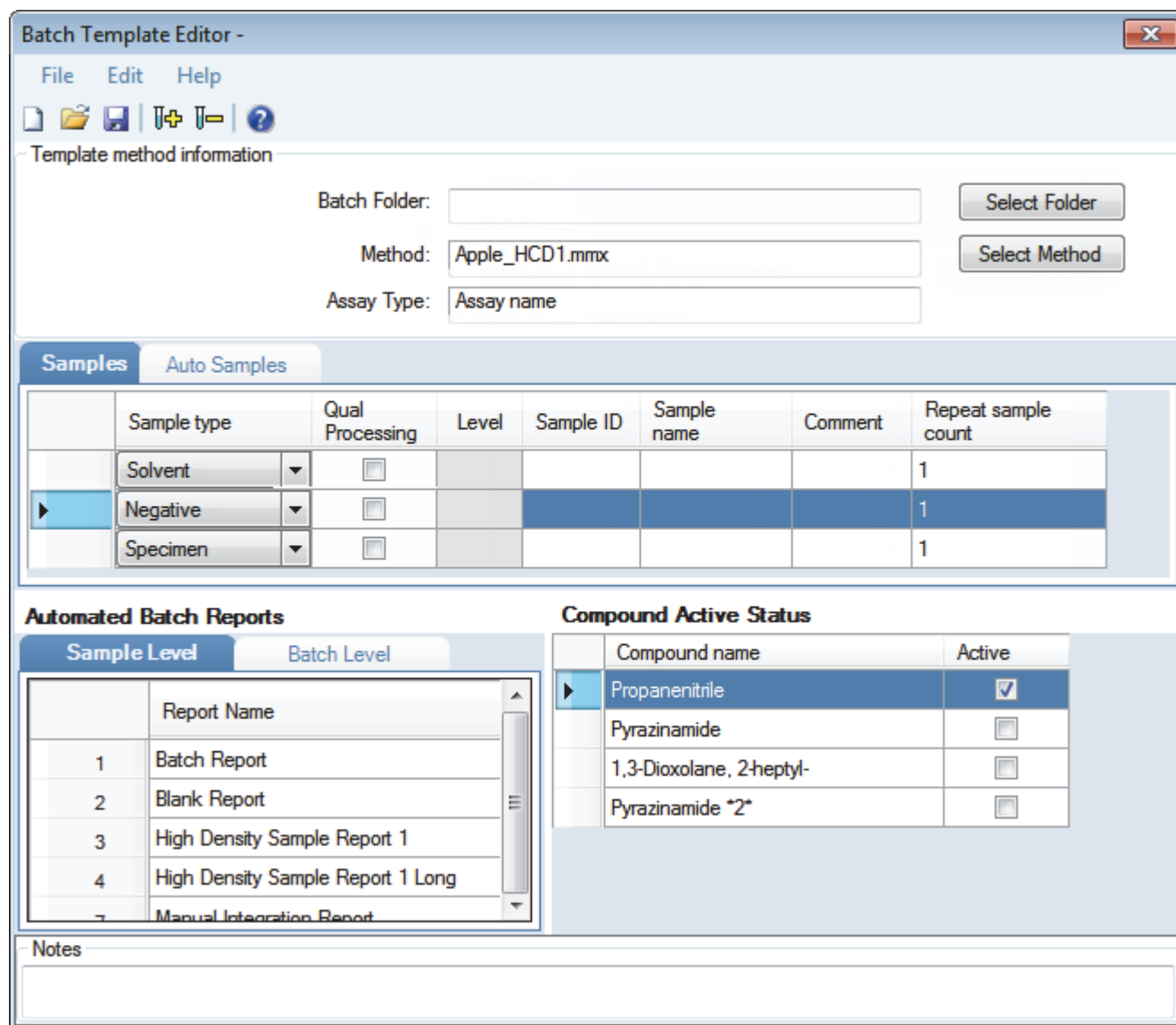
Table 117. Batch Template Editor parameters (Sheet 1 of 2)

Parameter	Description
Template Method Information	
Batch Folder	The project folder for the batch.
Select Folder	Opens the Select or Create Batch folder. See "Select or Create Batch Folder" on page 589.

Table 117. Batch Template Editor parameters (Sheet 2 of 2)

Parameter	Description
Method	The master method to use for the batch. The Select Method button opens the Open Method dialog box where you can select a different master method for the batch template.
Assay Type	The name for the analysis type to be targeted by the method. The assay type associates the method with the analysis of a compound or specific class of compounds (for example, an assay type of PAH might be used for the analysis of Polynuclear Aromatic Hydrocarbons). The application uses this assay type in the batch template. You can also select an appropriate combination of method and batch template.
Column values	
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Specimen, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative.
Level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined, alphanumeric string that identifies a sample.
Sample Name	A user-defined name that identifies a sample.
Comment	A user-defined comment for the sample.
Repeat Sample Count	Number of samples to create for this sample type.
Sample Level / Batch Level	
Report Name	The name of a report.
Type	Standard, Custom, or Target Screening
Print	Sends reports to the printer.
Create PDF	Saves reports as PDF files. Available only for standard and target screening reports.
Create XML	Saves reports as XML files. Available only for standard reports.
Create XLSM	Saves reports in Excel Macro-Enabled Workbook (.xlsm) format. Available only for custom reports.
Compound Active Status	
Compound Name	List of all compounds for the method.
Active	Compounds to identify in the selected sample.

Select or Create Batch Folder

Use the features on the Select or Create Batch Folder dialog box to display project folders or create, delete, or rename folders.

Figure 158. Select or Create Batch Folder
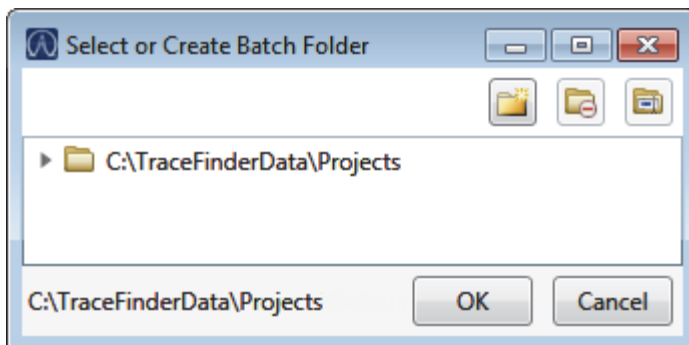
Table 118. Select or Create Batch Folder dialog box parameters

Parameter	Description
Icons	
 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.
 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	Lets you rename 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.
Shortcut menu commands	
Create Folder	Identical to the Create New Folder icon.
Delete Folder	Identical to the Delete Folder icon.
Rename Folder	Identical to the Rename Folder icon.
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.

Reports

This appendix contains information about standard, custom, ToxID, and target screening reports.

Contents

- Specifying Reports
- Report Flags
- Sample Standard Reports

The report engine can generate several different types of reports designed to meet the needs of the laboratory, the laboratory's customers, and key regulatory agencies that might review the results. The reports listed in this appendix meet the requirements of various methods and worldwide regulatory agencies and are designed to help track the performance of the system and method. The TraceFinder application can produce standard reports, custom reports, and reports specific to target screening and ToxID features.

Specifying Reports

As a user in a role with Reports permission, you can configure a list of reports that are available for the Method Development or Acquisition mode.

For detailed information about configuring reports in the Configuration console, see "Specifying the Reports" on page 40.

For detailed information about specifying reports when you create a method in the Method Development mode, see "Editing the Reports Page" on page 208.

For detailed information about viewing reports in the Acquisition mode, see "Selecting and Reviewing Reports" on page 354.

This section lists all available reports for the following report types:

- "Standard Reports" on page 592
- "Custom Reports" on page 593
- "Target Screening Reports" on page 593
- "ToxID Reports" on page 593

Standard Reports

For each standard report you generate, you can create a version in hardcopy print, as a PDF (.pdf) file, or in an XML (.xml) or XLSM (.xlsm) output format. In addition to the report type, you can specify a report title that appears at the top of each of your reports. The default report title is the report name.

The TraceFinder application can generate the following types of standard reports:

- Batch Report
- Batch Summary Report
- Batch Report Rev 1
- Calibration Report
- Calibration Curve Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- High Density Calibration Report
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Intelligent Sequencing Report
- Internal Standard Summary Report
- Ion Ratio Failure Report
- Manual Integration Report
- Method Report
- Negative Report
- Qualitative Peak Report
- Qualitative Summary Report
- Quality Control Report
- Quantitation Report
- Quantitation Report - 2
- Sample Report
- Sample Report Long
- Solvent Blank Report

To view an example of each type of standard report, see "Sample Standard Reports" on page 595.

Custom Reports

For each custom report you generate, you can create a hardcopy printout or an Excel Macro-Enabled Workbook (.xlsm) output file. The default report description is the report name. A user in the default ITAdmin or default LabDirector role can configure custom reports to generate a single report for an entire batch or create a separate report for each sample.

The TraceFinder application can generate the following types of custom reports:

- AltCalibrationReport
- Alternate BatchReport
- Alternate CalibrationReport
- Alternate ConfirmationReport
- Alternate MatrixSpikeReport
- Alternate SampleReport
- Alternate SummaryReport
- BatchReport
- BlankReport
- CalibrationDensityReport
- CalibrationReport
- CheckStandardReport
- CompoundCalibrationReport
- ConfirmationReport
- ConfirmationReport2
- HighDensitySampleReport1Long
- HighDensitySampleReport2Long
- HighDensitySampleReport3Long
- HighDensitySampleReport4
- HighDensitySampleReport5
- QuantitationReport
- SteroidAnalysisReport

Target Screening Reports

The TraceFinder application can generate the following types of target screening reports:

- Target Screening High Density Sample Report
- Target Screening Summary Report

ToxID Reports

ToxID reports are available only when you install the ToxID software and activate the ToxID features. For a detailed procedure for enabling ToxID features, see "ToxID" on page 65. The TraceFinder application can generate the following types of ToxID reports:

- Target Screening Long Report
- Target Screening Summary Report

Report Flags

When generating or viewing a report, you might see one of the following quantification or calibration flags listed on the page.

Table 119. Quantification flags

Flag	Definition
b	Compound was observed at a concentration in a Matrix Blank sample above the specified limit.
s	Compound was observed at a response in a solvent blank sample above the specified limit.
J	Compound was observed at a concentration above the limit of detection, but below the limit of quantitation.
I or *	Confirming/qualifying ion ratio for a compound was observed outside the target ratio range or the coelution between quantification and confirming/qualifying ion was larger than acceptable limit.
C	Compound was observed at a concentration above the specified carryover limit.
?	Compound was observed at a concentration above the specified linearity limit.
D	Compound was observed at a concentration below the specified limit of detection.
Q	Compound was observed at a concentration below the specified limit of quantitation.
POS	Compound was observed at a concentration above the specified cutoff.

Table 120. Calibration flags

Flag	Definition
D	Calibration for this compound exceeded the specified maximum percent relative standard deviation (%RSD).
F	Response factor for this compound was below the specified minimum response factor (Min RF).
R	Calibration for this compound was below the specified minimum correlation coefficient (r^2).
A	Back calculation of the calibration points for this compound exceeded the specified maximum percent difference (Max %D).
X	Calibration point for this compound was excluded from the overall calibration by manual selection.
X(ISNF)	Calibration point for this compound was excluded from the overall calibration because its associated internal standard was not found.

A flags failure is identified by an asterisk (*), a shaded row, or the word *Fail*.

Values on a report that are the result of a manual integration use an uppercase M to signify a manually integrated quantification ion and a lowercase m to signify a manually integrated qualifying/confirming ion. On alternate reports, manual integration uses a black box around the value.

Sample Standard Reports

This section shows samples of the following standard report types:

- Batch Report
- Batch Report Rev 1
- Calibration Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- High Density Calibration Report
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- Manual Integration Report
- Method Report
- Quality Control Report
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report

> **Tip** To easily view reports in landscape format, choose **View > Rotate View > Clockwise** from the Adobe Acrobat™ viewer menu.

Batch Report

Batch Report

Lab Names:	Thermo Lab							
Instrument:	TQU00637				Method:	011HPLR1_PDP_040511		
User:	TQU00637\RPC					PDP_040511		
Batch:	011HPLR1				Call File:	011HPLR1.calx		

File Name	Date/Time	Sample ID	Sample Name	Level	Sample Type	Vial Pos	Inj Vol	Conv Factor	Comment
LLOD_HP031711	3/17/2011 5:46:30 PM	1	LLOD_HP031711	N/A	Matrix Blank	5	5.000	1.0	
L1XLOQ_HP031711	3/17/2011 6:06:33 PM	2	L1XLOQ_HP031711	1XLOQ	Cal Std	5	5.000	1.0	
L2XLOQ_HP031711	3/17/2011 6:26:29 PM	3	L2XLOQ_HP031711	2XLOQ	Cal Std	5	5.000	1.0	
L4XLOQ_HP031711	3/17/2011 6:46:23 PM	4	L4XLOQ_HP031711	4XLOQ	Cal Std	5	5.000	1.0	
L6XLOQ_HP031711	3/17/2011 7:06:17 PM	5	L6XLOQ_HP031711	6XLOQ	Cal Std	5	5.000	1.0	
L10XLOQ_HP031711	3/17/2011 7:26:11 PM	6	L10XLOQ_HP031711	10XLOQ	Cal Std	5	5.000	1.0	
L16XLOQ_HP031711	3/17/2011 7:46:05 PM	7	L16XLOQ_HP031711	16XLOQ	Cal Std	5	5.000	1.0	
L32XLOQ_HP031711	3/17/2011 8:06:03 PM	8	L32XLOQ_HP031711	32XLOQ	Cal Std	5	5.000	1.0	
MeOH_01	3/17/2011 8:26:01 PM	9	MeOH	N/A	Unknown	5	5.000	1.0	
11_0041RB	3/17/2011 8:45:57 PM	10	11_0041RB	N/A	Unknown	5	5.000	1.0	
11_0040MB	3/17/2011 9:05:59 PM	11	11_0040MB	N/A	Unknown	5	5.000	1.0	
11_0037LCMS	3/17/2011 9:26:01 PM	12	11_0037LCMS	N/A	Unknown	5	5.000	1.0	
L2XLOQ_HP031711_01	3/17/2011 9:45:57 PM	13	L2XLOQ_HP031711	2XLOQ	Chk Std	5	5.000	1.0	
11_0001	3/17/2011 10:05:53 PM	14	11_0001	N/A	Unknown	5	5.000	1.0	
11_0002	3/17/2011 10:25:49 PM	15	11_0002	N/A	Unknown	5	5.000	1.0	
11_0003	3/17/2011 10:45:41 PM	16	11_0003	N/A	Unknown	5	5.000	1.0	
11_0004	3/17/2011 11:05:35 PM	17	11_0004	N/A	Unknown	5	5.000	1.0	
11_0005	3/17/2011 11:25:39 PM	18	11_0005	N/A	Unknown	5	5.000	1.0	
11_0006	3/17/2011 11:45:43 PM	19	11_0006	N/A	Unknown	5	5.000	1.0	
11_0007	3/18/2011 12:05:43 AM	20	11_0007	N/A	Unknown	5	5.000	1.0	
11_0008	3/18/2011 12:25:37 AM	21	11_0008	N/A	Unknown	5	5.000	1.0	
11_0009	3/18/2011 12:45:37 AM	22	11_0009	N/A	Unknown	5	5.000	1.0	
11_0010	3/18/2011 1:05:37 AM	23	11_0010	N/A	Unknown	5	5.000	1.0	
11_0011	3/18/2011 1:25:35 AM	24	11_0011	N/A	Unknown	5	5.000	1.0	
L2XLOQ_HP031711_02	3/18/2011 1:45:29 AM	25	L2XLOQ_HP031711	2XLOQ	Chk Std	5	5.000	1.0	
11_0012	3/18/2011 2:05:23 AM	26	11_0012	N/A	Unknown	5	5.000	1.0	
11_0013	3/18/2011 2:25:19 AM	27	11_0013	N/A	Unknown	5	5.000	1.0	
11_0014	3/18/2011 2:45:17 AM	28	11_0014	N/A	Unknown	5	5.000	1.0	
11_0015	3/18/2011 3:05:13 AM	29	11_0015	N/A	Unknown	5	5.000	1.0	
11_0016	3/18/2011 3:25:07 AM	30	11_0016	N/A	Unknown	5	5.000	1.0	
11_0017	3/18/2011 3:45:05 AM	31	11_0017	N/A	Unknown	5	5.000	1.0	
11_0018	3/18/2011 4:05:09 AM	32	11_0018	N/A	Unknown	5	5.000	1.0	
11_0019	3/18/2011 4:25:11 AM	33	11_0019	N/A	Unknown	5	5.000	1.0	
11_0020	3/18/2011 4:45:19 AM	34	11_0020	N/A	Unknown	5	5.000	1.0	
11_0021	3/18/2011 5:05:15 AM	35	11_0021	N/A	Unknown	5	5.000	1.0	
L2XLOQ_HP031711_03	3/18/2011 5:25:15 AM	36	L2XLOQ_HP031711	2XLOQ	Chk Std	5	5.000	1.0	
11_0022	3/18/2011 5:45:11 AM	37	11_0022	N/A	Unknown	5	5.000	1.0	
11_0023	3/18/2011 6:05:03 AM	38	11_0023	N/A	Unknown	5	5.000	1.0	

Batch Report Rev 1

Batch Report

Lab Name: Thermo Lab
Instrument: TQU00637
User: TQU00637RPC
Batch: 011HPLR1

Method: 011HPLR1_PDP_040511
PDP_040511
Cal File: 011HPLR1.calx

File Name	Date/Time	Sample ID	Sample Name	Level	Sample Type	Vial Pos	Inj Vol	Conv Factor	Comment
LLOD_HP031711	3/17/2011 5:46:30 PM	1	LLOD_HP031711	N/A	Matrix Blank	5	5.000	1.0	
L1XLOQ_HP031711	3/17/2011 6:06:33 PM	2	L1XLOQ_HP031711	1XLOQ	Cal Std	5	5.000	1.0	
L2XLOQ_HP031711	3/17/2011 6:26:29 PM	3	L2XLOQ_HP031711	2XLOQ	Cal Std	5	5.000	1.0	
L4XLOQ_HP031711	3/17/2011 6:46:23 PM	4	L4XLOQ_HP031711	4XLOQ	Cal Std	5	5.000	1.0	
L6XLOQ_HP031711	3/17/2011 7:06:17 PM	5	L6XLOQ_HP031711	6XLOQ	Cal Std	5	5.000	1.0	
L10XLOQ_HP031711	3/17/2011 7:26:11 PM	6	L10XLOQ_HP031711	10XLOQ	Cal Std	5	5.000	1.0	
L16XLOQ_HP031711	3/17/2011 7:46:05 PM	7	L16XLOQ_HP031711	16XLOQ	Cal Std	5	5.000	1.0	
L32XLOQ_HP031711	3/17/2011 8:06:03 PM	8	L32XLOQ_HP031711	32XLOQ	Cal Std	5	5.000	1.0	
MeOH_01	3/17/2011 8:26:01 PM	9	MeOH	N/A	Unknown	5	5.000	1.0	
11_0041RB	3/17/2011 8:45:57 PM	10	11_0041RB	N/A	Unknown	5	5.000	1.0	
11_0040MB	3/17/2011 9:05:59 PM	11	11_0040MB	N/A	Unknown	5	5.000	1.0	
11_0037LCMS	3/17/2011 9:26:01 PM	12	11_0037LCMS	N/A	Unknown	5	5.000	1.0	
L2XLOQ_HP031711_01	3/17/2011 9:45:57 PM	13	L2XLOQ_HP031711	2XLOQ	Chk Std	5	5.000	1.0	
11_0001	3/17/2011 10:05:53 PM	14	11_0001	N/A	Unknown	5	5.000	1.0	
11_0002	3/17/2011 10:25:49 PM	15	11_0002	N/A	Unknown	5	5.000	1.0	
11_0003	3/17/2011 10:45:41 PM	16	11_0003	N/A	Unknown	5	5.000	1.0	
11_0004	3/17/2011 11:05:35 PM	17	11_0004	N/A	Unknown	5	5.000	1.0	
11_0005	3/17/2011 11:25:39 PM	18	11_0005	N/A	Unknown	5	5.000	1.0	
11_0006	3/17/2011 11:45:43 PM	19	11_0006	N/A	Unknown	5	5.000	1.0	
11_0007	3/18/2011 12:05:43 AM	20	11_0007	N/A	Unknown	5	5.000	1.0	
11_0008	3/18/2011 12:25:37 AM	21	11_0008	N/A	Unknown	5	5.000	1.0	
11_0009	3/18/2011 12:45:37 AM	22	11_0009	N/A	Unknown	5	5.000	1.0	
11_0010	3/18/2011 1:05:37 AM	23	11_0010	N/A	Unknown	5	5.000	1.0	
11_0011	3/18/2011 1:25:35 AM	24	11_0011	N/A	Unknown	5	5.000	1.0	
L2XLOQ_HP031711_02	3/18/2011 1:45:29 AM	25	L2XLOQ_HP031711	2XLOQ	Chk Std	5	5.000	1.0	
11_0012	3/18/2011 2:05:23 AM	26	11_0012	N/A	Unknown	5	5.000	1.0	
11_0013	3/18/2011 2:25:19 AM	27	11_0013	N/A	Unknown	5	5.000	1.0	
11_0014	3/18/2011 2:45:17 AM	28	11_0014	N/A	Unknown	5	5.000	1.0	
11_0015	3/18/2011 3:05:13 AM	29	11_0015	N/A	Unknown	5	5.000	1.0	
11_0016	3/18/2011 3:25:07 AM	30	11_0016	N/A	Unknown	5	5.000	1.0	
11_0017	3/18/2011 3:45:05 AM	31	11_0017	N/A	Unknown	5	5.000	1.0	
11_0018	3/18/2011 4:05:09 AM	32	11_0018	N/A	Unknown	5	5.000	1.0	
11_0019	3/18/2011 4:25:11 AM	33	11_0019	N/A	Unknown	5	5.000	1.0	
11_0020	3/18/2011 4:45:19 AM	34	11_0020	N/A	Unknown	5	5.000	1.0	
11_0021	3/18/2011 5:05:15 AM	35	11_0021	N/A	Unknown	5	5.000	1.0	
L2XLOQ_HP031711_03	3/18/2011 5:25:15 AM	36	L2XLOQ_HP031711	2XLOQ	Chk Std	5	5.000	1.0	
11_0022	3/18/2011 5:45:11 AM	37	11_0022	N/A	Unknown	5	5.000	1.0	
11_0023	3/18/2011 6:05:03 AM	38	11_0023	N/A	Unknown	5	5.000	1.0	

Calibration Report

Lab Name:	Thermo Lab			
Instrument:	TQU00637	**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC		PDP_040511	
Batch:	011HPLR1	**Cali File:**	011HPLR1.calx	

Calibration Summary

Compound	Manually Integrated	Curve Type	A0 y-Intercept Mean RF	A1 Slope	A2	R^2 R^2 % RSD	Flag
Oxamyl_Oxime		Q	0e0	1.021e5	-9.21e0	0.9999	
Omethoate		Q	0e0	3.449e5	-2.743e2	0.9999	
Formetanate		Q	0e0	7.037e5	-8.207e1	0.9999	
Dinotefuran		Q	0e0	8.978e4	-3.798e1	0.9995	
Aldicarb_SO		Q	0e0	8.444e4	-1.968e1	0.9997	
Propamocarb		Q	0e0	2.953e5	1.094e2	0.9990	
Pymetrozine		Q	0e0	1.458e5	-1.625e2	0.9999	
Aldicarb_SO2		Q	0e0	1.304e5	-2.433e1	0.9999	
Oxamyl		Q	0e0	6.343e4	-9.365e0	0.9999	
Methomyl		Q	0e0	5.609e4	2.406e-2	0.9998	A
Flonicamid		Q	0e0	6.78e3	-6.227e-1	0.9999	
ODMS		Q	0e0	1.559e5	-3.779e1	1.0000	
5-OH_TBZ		Q	0e0	1.554e5	-8.3e1	1.0000	
Thiamethoxam		Q	0e0	9.218e4	-8.168e1	0.9999	
Monocrotophos		Q	0e0	2.546e5	3.747e0	0.9999	
Imidacloprid		Q	0e0	9.412e4	-1.542e1	0.9999	
Clothianidin		Q	0e0	6.899e4	-2.01e1	0.9999	
Thiabendazole		Q	0e0	2.318e5	-3.829e1	0.9998	
3-OH_Carbofuran		Q	0e0	2.673e5	-5.488e1	0.9999	
Acetamiprid		Q	0e0	1.465e5	-1.234e2	0.9999	
Cymoxanil		Q	0e0	1.907e4	-2.093e0	0.9999	
Thiacloprid		Q	0e0	1.804e5	-3.743e1	0.9998	
Methidathion_OA		Q	0e0	2.452e5	-4.327e1	0.9999	
Aldicarb		Q	0e0	9.107e4	-8.106e0	0.9999	
Azinphos_Me_OA		Q	0e0	7.722e4	-1.808e1	0.9993	
Metribuzin		Q	0e0	1.285e5	-6.658e1	0.9998	
Simazine		Q	0e0	5.641e4	-4.048e1	0.9997	
Propoxur_(S)		Q	0e0	2.644e5	-7.519e1	0.9999	
Pirimicarb		Q	0e0	4.722e5	-4.082e1	0.9998	
Bendiocarb		Q	0e0	1.491e5	-6.818e1	0.9997	
Carbofuran		Q	0e0	7.01e5	-2.286e2	0.9998	
Fenamiphos_SO		Q	0e0	1.522e4	-9.643e-1	0.9998	A
Tebuthiuron		Q	0e0	8.461e5	-2.67e2	0.9998	
Carboxin		Q	0e0	6.506e5	-1.708e2	1.0000	
Sulfentrazone		Q	0e0	1.374e4	-1.836e0	0.9998	
Fenamiphos_SO2		Q	0e0	9.059e4	-2.877e1	0.9999	
Carbaryl		Q	0e0	4.251e5	-4.87e1	0.9999	
Thiodicarb		Q	0e0	3.968e4	-3.693e0	0.9995	A
Phorate_Sulfoxide		Q	0e0	3.861e5	-1.033e2	0.9998	
Norflurazon_DM		Q	0e0	4.987e4	-1.219e1	0.9998	
Phorate_Sulfone		Q	0e0	2.959e5	-3.89e1	1.0000	
Atrazine		Q	0e0	3.679e5	-1.13e2	1.0000	
Isoprocarb		Q	0e0	9.685e4	3.858e0	0.9996	
Imazalil		Q	0e0	7.833e4	-4.144e0	1.0000	
Metalaxyl		Q	0e0	8.234e5	6.852e0	0.9999	
Diuron		Q	0e0	8.495e4	-1.208e1	0.9999	
Norflurazon		Q	0e0	5.513e4	-9.775e0	0.9999	
Chlorantraniliprole		Q	0e0	2.947e4	-1.6e0	0.9996	
Azinphos_Me		Q	0e0	7.972e4	-1.585e1	1.0000	
Benoxacor		Q	0e0	1.333e4	-8.821e-1	0.9999	
Fluridone		Q	0e0	5.003e5	-1.602e2	0.9999	
Pyrimethanil		Q	0e0	4.783e5	-1.313e0	0.9999	
Azoxystrobin		Q	0e0	7.944e5	-3.268e2	1.0000	

Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard; Note: Amounts displayed for Internal standards represent the ISTD Response.

Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.

Calibration Report

Lab Name: Thermo Lab
Instrument: TQU00637 **Method:** 011HPLR1_PDP_040511
User: TQU00637\RPC PDP_040511
Batch: 011HPLR1 **Cali File:** 011HPLR1.calx

Calibration Data Points

Compound	Curve Type	1XLOQ	2XLOQ	4XLOQ	6XLOQ	10XLOQ	16XLOQ	32XLOQ
Oxamyl_Oxime	Q	4301979	8239118	16242623	23873974	39827173	61070387	115624994
Omethoate	Q	1767322	3484419	6936118	10019480	16562654	25318124	47692071
Formetanate	Q	14839193	28774173	55703047	83034780	140328387	215487571	418192129
Dinotefuran	Q	1957462	3754131	7124741	10430815	16753892	24286005	41994838
Aldicarb_SO	Q	1800889	3431833	6655525	10063684	16448105	24529724	46055255
Propamocarb	Q	4981586	9714037	23426813	33421290	62325833	109908202	233040768
Pymetrozine	Q	827514	1491832	2850157	4285647	6910457	10568034	19185279
Aldicarb_SO2	Q	2773066	5247744	10263769	15236469	25734192	39154955	73839209
Oxamyl	Q	1360327	2563147	4952614	7533418	12426641	19210270	36777897
Methomyl	Q	2737537	4939807	9115295	13452238	22783824	35397006	71931672
Flonicamid	Q	390564	802238	1626266	2324940	3876593	5915996	10725410
ODMS	Q	1662957	3110348	6149507	9205405	15380974	23845736	46047319
5-OH_TBZ	Q	1563076	3024611	6173603	9057919	14758723	22647279	41244357
Thiamethoxam	Q	473839	910788	1823911	2662361	4489338	6790735	12666340
Monocrotophos	Q	2676623	5322359	10272373	15475446	25680186	40444172	81911360
Imidacloprid	Q	1961674	3825066	7339375	11168910	18451926	28278482	53957135
Clothianidin	Q	714437	1377702	2705701	4075866	6843503	10397614	20034742
Thiabendazole	Q	2395330	4756375	9238564	13690129	23391302	35599065	70334577
3-OH_Carbofuran	Q	5631688	10797837	21032050	31558082	51838968	79183682	148721201
Acetamiprid	Q	770010	1489167	2851066	4289654	7143229	10810031	20289765
Cymoxanil	Q	377047	756131	1497988	2306694	3788308	5818639	11376041
Thiacloprid	Q	941310	1842377	3581247	5550042	9091552	13943056	27954176
Methidathion_OA	Q	5135521	9703625	18972892	29071643	47865654	73550478	139292777
Aldicarb	Q	1907088	3842466	7306696	11001829	17988401	28021382	55021609
Azinphos_Me_OA	Q	1653176	3209908	6311122	9387092	15079442	22160680	42137270
Metribuzin	Q	1382329	2590504	5034977	7543546	12429050	18563473	34333097
Simazine	Q	600586	1153840	2195023	3290653	5346202	7846242	13927839
Propoxur_(S)	Q	5511712	10559750	20690769	30998535	50521949	76084707	138563122
Pirimicarb	Q	20377224	38877301	76042738	114813774	183271544	281193286	538368936
Bendiocarb	Q	1600951	3142333	5931661	8910739	14446667	21691320	40789937
Carbofuran	Q	7314397	14139593	27712966	41779139	69378009	104524513	201180038
Fenamiphos_SO	Q	121310	301661	586312	869804	1528556	2435404	4766884
Tebuthiuron	Q	4394378	8642882	16607479	25289637	42667565	65032815	128681978
Carboxin	Q	6534810	12905965	25606866	38078875	63816950	99587153	190687947
Sulfentrazone	Q	279987	562967	1047875	1656952	2720819	4160971	8048554
Fenamiphos_SO2	Q	837268	1748158	3488544	5345562	8905884	13692958	26046963
Carbaryl	Q	4473316	8624723	17143920	25672675	42556304	65943386	131179439
Thiodicarb	Q	490260	1248479	3213413	4825393	7837944	12292695	23881048
Phorate_Sulfoxide	Q	4159733	7765608	15382246	23084301	38335816	58206610	113125292
Norflurazon_DM	Q	1052465	1986723	3983707	5792912	9714334	14483066	26957917

Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard; Note: Amounts displayed for internal standards represent the ISTD Response.
Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.
Manually Integrated

<div align="center">**Calibration Report**</div>

Lab Name:	Thermo Lab				Page 7 of 7
Instrument:	TQU00637		**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC			PDP_040511	
Batch:	011HPLR1		**Cali File:**	011HPLR1.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	2	L1XLOQ_HP031711	1XLOQ	L1XLOQ_HP031711	3/17/2011 6:06:33 PM	
5	3	L2XLOQ_HP031711	2XLOQ	L2XLOQ_HP031711	3/17/2011 6:26:29 PM	
5	4	L4XLOQ_HP031711	4XLOQ	L4XLOQ_HP031711	3/17/2011 6:46:23 PM	
5	5	L6XLOQ_HP031711	6XLOQ	L6XLOQ_HP031711	3/17/2011 7:06:17 PM	
5	6	L10XLOQ_HP031711	10XLOQ	L10XLOQ_HP031711	3/17/2011 7:26:11 PM	
5	7	L16XLOQ_HP031711	16XLOQ	L16XLOQ_HP031711	3/17/2011 7:46:05 PM	
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard; Note: Amounts displayed for internal standards represent the ISTD Response.

Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.

Manually Integrated

Calibration Density Report

Page 1 of 1

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	**Method:**	Preview2_EPA536-Triazines
User:	AMER\jamie.humphries		EPA536-Triazines
Batch:	Preview2	**Cali File:**	Preview2.calx

Chromatogram Report

Page 1 of 1

Lab Name:	Thermo Lab			
Instrument:	TQU00637	**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC		PDP_040511	
Batch:	011HPLR1	**Cali File:**	011HPLR1.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Compound Calibration Report

Compound Calibration Report

Lab Name:	Thermo Lab	
Instrument:	TQU00637	
User:	TQU00637RPC	
Batch:	011HPLR1	

Method:	011HPLR1_PDP_040511	
	PDP_040511	
Cal File	011HPLR1.calx	

Compound Name: Dinotefuran

Dinotefuran

$Y = -3.798e1X^2 + 8.978e4X$; R^2: 0.9995; Origin: Force; W: Equal; Area

Quadratic

Pass
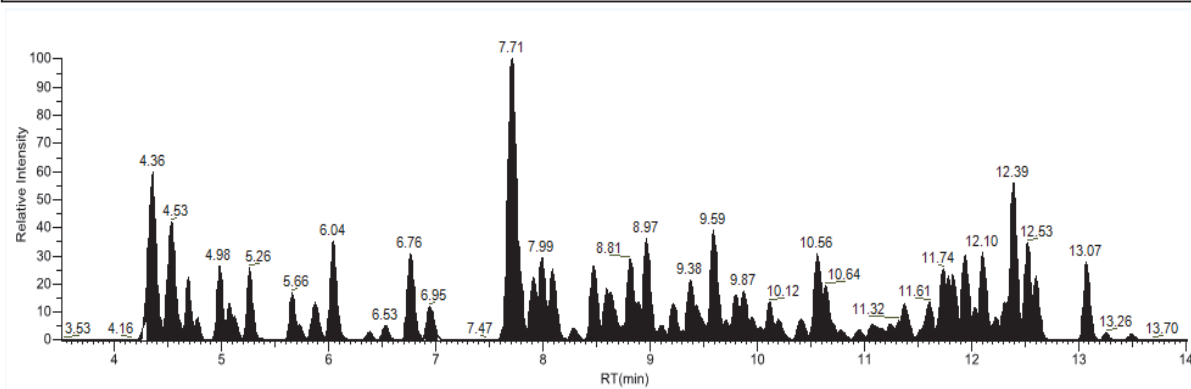
Level	Std Amount	Std Area	IS Amount	IS Area	Response factor	Calc Amt	Units	% CV	% RSD
1XLOQ	20.00	1957462			97873.106	22.01	PPB	N/A	N/A
2XLOQ	40.00	3754131			93853.284	42.58	PPB	N/A	N/A
4XLOQ	80.00	7124741			89059.260	82.22	PPB	N/A	N/A
6XLOQ	120.00	10430815			86923.457	122.54	PPB	N/A	N/A
10XLOQ	200.00	16753892			83769.461	204.27	PPB	N/A	N/A
16XLOQ	320.00	24286005			75893.767	311.59	PPB	N/A	N/A
32XLOQ	640.00	41994838			65616.934	642.34	PPB	N/A	N/A

Manually Integrated:

Calibration Flags: D =RSD, F = Response factor, R = R Squared, A = Amount

Page 2 of 2

Compound Calibration Report

Lab Name:	Thermo Lab	**Method:**	011HPLR1_PDP_040511	
Instrument:	TQU00637		PDP_040511	
User:	TQU00637\RPC	**Cal File**	011HPLR1.calx	
Batch:	011HPLR1			

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	2	L1XLOQ_HP031711	1XLOQ	L1XLOQ_HP031711	3/17/2011 6:06:33 PM	
5	3	L2XLOQ_HP031711	2XLOQ	L2XLOQ_HP031711	3/17/2011 6:26:29 PM	
5	4	L4XLOQ_HP031711	4XLOQ	L4XLOQ_HP031711	3/17/2011 6:46:23 PM	
5	5	L6XLOQ_HP031711	6XLOQ	L6XLOQ_HP031711	3/17/2011 7:06:17 PM	
5	6	L10XLOQ_HP031711	10XLOQ	L10XLOQ_HP031711	3/17/2011 7:26:11 PM	
5	7	L16XLOQ_HP031711	16XLOQ	L16XLOQ_HP031711	3/17/2011 7:46:05 PM	
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Manually Integrated:

Calibration Flags: D =RSD, F = Response factor, R = R Squared, A = Amount

Compound Calibration Report - Alternate

Lab Name: Thermo Lab
Instrument: TQU00637
User: TQU00637\RPC
Batch: 011HPLR1

Compound Calibration Report - Alternate

Method: 011HPLR1_PDP_040511
PDP_040511
Cal File 011HPLR1.calx

Compound Name: Dinotefuran

Dinotefuran
Y = –3.798e1X^2 + 8.978e4X; R^2: 0.9995; Origin: Force; W: Equal; Area

Quadratic
Pass

Level	File Name	Std Amount	Std Area	IS Amount	IS Area	Response factor	Calc Amt	Units	Min Range	Max Range	% RSD	Flags
1XLOQ	L1XLOQ_HP031711	20.00	1957462			97873.106	22.01	PPB	16.00	24.00	N/A	
2XLOQ	L2XLOQ_HP031711	40.00	3754131			93853.284	42.58	PPB	32.00	48.00	N/A	
4XLOQ	L4XLOQ_HP031711	80.00	7124741			89059.260	82.22	PPB	64.00	96.00	N/A	
6XLOQ	L6XLOQ_HP031711	120.00	10430815			86923.457	122.54	PPB	96.00	144.00	N/A	
10XLOQ	L10XLOQ_HP031711	200.00	16753892			83769.461	204.27	PPB	160.00	240.00	N/A	
16XLOQ	L16XLOQ_HP031711	320.00	24286005			75893.767	311.59	PPB	256.00	384.00	N/A	
32XLOQ	L32XLOQ_HP031711	640.00	41994838			65616.934	642.34	PPB	512.00	768.00	N/A	

Manually Integrated:

Calibration Flags: D =RSD, F = Response factor, R = R Squared, A = Amount

Compound Calibration Report - Alternate

Lab Name:	Thermo Lab
Instrument:	TQU00637
User:	TQU00637\RPC
Batch:	011HPLR1

Method:	011HPLR1_PDP_040511
	PDP_040511
Cal File	011HPLR1.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	2	L1XLOQ_HP031711	1XLOQ	L1XLOQ_HP031711	3/17/2011 6:06:33 PM	
5	3	L2XLOQ_HP031711	2XLOQ	L2XLOQ_HP031711	3/17/2011 6:26:29 PM	
5	4	L4XLOQ_HP031711	4XLOQ	L4XLOQ_HP031711	3/17/2011 6:46:23 PM	
5	5	L6XLOQ_HP031711	6XLOQ	L6XLOQ_HP031711	3/17/2011 7:06:17 PM	
5	6	L10XLOQ_HP031711	10XLOQ	L10XLOQ_HP031711	3/17/2011 7:26:11 PM	
5	7	L16XLOQ_HP031711	16XLOQ	L16XLOQ_HP031711	3/17/2011 7:46:05 PM	
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Manually Integrated:

Calibration Flags: D =RSD, F = Response factor, R = R Squared, A = Amount

Confirmation Report

Lab Name:	Thermo Lab			Page 1 of 1
Instrument:	TQU00637	**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC		PDP_040511	
Batch:	011HPLR1	**Cal File:**	011HPLR1.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Dinotefuran

	Injected	Sample
Conc:	642.34 PPB	642.34 PPB

Retention Time:	4.52
Area:	41994838
Height:	8893885

Quan Ion: 203.11->129.14
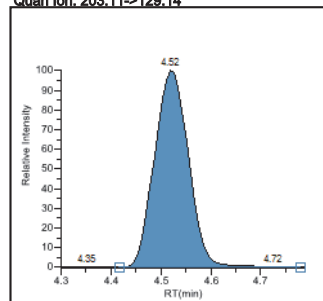
Calibration Curve
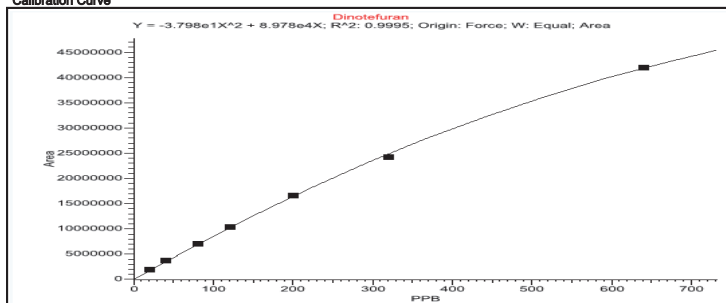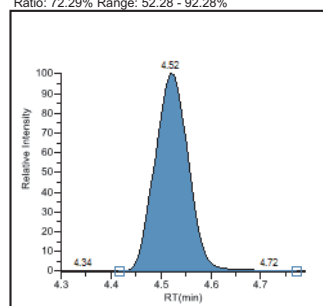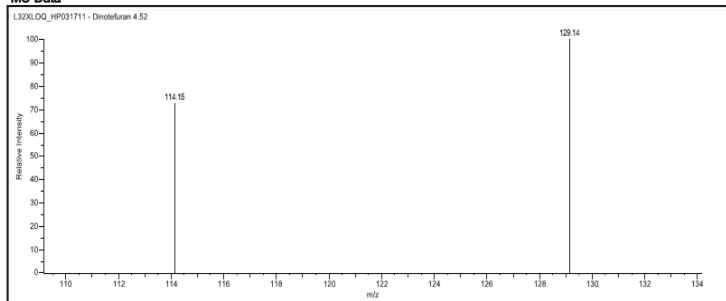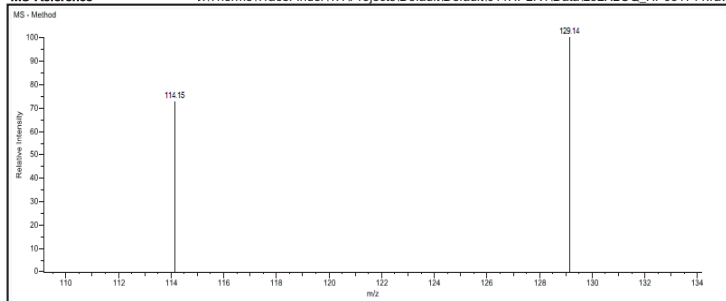
Dinotefuran
$Y = -3.798e1X^2 + 8.978e4X; R^2: 0.9995; Origin: Force; W: Equal; Area$

Qual Ion 1: 203.11->114.15
Ratio: 72.29% Range: 52.28 - 92.28%

MS-Data

MS-Reference   :\Thermo\TraceFinder\1.1\Projects\Default\Default\011HPLR1\Data\L32XLOQ_HP031711.raw

Overlay
RT: 4.52 | L32XLOQ_HP031711
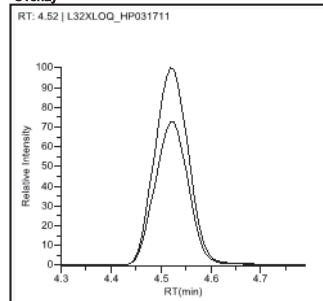
Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Confirmation Report 2

Lab Name:	Thermo Lab					
Instrument:	TQU00637		**Method:**	011HPLR1_PDP_040511		
User:	TQU00637\RPC			PDP_040511		
Batch:	011HPLR1		**Cali File:**	011HPLR1.calx		

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Compound Name:	Dinotefuran
Injected Conc:	642.34 PPB
Sample Conc:	642.34 PPB
Retention Time:	4.52
Area (Quan):	41994838
Height (Quan):	8893885
Qual Ratio 1:	Pass
Qual Ratio 2:	Pass

Quan Ion: 203.11->129.14
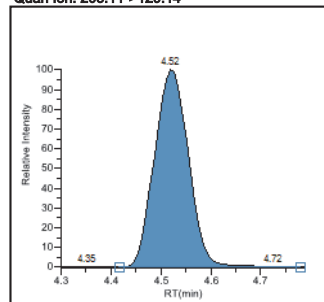
Qual Ion 1: 203.11->114.15

Ratio: 72.29% Range: 52.28 - 92.28%
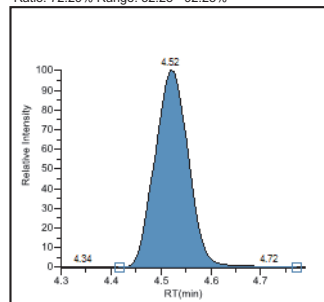
MS-Data
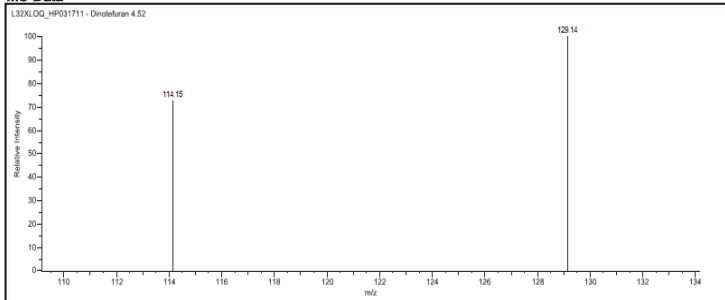
MS-Reference hermo\TraceFinder\1.1\Projects\Default\Default\011HPLR1\Data\L32XLOQ_HP031711.raw

Overlay

High Density Calibration Report

Lab Name:	Thermo Lab			Page 1 of 14
Instrument:	TQU00637	**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC		PDP_040511	
Batch:	011HPLR1	**Cali File:**	011HPLR1.calx	
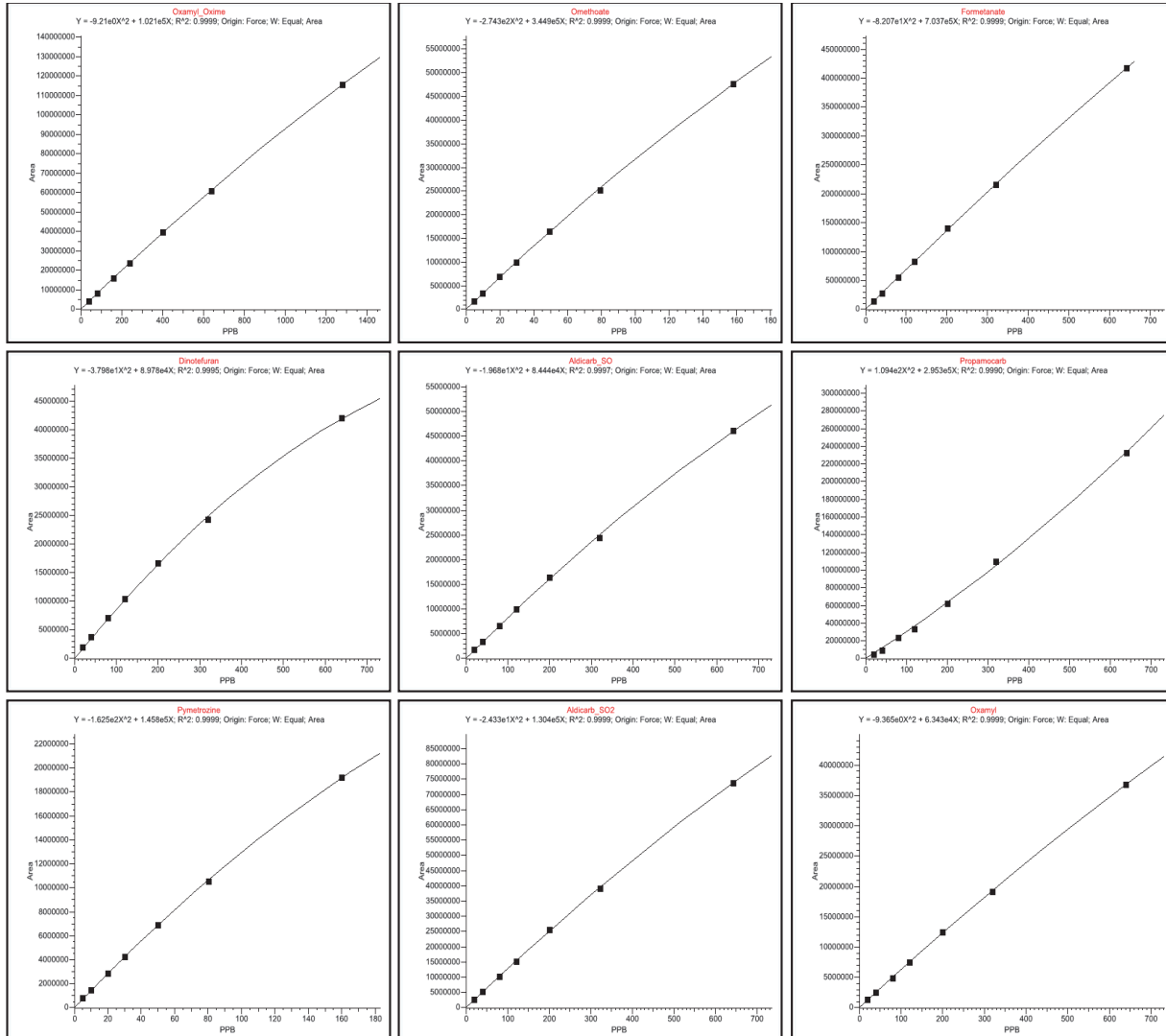
High Density Internal Standard Report

Lab name:	Thermo Fisher Laboratory				Page 1 of 1
Instrument:	Thermo Scientific Instrument		Method:	Drug_A_Drug_A	
User:	AMER\jamie.humphries			Drug_A	
Batch:	Drug_A		Cali File:	Drug_A.calx	

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
Amount: 5.581 ng/mL
TAmount: 6.000 ng/mL

Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %

Qual m/z: 488.20
Area: 32066
Ratio: 14.09 %
Range: 11.43 % - 17.14 %

Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

High Density Internal Standard Report Long

Lab name:	Thermo Fisher Laboratory			Page 1 of 1
Instrument:	Thermo Scientific Instrument	Method:	Drug_A_Drug_A	
User:	AMER\jamie.humphries		Drug_A	
Batch:	Drug_A	Cali File:	Drug_A.calx	

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

Drug_A
Quan m/z: 371.20
Total Area: 227568
Peak Area: 227568
RT: 1.95min (1.95)
Amount: 5.581 ng/mL
TAmount: 6.000 ng/mL
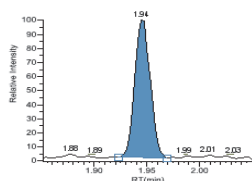
Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %

Qual m/z: 488.20
Area: 32066
Ratio: 14.09 %
Range: 11.43 % - 17.14 %

Int_Std
Quan m/z: 380.20
Total Area: 678044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Cutoff; n=Negative; b=Solvent blank; H=Hydrolysis

High Density Sample Report 1

High Density Sample Report 1

Lab Name:	Thermo Lab		Page 1 of 5
Instrument:	TQU00637	**Method:**	011HPLR1_PDP_040511
User:	TQU00637\RPC		PDP_040511
Batch:	011HPLR1	**Cali File:**	011HPLR1.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Oxamyl_Oxime
Quan m/z: 72.10
TotalArea: 115624994
Peak Area: 115624994
RT: 4.32min (4.31)
TAmount: 1280.00 PPB
Amount: 1280.93 PPB

Omethoate
Quan m/z: 183.04
TotalArea: 47692071
Peak Area: 47692071
RT: 4.34min (4.34)
TAmount: 158.00 PPB
Amount: 158.19 PPB

Formetanate
Quan m/z: 165.10
TotalArea: 418192129
Peak Area: 418192129
RT: 4.36min (4.35)
TAmount: 642.00 PPB
Amount: 642.46 PPB

Dinotefuran
Quan m/z: 129.14
TotalArea: 41994838
Peak Area: 41994838
RT: 4.52min (4.51)
TAmount: 640.00 PPB
Amount: 642.34 PPB

Aldicarb_SO
Quan m/z: 132.05
TotalArea: 46055255
Peak Area: 46055255
RT: 4.52min (4.52)
TAmount: 640.00 PPB
Amount: 641.29 PPB

Propamocarb
Quan m/z: 102.00
TotalArea: 233040768
Peak Area: 233040768
RT: 4.53min (4.53)
TAmount: 640.00 PPB
Amount: 638.19 PPB

Pymetrozine
Quan m/z: 105.10
TotalArea: 19185279
Peak Area: 19185279
RT: 4.57min (4.56)
TAmount: 160.00 PPB
Amount: 160.15 PPB

Aldicarb_SO2
Quan m/z: 148.04
TotalArea: 73839209
Peak Area: 73839209
RT: 4.69min (4.68)
TAmount: 643.00 PPB
Amount: 643.38 PPB

Oxamyl
Quan m/z: 90.00
TotalArea: 36777897
Peak Area: 36777897
RT: 4.78min (4.77)
TAmount: 640.00 PPB
Amount: 640.38 PPB

Methomyl
Quan m/z: 88.10
TotalArea: 71931672
Peak Area: 71931672
RT: 4.98min (4.98)
TAmount: 1280.00 PPB
Amount: 1281.62 PPB

Flonicamid
Quan m/z: 203.00
TotalArea: 10725410
Peak Area: 10725410
RT: 5.04min (5.03)
TAmount: 1920.00 PPB
Amount: 1920.54 PPB

ODMS
Quan m/z: 169.00
TotalArea: 46047319
Peak Area: 46047319
RT: 5.07min (5.07)
TAmount: 320.00 PPB
Amount: 320.14 PPB

5-OH_TBZ
Quan m/z: 147.10
TotalArea: 41244357
Peak Area: 41244357
RT: 5.12min (5.11)
TAmount: 320.00 PPB
Amount: 320.15 PPB

Thiamethoxam
Quan m/z: 181.10
TotalArea: 12666340
Peak Area: 12666340
RT: 5.13min (5.12)
TAmount: 160.00 PPB
Amount: 160.12 PPB

Monocrotophos
Quan m/z: 193.00
TotalArea: 81911360
Peak Area: 81911360
RT: 5.26min (5.26)
TAmount: 320.00 PPB
Amount: 320.27 PPB

Imidacloprid
Quan m/z: 209.06
TotalArea: 53957135
Peak Area: 53957135
RT: 5.66min (5.65)
TAmount: 640.00 PPB
Amount: 640.52 PPB

Clothianidin
Quan m/z: 169.10
TotalArea: 20034742
Peak Area: 20034742
RT: 5.73min (5.71)
TAmount: 320.00 PPB
Amount: 320.31 PPB

Thiabendazole
Quan m/z: 131.10
TotalArea: 70334577
Peak Area: 70334577
RT: 5.88min (5.86)
TAmount: 320.00 PPB
Amount: 320.35 PPB

3-OH_Carbofuran
Quan m/z: 163.08
TotalArea: 148721201
Peak Area: 148721201
RT: 6.04min (6.03)
TAmount: 640.00 PPB
Amount: 640.60 PPB

Acetamiprid
Quan m/z: 126.10
TotalArea: 20289765
Peak Area: 20289765
RT: 6.08min (6.07)
TAmount: 160.00 PPB
Amount: 160.15 PPB

Cymoxanil
Quan m/z: 128.14
TotalArea: 11376041
Peak Area: 11376041
RT: 6.38min (6.37)
TAmount: 641.00 PPB
Amount: 641.64 PPB

Thiacloprid
Quan m/z: 126.10
TotalArea: 27954176
Peak Area: 27954176
RT: 6.53min (6.51)
TAmount: 160.00 PPB
Amount: 160.25 PPB

Methidathion_OA
Quan m/z: 145.00
TotalArea: 139292777
Peak Area: 139292777
RT: 6.76min (6.75)
TAmount: 640.00 PPB
Amount: 640.35 PPB

Aldicarb
Quan m/z: 116.05
TotalArea: 55021609
Peak Area: 55021609
RT: 6.95min (6.93)
TAmount: 640.00 PPB
Amount: 640.68 PPB

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

High Density Sample Report 1 Long

Lab Name:	Thermo Lab			Page 1 of 10
Instrument:	TQU00637	**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC		PDP_040511	
Batch:	011HPLR1	**Cali File:**	011HPLR1.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Oxamyl_Oxime
Quan m/z: 72.10
TotalArea: 115624994
Peak Area: 115624994
RT: 4.32min (4.31)
TAmount: 1280.00 PPB
Amount: 1280.93 PPB

Omethoate
Quan m/z: 183.04
TotalArea: 47692071
Peak Area: 47692071
RT: 4.34min (4.34)
TAmount: 158.00 PPB
Amount: 158.19 PPB

Formetanate
Quan m/z: 165.10
TotalArea: 418192129
Peak Area: 418192129
RT: 4.36min (4.35)
TAmount: 642.00 PPB
Amount: 642.46 PPB

Dinotefuran
Quan m/z: 129.14
TotalArea: 41994838
Peak Area: 41994838
RT: 4.52min (4.51)
TAmount: 640.00 PPB
Amount: 642.34 PPB

Aldicarb_SO
Quan m/z: 132.05
TotalArea: 46055255
Peak Area: 46055255
RT: 4.52min (4.52)
TAmount: 640.00 PPB
Amount: 641.29 PPB

Propamocarb
Quan m/z: 102.00
TotalArea: 233040768
Peak Area: 233040768
RT: 4.53min (4.53)
TAmount: 640.00 PPB
Amount: 638.19 PPB

Pymetrozine
Quan m/z: 105.10
TotalArea: 19185279
Peak Area: 19185279
RT: 4.57min (4.56)
TAmount: 160.00 PPB
Amount: 160.15 PPB

Aldicarb_SO2
Quan m/z: 148.04
TotalArea: 73839209
Peak Area: 73839209
RT: 4.69min (4.68)
TAmount: 643.00 PPB
Amount: 643.38 PPB

Oxamyl
Quan m/z: 90.00
TotalArea: 36777897
Peak Area: 36777897
RT: 4.78min (4.77)
TAmount: 640.00 PPB
Amount: 640.38 PPB

Methomyl
Quan m/z: 88.10
TotalArea: 71931672
Peak Area: 71931672
RT: 4.98min (4.98)
TAmount: 1280.00 PPB
Amount: 1281.62 PPB

Flonicamid
Quan m/z: 203.00
TotalArea: 10725410
Peak Area: 10725410
RT: 5.04min (5.03)
TAmount: 1920.00 PPB
Amount: 1920.54 PPB

ODMS
Quan m/z: 169.00
TotalArea: 46047319
Peak Area: 46047319
RT: 5.07min (5.07)
TAmount: 320.00 PPB
Amount: 320.14 PPB

Flag legend: LOD<J<LOQ; i=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

High Density Sample Report 2

High Density Sample Report 2

Lab Name:	Thermo Lab			Page 1 of 10
Instrument:	TQU00637	Method:	011HPLR1_PDP_040511	
User:	TQU00637\RPC		PDP_040511	
Batch:	011HPLR1	Call File:	011HPLR1.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Oxamyl_Oxime
Quan m/z: 72.10
TotalArea: 115624994
Peak Area: 115624994
RT: 4.32min (4.31)
Amount: 1280.93 PPB
TAmount: 1280.00 PPB

Qual m/z: 90.06
Area: 8374691
Range: 0.00 % - 27.25 %

Omethoate
Quan m/z: 183.04
TotalArea: 47692071
Peak Area: 47692071
RT: 4.34min (4.34)
Amount: 158.19 PPB
TAmount: 158.00 PPB

Qual m/z: 125.03
Area: 35413809
Ratio: 74.26 %
Range: 53.49 % - 93.49 %

Formetanate
Quan m/z: 165.10
TotalArea: 418192129
Peak Area: 418192129
RT: 4.36min (4.35)
Amount: 642.46 PPB
TAmount: 642.00 PPB

Qual m/z: 120.00
Area: 33553959
Ratio: 8.02 %
Range: 0.00 % - 28.09 %

Dinotefuran
Quan m/z: 129.14
TotalArea: 41994838
Peak Area: 41994838
RT: 4.52min (4.51)
Amount: 642.34 PPB
TAmount: 640.00 PPB

Qual m/z: 114.15
Area: 30358995
Ratio: 72.29 %
Range: 52.28 % - 92.28 %

Aldicarb_SO
Quan m/z: 132.05
TotalArea: 46055255
Peak Area: 46055255
RT: 4.52min (4.52)
Amount: 641.29 PPB
TAmount: 640.00 PPB

Qual m/z: 89.10
Area: 30100441
Range: 48.87 % - 88.87 %

Propamocarb
Quan m/z: 102.00
TotalArea: 233040768
Peak Area: 233040768
RT: 4.53min (4.53)
Amount: 638.19 PPB
TAmount: 640.00 PPB

Qual m/z: 144.00
Area: 97076996
Ratio: 41.66 %
Range: 19.38 % - 59.38 %

Pymetrozine
Quan m/z: 105.10
TotalArea: 19185279
Peak Area: 19185279
RT: 4.57min (4.56)
Amount: 160.15 PPB
TAmount: 160.00 PPB

Qual m/z: 78.11
Area: 2406306
Ratio: 12.54 %
Range: 0.00 % - 32.18 %

Aldicarb_SO2
Quan m/z: 148.04
TotalArea: 73839209
Peak Area: 73839209
RT: 4.69min (4.68)
Amount: 643.38 PPB
TAmount: 643.00 PPB

Qual m/z: 86.00
Area: 43918555
Ratio: 59.48 %
Range: 40.81 % - 80.81 %

Oxamyl
Quan m/z: 90.00
TotalArea: 36777897
Peak Area: 36777897
RT: 4.78min (4.77)
Amount: 640.38 PPB
TAmount: 640.00 PPB

Qual m/z: 219.70
Area: 3371404
Range: 0.00 % - 31.32 %

Methomyl
Quan m/z: 88.10
TotalArea: 71931672
Peak Area: 71931672
RT: 4.98min (4.98)
Amount: 1281.62 PPB
TAmount: 1280.00 PPB

Qual m/z: 106.03
Area: 73876485
Ratio: 102.70 %
Range: 85.41 % - 125.41 %

Flonicamid
Quan m/z: 203.00
TotalArea: 10725410
Peak Area: 10725410
RT: 5.04min (5.03)
Amount: 1920.54 PPB
TAmount: 1920.00 PPB

Qual m/z: 98.00
Area: 5546720
Ratio: 51.72 %
Range: 32.77 % - 72.77 %

ODMS
Quan m/z: 169.00
TotalArea: 46047319
Peak Area: 46047319
RT: 5.07min (5.07)
Amount: 320.14 PPB
TAmount: 320.00 PPB

Qual m/z: 108.95
Area: 21960912
Ratio: 47.69 %
Range: 29.22 % - 69.22 %

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank
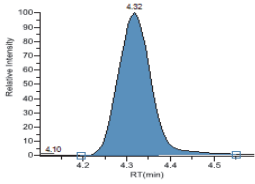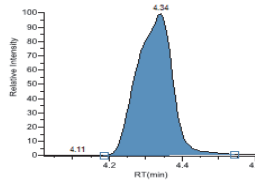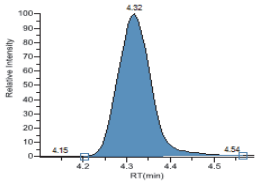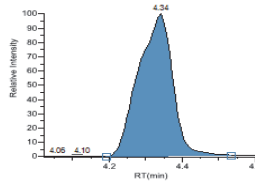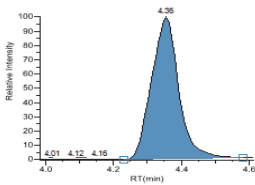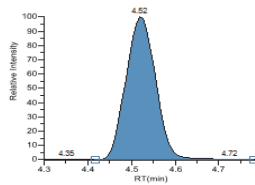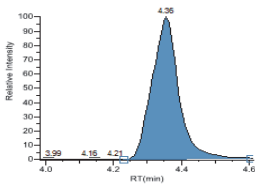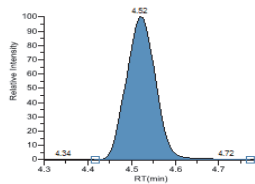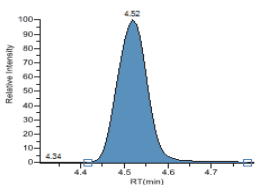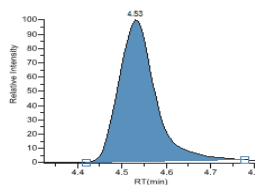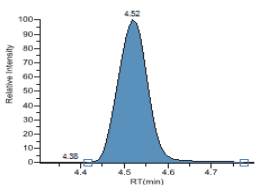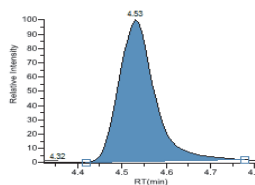
High Density Sample Report 2 Long

Lab Name:	Thermo Lab		Page 1 of 20
Instrument:	TQU00637	**Method:**	011HPLR1_PDP_040511
User:	TQU00637\RPC		PDP_040511
Batch:	011HPLR1	**Cali File:**	011HPLR1.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Oxamyl_Oxime
Quan m/z: 72.10
TotalArea: 115624994
Peak Area: 115624994
RT: 4.32min (4.31)
Amount: 1280.93 PPB
TAmount: 1280.00 PPB

Area: 8374691
Ratio: 7.24 %
Range: 0.00 % - 27.25 %

Omethoate
Quan m/z: 183.04
TotalArea: 47692071
Peak Area: 47692071
RT: 4.34min (4.34)
Amount: 158.19 PPB
TAmount: 158.00 PPB

Qual m/z: 125.03
Area: 35413809
Ratio: 74.26 %
Range: 53.49 % - 93.49 %

Formetanate
Quan m/z: 165.10
TotalArea: 418192129
Peak Area: 418192129
RT: 4.36min (4.35)
Amount: 642.46 PPB
TAmount: 642.00 PPB

Area: 33553959
Ratio: 8.02 %
Range: 0.00 % - 28.09 %

Dinotefuran
Quan m/z: 129.14
TotalArea: 41994838
Peak Area: 41994838
RT: 4.52min (4.51)
Amount: 642.34 PPB
TAmount: 640.00 PPB

Qual m/z: 114.15
Area: 30358995
Ratio: 72.29 %
Range: 52.28 % - 92.28 %

Aldicarb_SO
Quan m/z: 132.05
TotalArea: 46055255
Peak Area: 46055255
RT: 4.52min (4.52)
Amount: 641.29 PPB
TAmount: 640.00 PPB

Area: 30100441
Ratio: 65.36 %
Range: 48.87 % - 88.87 %

Propamocarb
Quan m/z: 102.00
TotalArea: 233040768
Peak Area: 233040768
RT: 4.53min (4.53)
Amount: 638.19 PPB
TAmount: 640.00 PPB

Qual m/z: 144.00
Area: 97076996
Ratio: 41.66 %
Range: 19.38 % - 59.38 %

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

High Density Sample Report 3

High Density Sample Report 3

Lab Name:	Thermo Lab					Page 1 of 20
Instrument:	TQU00637			**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC				PDP_040511	
Batch:	011HPLR1			**Cali File:**	011HPLR1.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Oxamyl_Oxime
Quan m/z: 72.10
TotalArea: 115624994
Peak Area: 115624994
RT: 4.32 min (4.31)
Amount: 1280.93 PPB
TAmount: 1280.00 PPB

Qual m/z: 90.06
Area: 8374691
Ratio: 7.24 %
Range: 0.00 % - 27.25 %

Omethoate
Quan m/z: 183.04
TotalArea: 47692071
Peak Area: 47692071
RT: 4.34 min (4.34)
Amount: 158.19 PPB
TAmount: 158.00 PPB

Qual m/z: 125.03
Area: 35413809
Ratio: 74.26 %
Range: 53.49 % - 93.49 %

Formetanate
Quan m/z: 165.10
TotalArea: 418192129
Peak Area: 418192129
RT: 4.36 min (4.35)
Amount: 642.46 PPB
TAmount: 642.00 PPB

Qual m/z: 120.00
Area: 33553959
Ratio: 8.02 %
Range: 0.00 % - 28.09 %

Dinotefuran
Quan m/z: 129.14
TotalArea: 41994838
Peak Area: 41994838
RT: 4.52 min (4.51)
Amount: 642.34 PPB
TAmount: 640.00 PPB

Qual m/z: 114.15
Area: 30358995
Ratio: 72.29 %
Range: 52.28 % - 92.28 %

Aldicarb_SO
Quan m/z: 132.05
TotalArea: 46055255
Peak Area: 46055255
RT: 4.52 min (4.52)
Amount: 641.29 PPB
TAmount: 640.00 PPB

Qual m/z: 89.10
Area: 30100441
Ratio: 65.36 %
Range: 48.87 % - 88.87 %

Propamocarb
Quan m/z: 102.00
TotalArea: 233040768
Peak Area: 233040768
RT: 4.53 min (4.53)
Amount: 638.19 PPB
TAmount: 640.00 PPB

Qual m/z: 144.00
Area: 97076996
Ratio: 41.66 %
Range: 19.38 % - 59.38 %

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank;
s=Solvent blank

High Density Sample Report 3 Long

				Page 1 of 40

Lab Name: Thermo Lab

Instrument: TQU00637

User: TQU00637\RPC

Batch: 011HPLR1

Method: 011HPLR1_PDP_040511

PDP_040511

Cali File: 011HPLR1.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Oxamyl_Oxime

Quan m/z: 72.10

TotalArea: 115624994

Peak Area: 115624994

RT: 4.32min (4.31)

Amount: 1280.93 PPB

TAmount: 1280.00 PPB

Qual m/z: 90.06

Area: 8374691

Ratio: 7.24 %

Range: 0.00 % - 27.25 %

Omethoate

Quan m/z: 183.04

TotalArea: 47692071

Peak Area: 47692071

RT: 4.34min (4.34)

Amount: 158.19 PPB

TAmount: 158.00 PPB

Qual m/z: 125.03

Area: 35413809

Ratio: 74.26 %

Range: 53.49 % - 93.49 %

Formetanate

Quan m/z: 165.10

TotalArea: 418192129

Peak Area: 418192129

RT: 4.36min (4.35)

Amount: 642.46 PPB

TAmount: 642.00 PPB

Qual m/z: 120.00

Area: 33553959

Ratio: 8.02 %

Range: 0.00 % - 28.09 %

Internal Standard Summary Report

Internal Standard Summary Report

Lab name:	Thermo Fisher Laboratory					
Instrument:	Thermo Scientific Instrument		Method:	Drug_A_Drug_A		
User:	AMER\jamie.humphries			Drug_A		
Batch:	Drug_A		Cali File:	Drug_A.calx		

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	cal 1 = 6 ng/mL	cal_1	level 1		4/17/2008 5:05:47 PM	

Compound	Std Response	Min	Max	Sample Response
Int_Std	655596	327798(50.00%)	983394(150.00%)	678044

Compound	Std RT	Min	Max	Sample RT
Int_Std	1.93	1.68(-0.25)	2.18(+0.25)	1.93

* = Fail   Manually integrated [＿＿＿＿＿]

Ion Ratio Failure Report

Ion Ratio Failure Report

Lab Name:	Thermo Lab
Instrument:	TQU00637
User:	TQU00637RPC
Batch:	011HPLR1

Method:	011HPLR1_PDP_040511
	PDP_040511
Call File:	011HPLR1.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

Compound	Response	Quan Ion	Quan Response	Qual Ion	Qual Response	Ratio	Range
Sethoxydim_I	Area	178.02	4002074	220.05	2971396	74.25	34.09-74.09
Buprofezin	Area	106.10	39861606	201.10	168167286	421.88	369.96-409.96

Manually Integrated

Manual Integration Report

Lab Name:	Thermo Lab					
Instrument:	TQU00637			**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC				PDP_040511	
Batch:	011HPLR1			**Call File:**	011HPLR1.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

3-OH_Carbofuran
m/z: 163.08
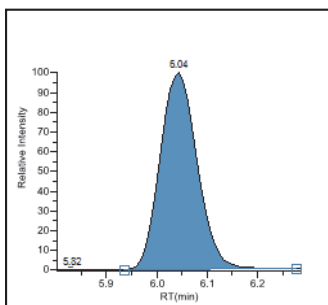
Method Integration

Apex RT:	6.04
Height:	30046630
Area:	148721201
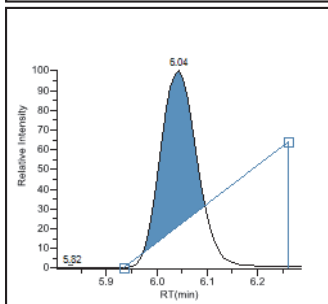
Manual Integration

Apex RT:	6.04
Height:	23956657
Area:	94907912

Method Report

Method name:	Drug_A_Drug_A	Page number:	Page 1 of 11
Master method name:	Drug_A		
Current calibration file:	Drug_A.calx		
Assay type:	Drug_A	Ion range calc method:	Average
Inj vol:	1.000		
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid		

Compound Identification:

Compound	Quan mass	RT	Window	View width	Use as reference	Reference compound
Int_Std	380.20	1.94	10.00	0.40	Yes	
Drug_A	371.20	1.95	10.00	0.40	No	Int_Std

Method name:	Drug_A_Drug_A	Page number:	Page 2 of 11
Master method name:	Drug_A		
Current calibration file:	Drug_A.calx		
Assay type:	Drug_A	Ion range calc method:	Average
Inj vol:	1.000		
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid		

Compound Calibration:

Compound	Response	Calibration	Curve type	Weighting	Origin	Units	ISTD Name	ISTD Units
Drug_A	Area	Internal	Linear	Equal	Ignore	ng/mL	Int_Std	ng/mL

Method name:	Drug_A_Drug_A	Page number:	Page 3 of 11
Master method name:	Drug_A		
Current calibration file:	Drug_A.calx		
Assay type:	Drug_A	Ion range calc method:	Average
Inj vol:	1.000		
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid		

QAQC Limits:

Compound	LOD	LOQ	Cutoff	ULOL	Carryover
Drug_A	1.500	1.500	15.000	1000.000	1000.000

Method name:	Drug_A_Drug_A	Page number:	Page 4 of 11
Master method name:	Drug_A		
Current calibration file:	Drug_A.calx		
Assay type:	Drug_A	Ion range calc method:	Average
Inj vol:	1.000		
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid		

Groups:

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 5 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid				

Report options:

Quan report options

Report concentration:	Always
Decimal places to be reported:	3
Show chromatogram on Quantitation report:	True
Display valid compounds only	False

Qual options

Sort Qual results by:	Search Index
Enable limiting peaks:	False
Limit Peaks to :	

User interface options

Shade row when sample is outside of evaluation criteria:	False
Separate ion overlay display :	True
Use alternative calibration report format:	False
Display quan flags and legend	True

ToxLab Forms settings

Quan flags

Flag values below LOD:	True
Flag values below LOQ:	True
Flag values above Cutoff:	True
Flag values above ULOL:	True
Flag values above Carryover:	True
Flag values between LOD and LOQ:	True

Calculated amount option

Calculate concentration as:	Truncated

Tune time tracking options

Enable tune time tracking:	False
Tune file lifetime (hrs):	N/A

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 6 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid				

QAQC Calibration:

Compound	Max RSD (%)	Min RF	R^2 threshold	Max amt diff (%)
Drug_A	20.00	0.00	0.990	20.000

Method Report

Method name:	Drug_A_Drug_A			Page number:	Page 7 of 11
Master method name:	Drug_A				
Current calibration file:	Drug_A.calx				
Assay type:	Drug_A	Ion range calc method:	Average		
Inj vol:	1.000				
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid				

QAQC QC Check:

Compound	Max RF diff (%)	Min RF
Drug_A	20.00	0.000

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 8 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid			

QAQC Negative:

Compound	Criterion	Max value
Drug_A	% of LOD	1.500

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 9 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid			

QAQC ISTD:

Compound	Min recovery (%)	Max recovery (%)	Min RT (-min)	Max RT (+min)
Int_Std	50.00	150.00	0.25	0.25

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 10 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid			

QAQC Solvent Blank:

Compound	Method	Upper Limit %
Int_Std	None	
Drug_A	Quan Ion RT	0

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 11 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x3, Ext: EPA536 Triazines, Ext: Anabolic Steroids, Ext: Melamine and Cyanuric Acid			

QAQC Hydrolysis:

CompoundName	EvaluationMethod	LowerLimit	UpperLimit
Drug_A	Range	15.000	23.000

Method Validation Report

Lab name:	Thermo Fisher Laboratory		Page 1 of 3
Instrument:	Thermo Scientific Instrument	**Method:**	Preview2_EPA536-Triazines
User:	AMER\jamie.humphries		EPA536-Triazines
Batch:	Preview2	**Cali File:**	Preview2.calx

Method Validation Summary

Compound	Avg Conc	Theo Conc	% Diff	Min Conc	Max Conc	% RSD	Max % RSD	
DIA D-5	295652					0.00		IS
DIA	0.358	0.500	-28.34	0.250	0.750	0.00	20.00	
DEA D-7	1778658					0.00		IS
DEA	0.602	0.500	20.45	0.250	0.750	0.00	20.00	
Cyanazine D-5	2224244					0.00		IS
Cyanazine	0.565	0.500	12.90	0.250	0.750	0.00	20.00	
Simazine D-10	505462					0.00		IS
Simazine	0.607	0.500	21.49	0.250	0.750	0.00	20.00	
Atrazine D-5	2334865					0.00		IS
Atrazine	0.512	0.500	2.46	0.250	0.750	0.00	20.00	
Propazine	0.757	0.500	51.41	0.250	0.750	0.00	20.00 <<<	
Propazine D-14	272050					0.00		IS

Manually integrated [   ]   **<<< = Failure**

Method Validation Report

Lab name:	Thermo Fisher Laboratory		Page 2 of 3
Instrument:	Thermo Scientific Instrument	**Method:**	Preview2_EPA536-Triazines
User:	AMER\jamie.humphries		EPA536-Triazines
Batch:	Preview2	**Cali File:**	Preview2.calx

Method Validation Report Data

Compound	1
DIA D-5	295652
DIA	0.358
DEA D-7	1778658
DEA	0.602
Cyanazine D-5	2224244
Cyanazine	0.565
Simazine D-10	505462
Simazine	0.607
Atrazine D-5	2334865
Atrazine	0.512
Propazine	0.757
Propazine D-14	272050

Manually integrated [ ]

<<< = Failure

Method Validation Report

Lab name:	Thermo Fisher Laboratory			Page 3 of 3
Instrument:	Thermo Scientific Instrument	**Method:**	Preview2_EPA536-Triazines	
User:	AMER\jamie.humphries		EPA536-Triazines	
Batch:	Preview2	**Cali File:**	Preview2.calx	

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:10	SampleID003	500ppt-003	N/A	D003	6/26/2007 10:18:49 PM	New Dilutions 6/26/2007 F

Manually integrated ☐   **<<< = Failure**

MSMSD Report

Lab name:	Thermo Fisher Laboratory		Page 1 of 1
Instrument:	Thermo Scientific Instrument	**Method:**	Preview2_EPA536-Triazines
User:	AMER\jamie.humphries		EPA536-Triazines
Batch:	Preview2	**Cali File:**	Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:1	SampleID021	DACTTest001	N/A	D021	6/27/2007 11:42:07 AM	New dilution of DACT

SampleID021

Compound	Unknown Conc	Spike Amt	MS Conc	% Rec	Lower Limit %	Upper Limit %	Rec Fails
DIA	0.000	0.500	0.000	0.00	50.00	150.00	0
DEA	0.000	0.500	0.000	0.00	50.00	150.00	0
Cyanazine	0.000	0.500	0.000	0.00	50.00	150.00	0
Simazine	0.000	0.500	0.000	0.00	50.00	150.00	0
Atrazine	0.000	0.500	0.000	0.00	50.00	150.00	0
Propazine	0.000	0.500	0.000	0.00	50.00	150.00	0

Quality Control Report

Lab name:	Thermo Fisher Laboratory					Page 1 of 1
Instrument:	Thermo Scientific Instrument		Method:	Drug_A_Drug_A		
User:	AMER\jamie.humphries			Drug_A		
Batch:	Drug_A		Cali File:	Drug_A.calx		

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
7	qc 40% = 6 ng/mL	qc_40	level 40		4/17/2008 5:07:57 PM	

Compound	Curve Type	Daily RF	Mean RF	Min RF	RF %D	Max RF % D	QC amt	Calc amt	Amt %D	Max Amt %D	Flag
Drug_A	L		0.000				6.000	5.603	-6.62	20.00	Pass

Internal standard summary:

Compound	Std Response	Min	Max	Sample Response
Int_Std	655596	327798(50.00%)	983394(150.00%)	639922
	Std RT	Min	Max	Sample RT
Int_Std	1.93	1.68(-0.25)	2.18(+0.25)	1.93

Manually integrated [   ] * = Fail;Curve Type: A=Average RF; L=Linear; Q=Quadratic;R=Recovery limits exceeded

Quantitation Report

Quantitation Report

Lab Name:	Thermo Lab		Method:	011HPLR1_PDP_040511
Instrument:	TQU00637			PDP_040511
User:	TQU00637RPC			
Batch:	011HPLR1		Call File:	011HPLR1.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	8	L32XLOQ_HP031711	32XLOQ	L32XLOQ_HP031711	3/17/2011 8:06:03 PM	

C:\Thermo\TraceFinder1.1\Projects\Default\Default\011HPLR1\Data\L32XLOQ_HP031711.raw
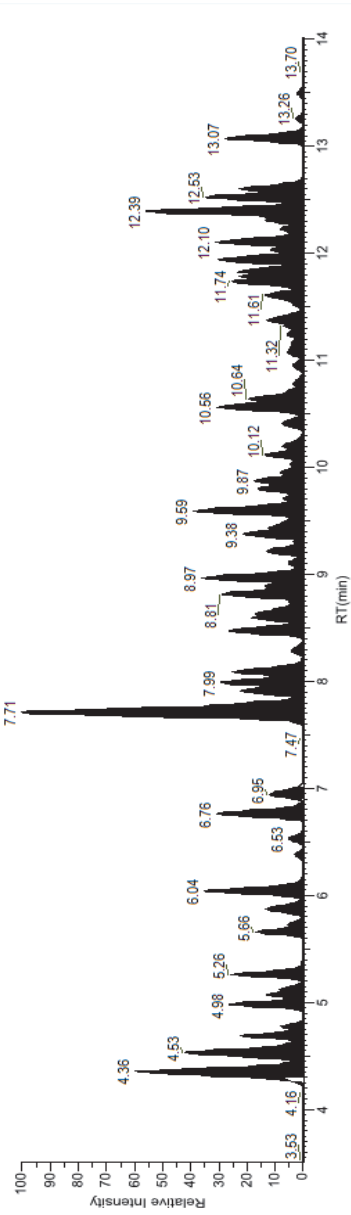
Surrogates

	RT	Qlon	Response	Average RF/Response Ratio	Injected Conc	Units	Calculated Conc	Units	Curve Type	Flags
Propoxur_(S)	7.70	111.10	138563122	0.00	640.78	PPB	640.78	PPB	Quadratic	

Target Compounds

	RT	Qlon	Response	Average RF/Response Ratio	Injected Conc	Units	Calculated Conc	Units	Curve Type	Flags
Oxamyl_Oxime	4.32	72.10	115624994	0.00	1280.93	PPB	1280.93	PPB	Quadratic	
Omethoate	4.34	183.04	47692071	0.00	158.19	PPB	158.19	PPB	Quadratic	
Formetanate	4.36	165.10	418192129	0.00	642.46	PPB	642.46	PPB	Quadratic	
Dinotefuran	4.52	129.14	41994838	0.00	642.34	PPB	642.34	PPB	Quadratic	
Aldicarb_SO	4.52	132.05	46055255	0.00	641.29	PPB	641.29	PPB	Quadratic	
Propamocarb	4.53	102.00	233040768	0.00	638.19	PPB	638.19	PPB	Quadratic	
Pymetrozine	4.57	105.10	19185279	0.00	160.15	PPB	160.15	PPB	Quadratic	
Aldicarb_SO2	4.69	148.04	73839209	0.00	643.38	PPB	643.38	PPB	Quadratic	
Oxamyl	4.78	90.00	36777897	0.00	640.38	PPB	640.38	PPB	Quadratic	

Manually Integrated

Flag legend: LOD=J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Quantitation Report - 2

MS Integ Params:	PDP_040511
Quant Method:	011HPLR1_PDP_040511
Title:	Assay
Last Update:	6/2/2011 9:47:56 AM
Data Acq Method:	PDP_010411
Operator:	TQU0637tRPC
Instr:	TQU00637
Response Via:	011HPLR1.calx

Quantitation Report - 2

Quant Time:	4/19/2011 3:39:05 PM
Data File:	L32XLOQ_HP031711
Acq On:	3/17/2011 8:06:03 PM
Sample:	L32XLOQ_HP031711
Comment:	
Vial:	5
Multiplr:	1.000
Quant Results File:	C:\Thermo\TraceFinder1.1\Projects\Default\Default\011HPLR1\Data\L32XLOQ_HP031711.rsx

Surrogates

Compound Name	RT	Qion	Response	Conc	Units	Dev (min)	Spike Amt	Recovery	Flags
28 Propoxur_(S)	7.70	111.10	138563122	640.78	PPB	0.01	40.00	1601.95	

Target Compounds

Compound Name	RT	Qion	Response	Conc	Units	Dev (min)	Flags
1 Oxamyl_Oxime	4.32	72.10	115624994	1280.93	PPB	0.01	
2 Omethoate	4.34	183.04	47692071	158.19	PPB	0.01	
3 Formetanate	4.36	165.10	418192129	642.46	PPB	0.01	
4 Dinotefuran	4.52	129.14	41994838	642.34	PPB	0.01	
5 Aldicarb_SO	4.52	132.05	46055255	641.29	PPB	0.00	
6 Propamocarb	4.53	102.00	233040768	638.19	PPB	0.00	
7 Pymetrozine	4.57	105.10	19185279	160.15	PPB	0.01	
8 Aldicarb_SO2	4.69	148.04	73839209	643.38	PPB	0.01	
9 Oxamyl	4.78	90.00	36777897	640.38	PPB	0.01	
10 Methomyl	4.98	88.10	71931672	1281.62	PPB	0.01	
11 Flonicamid	5.04	203.00	10725410	1920.54	PPB	0.01	
12 ODMS	5.07	169.00	46047319	320.14	PPB	0.00	
13 5-OH_TBZ	5.12	147.10	41244357	320.15	PPB	0.01	
14 Thiamethoxam	5.13	181.10	12666340	160.12	PPB	0.01	
15 Monocrotophos	5.26	193.00	81911360	320.27	PPB	0.01	
16 Imidacloprid	5.66	209.06	53957135	640.52	PPB	0.01	
17 Clothianidin	5.73	169.10	20034742	320.31	PPB	0.01	
18 Thiabendazole	5.88	131.10	70334577	320.35	PPB	0.01	
19 3-OH_Carbofuran	6.04	163.08	94907912	537.87	PPB	0.01	—

Manually integrated

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit; D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Quantitation Report - 2

Target Compounds

Compound Name	RT	QIon	Response	Conc	Units	Dev (min)	Flags
52 Pyrimethanil	9.31	107.00	15176188	320.09	PPB	0.02	
53 Azoxystrobin	9.38	372.10	118737360	160.00	PPB	0.01	
54 Fenobucarb	9.43	95.00	68157960	320.10	PPB	0.01	
55 Linuron	9.48	160.10	31079975	639.90	PPB	0.02	
56 Dimethomorph_I	9.55	301.10	8049921	92.89	PPB	0.00	
57 Fenamidone	9.58	92.10	11883329	320.00	PPB	0.01	
58 Methiocarb	9.59	169.00	188527803	644.38	PPB	0.01	
59 Boscalid	9.70	307.10	16765638	320.43	PPB	0.01	
60 Fludioxonil	9.72	158.00	11536347	640.67	PPB	0.02	
61 Mandipropamid	9.70	328.21	36436634	320.31	PPB	0.00	
62 Sethoxydim_I	9.74	178.02	4002074	22.38	PPB	0.02	I
63 Promecarb	9.80	109.02	72069251	320.27	PPB	0.01	
64 Flutolanil	9.81	262.00	59962817	160.05	PPB	0.01	
65 Fluopicolide	9.83	173.00	29652715	160.16	PPB	0.01	
66 Methoxyfenozide	9.87	149.00	68163623	319.95	PPB	0.01	
67 Dimethomorph_II	9.88	301.10	24249261	227.43	PPB	0.00	
68 Clethodim_I	9.94	164.09	30569148	512.02	PPB	0.02	
69 Triadimefon	9.95	197.00	34892978	640.89	PPB	0.01	
70 Imiprothrin_I	10.02	151.10	9384265	68.41	PPB	0.01	
71 Myclobutanil	10.03	70.10	20569388	639.97	PPB	0.02	
72 Bifenazate	10.12	170.10	47077629	319.44	PPB	0.01	
73 Triadimenol	10.16	70.00	17384509	1924.45	PPB	0.02	
74 Spirotetramat	10.20	216.15	28050091	159.99	PPB	0.01	
75 Imiprothrin_II	10.22	123.09	10608234	248.90	PPB	0.01	I
76 Cyazofamid	10.41	108.00	50568848	642.61	PPB	0.03	
77 Fenbuconazole	10.54	125.00	26717669	640.05	PPB	0.02	
78 Chlorpyrifos_OA	10.56	278.00	125363774	641.05	PPB	0.02	
79 Uniconazole	10.61	125.08	9243171	2559.62	PPB	0.02	
80 Diflubenzuron	10.62	158.02	27577198	1280.31	PPB	0.03	
81 Tebufenozide	10.64	133.00	114645763	320.30	PPB	0.03	
82 Flubendiamide	10.71	408.07	20125339	320.06	PPB	0.02	

L32XLOQ_HP031711

Flag legend: LOD=<J=<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Page 3 of 65
6/2/2011 11:40:51AM

Manually integrated   PDP_040511

Solvent Blank Report

Solvent Blank Report

Page 1 of 4

Lab Name:	Thermo Lab				
Instrument:	TQU00637		**Method:**	011HPLR1_PDP_040511	
User:	TQU00637\RPC			PDP_040511	
Batch:	011HPLR1		**Cali File:**	011HPLR1.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
5	1	LLOD_HP031711	N/A	LLOD_HP031711	3/17/2011 5:46:30 PM	

Surrogates	RT	QIon	Response	Method	Upper Limit
Propoxur_(S)	7.69	111.10	1553885	None	

Target Compounds	RT	QIon	Response	Method	Upper Limit
Oxamyl_Oxime	4.32	72.10	1291350	None	
Omethoate	4.34	183.04	540508	None	
Formetanate	4.35	165.10	4408552	None	
Dinotefuran	4.52	129.14	608336	None	
Aldicarb_SO	4.51	132.05	538697	None	
Propamocarb	4.53	102.00	750180	None	
Pymetrozine	4.56	105.10	231305	None	
Aldicarb_SO2	4.68	148.04	842061	None	
Oxamyl	4.77	90.00	408081	None	
Methomyl	4.98	88.10	973424	None	
Flonicamid	5.05	203.00	121206	None	
ODMS	5.07	169.00	495002	None	
5-OH_TBZ	5.12	147.10	427244	None	
Thiamethoxam	5.12	181.10	149534	None	
Monocrotophos	5.26	193.00	820046	None	
Imidacloprid	5.66	209.06	611636	None	
Clothianidin	5.71	169.10	216332	None	
Thiabendazole	5.87	131.10	692435	None	
3-OH_Carbofuran	6.03	163.08	1717688	None	
Acetamiprid	6.07	126.10	239740	None	
Cymoxanil	6.38	128.14	108494	None	
Thiacloprid	6.51	126.10	299625	None	
Methidathion_OA	6.75	145.00	1537066	None	
Aldicarb	6.94	116.05	563453	None	
Azinphos_Me_OA	6.95	132.00	485885	None	
Metribuzin	7.65	187.16	437173	None	
Simazine	7.69	104.10	182755	None	
Pirimicarb	7.71	182.08	6037105	None	

Manually Integrated

Isotopic Pattern Details

For target screening, the TraceFinder application calculates an isotopic pattern score based on the settings in the method. The application displays this score in the Data Review view. This appendix describes the isotopic distribution concepts and provides calculation details with examples for the isotopic pattern score.

Contents

- Isotopic Distribution in Exact Mass Spectra
- Isotopic Pattern Score Calculations

Isotopic Distribution in Exact Mass Spectra

To determine the elemental compositions for target screening, the TraceFinder application uses an isotopic pattern matching algorithm that considers the isotope accurate mass and intensity ratios. Using a single exact mass, usually the monoisotopic mass of a measured isotope pattern, the application calculates all possible elemental compositions that lie within a mass tolerance window. You can filter this list of possible elemental compositions and narrow the results by using the natural isotopic distribution of elements.

Natural Isotopic Distribution

The following table lists the natural isotopic distribution of the most common elements.

Table 121. Natural isotopic distribution (Sheet 1 of 2)

Element	Isotope	Isotope order	Exact mass	Mass difference	Abundance (%)
Hydrogen	^{1}H	A0	1.0078		99.9985
	^{2}H	A1	2.014102	+1.006302	0.015
Carbon	^{12}C	A0	12.0		98.890
	^{13}C	A1	13.003355	+1.003355	1.110
Nitrogen	^{14}N	A0	14.003074		99.634
	^{15}N	A1	15.00109	+0.998016	0.366

Table 121. Natural isotopic distribution (Sheet 2 of 2)

Element	Isotope	Isotope order	Exact mass	Mass difference	Abundance (%)
Oxygen	^{16}O	A0	15.994915		99.762
	^{17}O	A1	16.999132	+1.004217	0.038
	^{18}O	A2	17.999161	+2.004246	0.200
Fluorine	^{19}F	A0	18.99840		100
Phosphorus	^{31}P	A0	30.971459		100
Sulfur	^{32}S	A0	31.972071		95.020
	^{33}S	A1	32.971459	+0.999388	0.750
	^{34}S	A2	33.967867	+1.995796	4.210
	^{36}S	A4	35.967081	+3.995010	0.020

where

- A0 represents the monoisotopic peak, which is the most abundant and usually the isotope with the lowest mass.

  For example: ^{1}H, ^{12}C, ^{14}N, ^{16}O, ^{19}F, ^{31}P, and ^{32}S

- A1 represents the isotope where one atom in the molecule is statistically replaced by one other atom approximately 1 amu heavier.

  For example: ^{2}H, ^{13}C, ^{15}N, ^{17}O, and ^{33}S

- A2 represents the isotope where:

  Two atoms in the molecule are statistically replaced by two other atoms, each approximately 1 amu heavier.

  –or–

  One atom is replaced by another atom approximately 2 amu heavier.

  For example: ^{18}O and ^{34}S

- A3 represents the isotope where:

  Three atoms in the molecule are statistically replaced by three other atoms, each approximately 1 amu heavier.

  –or–

  One atom is replaced by another atom approximately 1 amu heavier and one atom is replaced by another atom approximately 2 amu heavier.

  –or–

  One atom is replaced by another atom approximately 3 amu heavier.

- A4 represents the isotope where:

  Four atoms in the molecule are statistically replaced by four other atoms, each approximately 1 amu heavier.

  –or–

  Two atoms are replaced by two other atoms, each approximately 1 amu heavier, and one atom is replaced by another atom approximately 2 amu heavier.

  –or–

  One atom is replaced by another atom approximately 2 amu heavier, and one other atom is replaced by another atom approximately 2 amu heavier.

  –or–

  One atom is replaced by another atom approximately 1 amu heavier, and one atom is replaced by another atom approximately 3 amu heavier.

  –or–

  One atom is replaced by another atom approximately 4 amu heavier.

  For example: ^{36}S

- Mass difference is the difference in mass between the A0 isotope and another isotope (A1, A2, A3, A4, and so on) of the same element.

- Abundance is the percentage of occurrence of each isotope normally in nature.

In the following figure, the *x* axis shows the mass difference of A1 relative to the monoisotopic peak (A0) of the ^{13}C, ^{15}N, and ^{33}S isotopes. The *y* axis shows relative abundance in intensity.

Figure 159. Mass difference and abundance of A1 relative to A0
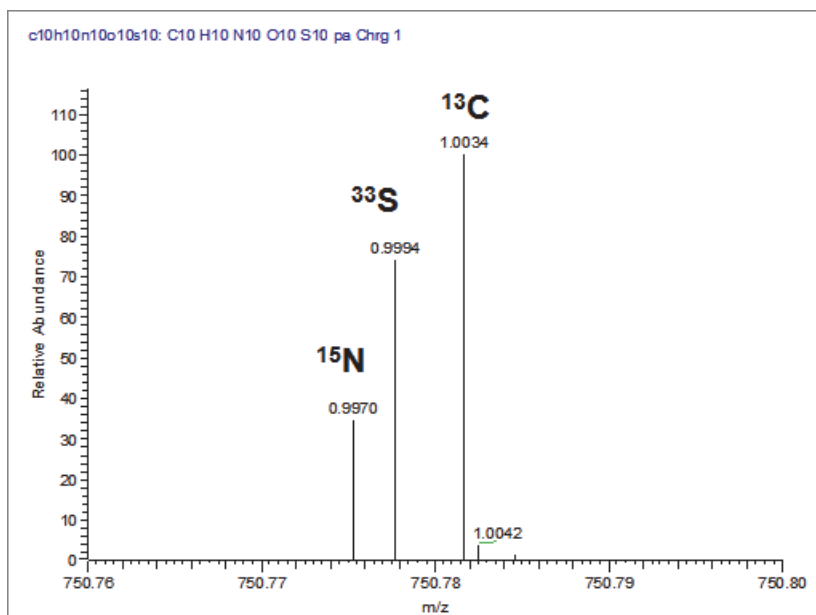
In the following figure, the *x* axis shows the mass difference of A2 relative to the monoisotopic peak (A0) of the ^{18}O, ^{34}S, and $^{13}C2$ isotopes. The *y* axis shows relative abundance in intensity.

Figure 160. Mass difference and abundance of A2 relative to A0
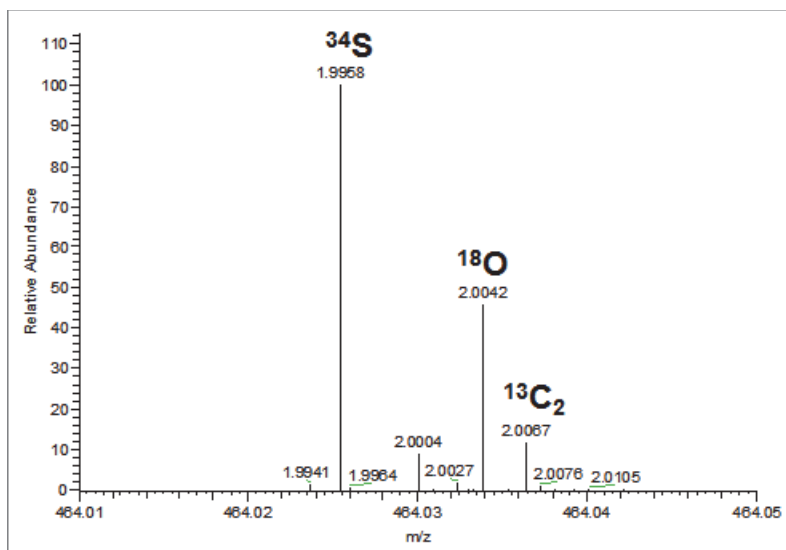
Note For a particular isotopic spectrum, the mass difference is always the same between the A0 isotope and the other isotopes (A1, A2, and so on) of each specific element, but the intensity varies according to the composition of the molecule—that is, the number of each element in the molecule.

Isotopic Pattern Score Calculations

The TraceFinder application follows the same isotopic distribution logic as described in "Isotopic Distribution in Exact Mass Spectra" on page 633, but in a different order and with numerical limits and scores to optimize automatic processing. After the TraceFinder application determines the possible elemental compositions for a particular compound of interest, it calculates a expected isotope pattern for each elemental composition candidate and an isotopic pattern score to represent the fit between the expected and measured isotope patterns.

The following example describes the isotopic pattern score data and provides the score calculation details for one specific data set.

Data Set Example

For this example, use the "Pesticides Screening Example" data set installed in the …\TraceFinderData folder. In the Data Review view, select the **Apple_PosHCD__40_5_01** sample and the **Metribuzin** target compound.

For this compound, note that the Isotopic Pattern Score column shows 90% and the Num Isotopes Matched column shows "2 of 3" in the Compounds pane in the Data Review. The compound's formula is C8H14N4OS and its adduct is H, so the modeled isotopic pattern is C8H15N4OS.

Figure 161. Isotopic data for Metribuzin

In the Spectrum pane, click the Isotopes tab and zoom in to view the expected isotopic pattern spectrum compared to the acquired, measured spectrum. The resulting isotopic pattern score should correlate to a visual inspection of the difference between the expected isotope display and the measured display for the target compound.

Figure 162. Isotopic pattern spectra (stacked)
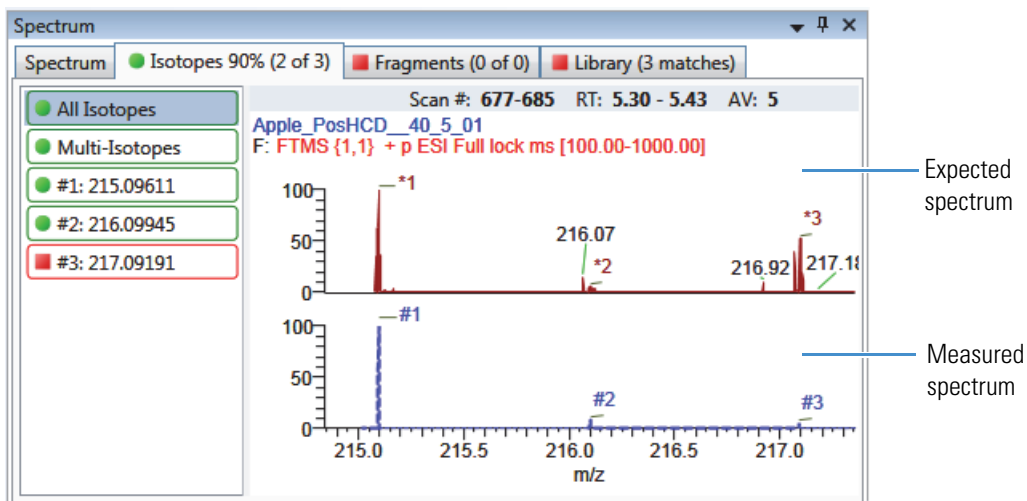
For this example, the processing method used to process the data contains the following isotopic pattern settings for target screening:

- Fit threshold = 90%

- Allowed Mass Deviation = 5 ppm

- Allowed Intensity Deviation = 10%

- Use Internal Mass Calibration = Cleared

The data for the **Metribuzin** compound is as follows:

Measured	Expected
A0 *m/z* = 215.09602	A0 *m/z* = 215.09611
A0 Noise = 1482	–
A0 intensity = 4.75E4	A0 intensity = 8.55E5

Because the measured and the expected spectra have different intensities, the spectral noise threshold must proportionally apply to the expected spectrum to decide which peaks are expected in the measured data.

Noise threshold (expected) = *Noise of A0 (measured) × Intensity of A0 (expected) ÷ Intensity of A0 (measured)*

Following the previous formula, the expected noise threshold is 1482 × 8.55E5 ÷ 4.75E4 = 2.6676E4.

The expected ions in the measured spectrum are those whose intensities are above the expected noise threshold. The following tables lists the ions in the expected spectrum. A "✓" in the Above Threshold column indicates the expected ions.

Table 122. Ions in expected spectrum

Isotope order	m/z (expected)	Intensity (expected)	Above threshold	Present in measured spectrum
A0	215.09611	8.55E5	✓	Yes
A1	216.09945	7.50E4	✓	Yes
A2	217.09191	3.86E4	✓	Yes
A3	218.09521	3.39E3		No

Calculating Mass and Intensity Deviations

The expected number of ions is 3, as shown by those ions with a "✓" in the Above Threshold column of the Ions in expected spectrum table. These are the ions you focus on for the scoring calculations. This number "3" shows as the value of *y* in the Num Isotopes Matched column of the Compounds pane in the Data Review. It indicates the number of expected isotopic pattern peaks based on the Fourier transform (FT) noise in the spectrum.

In this case, you expect to see the three most intense expected peaks in the measured spectrum. The masses of those peaks are (in order of intensity from high to low): 215.09611, 216.09945, and 217.09191. When the measured spectrum is more intense or the noise level is lower, you find more peaks passing the noise threshold and expected in the measured spectrum, eventually including other isotopic peaks.

The following table shows the mass deviation (delta *m/z*) data for each of the expected ions.

Table 123. Mass deviation data for the expected ions

Isotope order	*m/z* (expected)	*m/z* (measured)	Delta *m/z* (ppm)
A0	215.09611	215.09602	–0.42
A1	216.09945	216.09879	–3.05
A2	217.09191	217.09712	24

where

Delta *m/z* (ppm) = 1 000 000 × ([*m/z (measured) – m/z (expected)*] ÷ *m/z (expected)*)

For example:

1 000 000 × ([216.09879 – 216.09945] ÷ 216.09945)] = –3.05 ppm

> **Tip** You can see the expected, measured, and delta *m/z* values on the Isotopes page of the Spectrum pane. The MS page (see "Isotopic pattern spectra (stacked)" on page 638) displays the profile measured *m/z* values, whereas the Isotopes page displays the centroid measured *m/z* values, which might be different.
>
> If you want more precision, you can see extra decimal digits for the A0 *m/z* values in an exported data file.

If the absolute value of the Delta *m/z* is less than 5 ppm (the Allowed Mass Deviation value set in the processing method), the TraceFinder application determines that this ion is found—that is, the ion is present in the measured spectrum. For this data set example, the application finds only the A0 and A1 ions, so "2" shows as the value of *x* in the Num Isotopes Matched column of the Compounds pane in the Data Review. The application does not find the A2 expected ion because the absolute value of its Delta *m/z* of 24 ppm is much higher than 5 ppm.

> **Note** You can see from zooming in on the isotopic pattern spectra (see "Isotopic pattern spectra (stacked)" on page 638) that there are measured peaks in the measured spectrum closely corresponding to the first two expected ions, but there is not a measured peak closely corresponding to the 217.09191 expected ion.

The following table lists the intensity deviation (delta intensity) data for each of the expected ions, relative to the A0 ion's expected intensity of 8.55E5 and measured intensity of 4.75E4.

Table 124. Intensity deviation data for the expected ions

Isotope order	*m/z* (expected)	Intensity (expected)	Relative intensity (expected, %)	Intensity (measured)	Relative intensity (measured, %)	Delta intensity
A0	215.09611	8.55E5	100	4.75E4	100	0
A1	216.09945	7.50E4	8.77	8.75E3	18.42	9.65
A2	217.09191	3.86E4	4.51	3.47E4	73.05	68.54

where

- Relative intensity (expected and measured) values are derived from the isotopic pattern spectra (see "Isotopic pattern spectra (stacked)" on page 638). Each value is a percentage of the isotope's intensity relative to the A0 ion's intensity.

  For example: 7.50E4 ÷ 8.55E5 = 8.77%

- Delta intensity = *Relative intensity (measured) – Relative intensity (expected)*

  For example: 18.42 – 8.77 = 9.65

In this example, the absolute values of the Delta *m/z* for the A0 and A1 ions (see " Mass deviation data for the expected ions" on page 640) are both less than the Allowed Mass Deviation of 5 ppm; therefore, the application considers that these two ions are present in the measured spectrum. The delta intensity of the A1 isotope ion is close to the Allowed Intensity Deviation of 10% and the delta intensity of the A2 isotope ion is much higher (see " Intensity deviation data for the expected ions" on page 641).

The TraceFinder application determines the isotopic pattern score value from a combination of the mass and intensity deviations between the expected and the measured spectra. In this case, the application reduces the isotopic pattern score value down to 90% from 100% to reflect the marginal quality of the intensities of the A1 and A2 isotopes and to penalize for not finding the A2 isotope.

Calculating Isotopic Pattern Score

To score the fit for an isotopic pattern, the TraceFinder application calculates each expected ion's fit and then combines the individual fit scores, weighted by their expected intensities.

For each expected ion peak, the application measures the *m/z* and intensity differences between the expected and the measured patterns. It then normalizes those differences (normalized deviation values) to the maximum allowed mass and intensity deviation values set in the processing method. The application then sums the normalized differences by vector addition (see "Vector sum of intensity (I) and mass (M) deviations" on page 642).

Figure 163. Measured and expected patterns
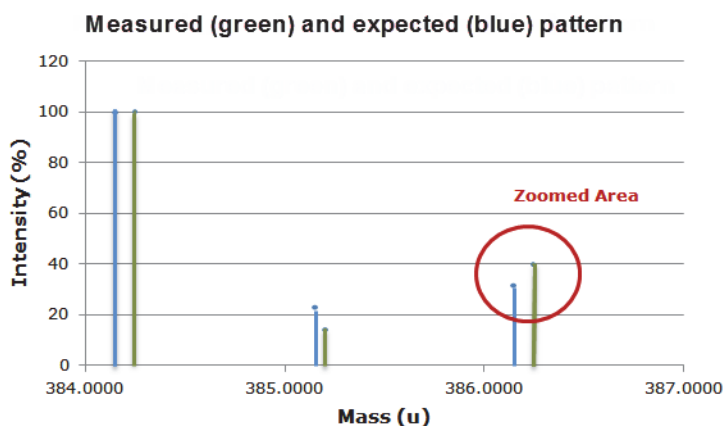
Figure 164. Vector sum of intensity (I) and mass (M) deviations
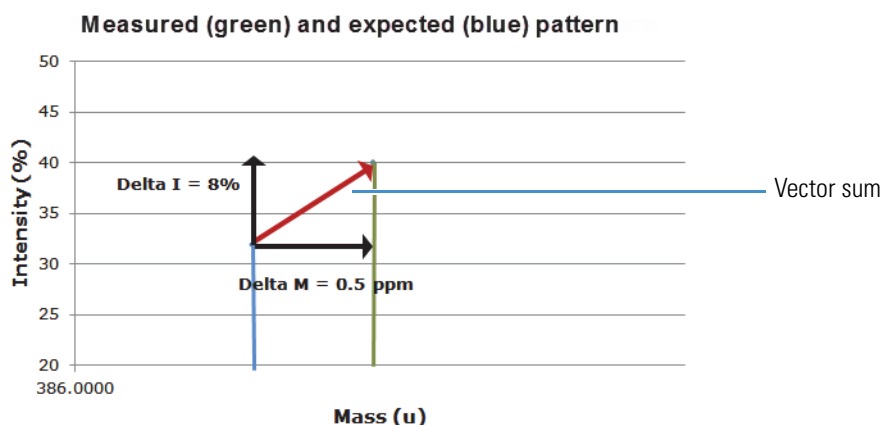
This example starts first with the intensity deviations. The Allowed Intensity Deviation value set in the processing method is 10%, so this is the normalization value. As shown in " Intensity deviation data for the expected ions" on page 641, the delta intensity value for the A1 isotope is close to 10%, resulting in a normalized intensity deviation close to 1.0.

Normalized Intensity Deviation

The following table lists the normalized intensity deviation data for each of the expected ions.

Table 125. Normalized intensity deviation data for the expected ions

Isotope order	*m/z* (expected)	Delta intensity	Allowed intensity deviation (%)	Normalized intensity deviation
A0	215.09611	0	10	0 ÷ 10 = 0.0
A1	216.09945	9.65	10	9.65 ÷ 10 = 0.965
A2	217.09191	68.54	10	68.54 ÷ 10 = 6.854

Next are the mass deviations. For mass deviations, you can control two settings in the processing method:

- The first setting is the Allowed Mass Deviation that functions as an outer limit in the same way as the Allowed Intensity Deviation functions as a limit for the intensity.

- The second setting is the Use Internal Mass Calibration check box. If you do not select this check box in the method, then the application considers any mass value within 2 ppm of the expected *m/z* as a perfect match (no deviation). If you select this check box, then the application considers only a mass value within 1 ppm of the expected *m/z* as a perfect match.

In this example, the Allowed Mass Deviation value set in the processing method is 5 ppm and the Use Internal Mass Calibration check box is cleared. The mass normalization is a bit more complex than the intensity normalization because mass values < 2 ppm (Use Internal Mass Calibration setting) from the expected *m/z* are considered to have no deviation from theory; however, for values between 2 ppm and 5 ppm (Allowed Mass Deviation value) from the expected *m/z*, the normalized deviation varies from 0 to 1.

The calculated normalized mass deviation value is as follows:

- 0 if absolute value (*Delta m/z*) < 2 ppm

  where 2 ppm is the value from the Use Internal Mass Calibration setting.

- [absolute value (*Delta m/z*) – 2 ppm] ÷ (5 ppm – 2 ppm) if absolute value (*Delta m/z*) ≥ 2 ppm

  where 2 ppm is the value from the Use Internal Mass Calibration setting and 5 ppm is the Allowed Mass Deviation value.

In this case, the absolute value of the mass deviation for the A0 ion is less than 2 ppm; therefore, its normalized mass deviation value is 0.

Normalized Mass Deviation

The following table lists the normalized mass deviation data for each of the expected ions.

Table 126. Normalized mass deviation for each of the expected ions

Isotope order	m/z (expected)	m/z (measured)	Delta m/z (ppm)	Internal calibration (ppm)	Allowed mass deviation (ppm)	Normalized mass deviation
A0	215.09611	306.10356	–0.42	2	5	0
A1	216.09945	307.10691	–3.05	2	5	0.35
A2	217.09191	308.11324	24	2	5	7.33

For example: $[(24 - 2)] \div (5 - 2) = 7.33$

To calculate the combined deviations, the application uses the Pythagorean theorem to calculate the vector sum of the normalized deviations. The calculation for the vector sum is as follows:

Vector sum = Square root [(*Normalized intensity deviation*)^2 + (*Normalized mass deviation*)^2].

However, if the vector sum > 1 then set it to 1.

Calculated Vector Sum

The following table lists the vector sum data for each of the expected ions.

Table 127. Calculated vector sum

Isotope order	m/z (expected)	Normalized intensity deviation	Normalized mass deviation	Vector sum
A0	215.09611	0	0	0
A1	216.09945	0.965	0.35	1
A2	217.09191	6.854	7.33	1

To calculate the final score, you must weigh the vector sum values and then express the result as a percentage value. Each ion's weighting contribution to the final isotopic pattern score is proportional to its intensity.

Weighting Factor Calculations

The following table lists the weighting factor of each of the three expected ions.

Table 128. Weighting factor calculations

Isotope order	m/z (expected)	Intensity (expected)	Weighting factor for final score
A0	215.09611	8.55E5	0.8827
A1	216.09945	7.50E4	0.0774
A2	217.09191	3.86E4	0.0399
		Sum = 9.686E5	Sum = 1.000

The weighting factor of each individual ion = *Intensity of each ion ÷ Sum of intensities of all expected ions*

For example: 8.55E5 ÷ 9.686E5 = 0.8827

When not all of the expected ions are present in the measured spectrum, the application applies a penalty value (1, 2, or 4) to the weighted deviation of each missing ion, lowering the final isotopic pattern score even further. The penalty value depends on how strong the ion signal is expected to be in the measured spectrum. For the A2 ion that is not found, the application sets its penalty to a value of 1, causing its vector sum value of 1 in Table 127 to be replaced with the penalty value of 1 in Table 129. In this case, it is the same number, but for other cases, the penalty value might be different from the vector sum value.

Calculated Isotopic Pattern Score

The following table lists the calculated isotopic pattern score using the weighting factors.

Table 129. Calculated isotopic pattern score

Isotope order	m/z (expected)	Deviation (vector sum or penalty)	Weighting factor	Weighted deviation
A0	215.09611	0 (vector sum)	0.8827	0
A1	216.09945	1 (vector sum)	0.0774	0.0774
A2	217.09191	1 (penalty)	0.0399	0.0399
				Sum = 0.12

where

- Weighted deviation of each individual ion = *Deviation × Weighting factor*

  For example: 1 × 0.0774 = 0.0774

- Isotopic pattern score = 100% × (1.0 – *Sum of all weighted deviation values*)

  For this example, the calculated isotopic pattern score of 100% × (1.0 – 0.12) is 88%, which is close to the 90% score displayed in the application.

> **Note** Use these calculations to approximate the score displayed in the application. The calculated score might not match exactly the score in the application because some internal calculation details are not listed here or there is discrepancy due to decimal digit rounding.
>
> In certain cases, closely matching isotopes exist because heavier isotopes contribute to the isotopic pattern observed in the mass spectra. For example, the isotopes 206.0941 and 206.1006 result from the contribution of one heavier isotope of carbon and one heavier isotope of nitrogen, respectively, together making up the split A1 isotopic peak. When the application performs isotopic pattern scoring, this situation appears as a main isotopic peak with a smaller peak to the side whose *m/z* is included in the calculations.

Finding the Noise Value

❖ **To find the noise value associated with a mass spectral peak**

1. On the Isotopes page of the Spectrum pane, to view the expected spectrum stacked above the measured spectrum, right-click the spectrum plot area and choose **Display Stack Spectra** from the shortcut menu.

2. Zoom in to the peak of interest.

   As an example, see "Isotopic pattern spectra (stacked)" on page 638 for the compound **Metribuzin**.

3. To view the averaged noise value (N) for a peak in the measured spectrum, right-click the spectrum plot area and choose **Show Noise Label** from the shortcut menu.
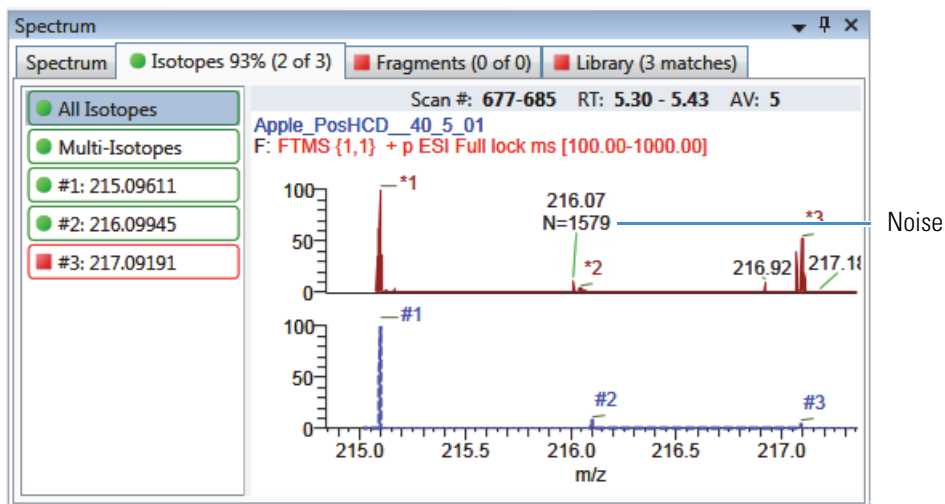
In this example, the averaged noise value for the peak is 1579.

Using Copy Down and Fill Down

This appendix describes the Copy Down and Fill Down commands that you can use to make entering column values easier.

- Use the Fill Down command for the Filename, Sample Name, Sample ID, and Vial Position columns.

- Use the Copy Down command for the Sample Type, Vial Position, Injection Volume, Conv Factor, Level, Comment, and other columns.

Follow these procedures:

- To automatically copy column values

- To automatically enter sequential column values

- To use Copy Down or Fill Down for a range of samples

❖ **To automatically copy column values**

1. Select the cell whose value you want to copy to all cells below it.

   Observe the difference between a selected and nonselected cell.

2. Right-click and choose **Copy Down** from the shortcut menu.

   The value is copied to all rows below the selected row.

❖ **To automatically enter sequential column values**

1. Enter a value for the first row of the fill down sequence.

   This does not have to be the first sample row. You can begin the fill down procedure from any row in the sequence.

2. Select the cell whose value is the first in the fill down sequence.

    Observe the difference between a selected and nonselected cell.

    Selected ——
Vial position
1

    Not selected ——
Vial position
1
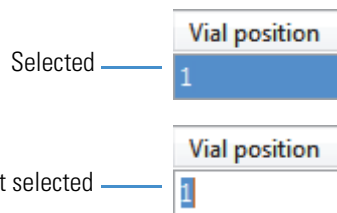
3. Right-click and choose **Fill Down** from the shortcut menu.

    The application enters sequential column values starting with the value in the selected row and ending with the last row in the column.

    You can repeatedly use the Fill Down command to create multiple sequences.

Vial position
A:A1
A:A2
A:A1
A:A2
A:A1
A:A2
A:A3
A:A4

    When you use the Fill Down command for the Vial Position column with an autosampler configured, the TraceFinder application knows the number of vial positions configured in your autosampler and numbers the positions accordingly.

Vial position
A:A1
A:A2
A:A3
A:A4
A:A5
A:A6
A:B1
A:B2
A:B3
A:B4
A:B5
A:B6

❖ **To use Copy Down or Fill Down for a range of samples**

1. To select a range of sample values, do one of the following:

   Drag your cursor to select a contiguous group of sample values.

   –or–

   Hold down the SHIFT key to select a contiguous group of sample values.

2. Right-click and choose the appropriate command from the shortcut menu.

   The column values are copied or entered sequentially starting with the value in the first selected row and ending with the last selected row.

Index

N

O

S