Thermo

TraceFinder

Version 2.1

User Guide

Optimized for Environmental and Food Safety

DOCUMENTATION SURVEY

Thermo
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Part of Thermo Fisher Scientific

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Software version: Thermo Foundation 2.0 SP1; Thermo Xcalibur 2.2 SP1; Microsoft Windows XP Professional SP3 or Windows 7 Professional; Thermo LC Devices 2.5 SP2; Thermo GC Devices 2.2

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

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Preface

The TraceFinder 2.1 application is the newest application in the series of Thermo Scientific GC/MS and LC/MS analytical software.

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❖ **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 Quick Reference 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 Help Contents, Index, or Search panes.

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

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

   The PDF opens in a new window.

Special Notices

This guide includes the following types of special notices:

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

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

System Requirements

Your system must meet these minimum requirements.

System	Requirements
Computer	• 2.33 GHz processor dual core with 4 GB RAM • CD/R-ROM drive • Video card and monitor capable of 1280 × 1024 resolution • 75 GB available on drive C • NTFS format
Instruments (supported or required)	Autosamplers: • TriPlus™ • AS3000 • Accela™ AS GC Devices: • FOCUS™ GC • Trace GC Ultra™ • Trace 1300 Series LC Devices: • Accela 1250 Pump • Accela Pump • Dionex™ • TLX-1 • LX2 • Agilent™ 1100 • Agilent 1200 GC/MS and LC/MS mass spectrometers
Software	• Microsoft™ Windows™ XP Professional SP3 or Windows 7 Professional • Microsoft Office 2007 SP2 or Microsoft Excel™ 2007 SP2 • Microsoft .NET Framework 4.0 Extended • Thermo Foundation™ 2.0 SP1 • Thermo Xcalibur™ 2.2 SP1 • Adobe™ Reader™ 10.0 • NIST™ 2008 • Thermo LC Devices 2.5 SP2 or Thermo GC Devices 2.2

System Activation

When you first start the TraceFinder application, a dialog box displays the number of days remaining in your 60-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:

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

The evaluation version is full-featured and automatically expires 60 days after activation. Any attempt to set back the system date automatically terminates this version. You can purchase and then activate the full version of the TraceFinder application at any time, during or after the free evaluation, without reinstalling the software.

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

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

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

❖ **To request an activation key**

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

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

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

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

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

   The application copies this XML text to the Clipboard.

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

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

❖ **To use your activation key**

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

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

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

   The License Activation window opens.

3. Click **Paste**.

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

4. Click **Set.**

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

Contacting Us

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

❖ **To contact Technical Support**

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

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

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

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

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

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

❖ **To copy manuals from the Internet**

Go to mssupport.thermo.com, agree to the Terms and Conditions, and then click **Customer Manuals** in the left margin of the window.

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

- Fill out a reader survey online at www.surveymonkey.com/s/PQM6P62.

- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

Introduction

This chapter describes general features of the TraceFinder software.

Contents

About the TraceFinder Application

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

The TraceFinder application can export SRM data in .xml format so that other applications can import the files into their databases.

The TraceFinder application can import the following file types:

- Sample lists in .csv or .xml format

  See "Defining the Sample List" on page 255.

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

  See "Working with Master Methods" on page 100 or "Working with Instrument Methods" on page 228.

- Compounds from files that use the datastore (.xml) format

  See "Adding Compounds, Quantitative Peaks, and Confirming Ions to a Datastore" on page 62.

- Batches, methods, or templates from the following applications:

  – TraceFinder 1.0

  – TraceFinder 1.1

  – TraceFinder 2.0

  – QuanLab Forms or EnviroLab Forms 2.5

  – QuanLab Forms or EnviroLab Forms 3.0

  See "Converting Legacy Data" on page 19.

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

Supported File Types

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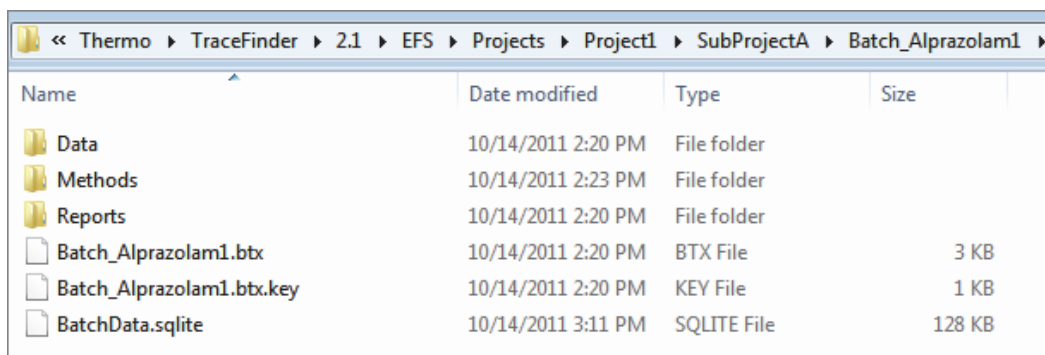
- Comma-separated values (.csv): A set of file formats used to store tabular data in which numbers and text are stored in plain textual form that can be read in a text editor. Lines in the text file represent rows of a table, and commas in a line separate fields in the tables row.

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

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

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

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

TraceFinder Directory Structure

The TraceFinder application creates folders for projects/subprojects/batches and templates in the C:\Thermo\TraceFinder\2.1\EFS directory. Within each batch folder, the application creates folders for data, methods, and reports.

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

Figure 1.   Example batch directory structure

Name	Date modified	Type	Size
Data	10/14/2011 2:20 PM	File folder	
Methods	10/14/2011 2:23 PM	File folder	
Reports	10/14/2011 2:20 PM	File folder	
Batch_Alprazolam1.btx	10/14/2011 2:20 PM	BTX File	3 KB
Batch_Alprazolam1.btx.key	10/14/2011 2:20 PM	KEY File	1 KB
BatchData.sqlite	10/14/2011 3:11 PM	SQLITE File	128 KB

« Thermo ▸ TraceFinder ▸ 2.1 ▸ EFS ▸ Projects ▸ Project1 ▸ SubProjectA ▸ Batch_Alprazolam1 ▸

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 environmental 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
- Configuration mode for user administration, project administration, datastore administration, and application administration
- Method Development mode for editing instrument methods, setting processing and error flag parameters, and setting report options
- 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 EnviroLab 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 EnviroLab Forms applications
- Standard and customized report formats

Features of the common workflow core include the following:

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

TraceFinder Workflow

The TraceFinder application is structured with a typical laboratory workflow in mind. 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 how the raw data is acquired and processed, how the error checking information evaluates the results, and how the results appear in reports.

2. Create and submit a batch 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 the dashboard and all the TraceFinder modes. You can begin another batch while you watch the real-time display of the currently acquiring batch.

   > **Note** At any time, you can quickly view the system status by looking in the lower right corner of the TraceFinder window. This area displays a green, yellow, or red 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 three groups: Standard, Custom, and Target Screening.

For additional information about standard, custom, or target screening reports and examples of each standard report type, see "Reports" on page 423. Examples of standard reports (as PDF files) are also located in the C:\Thermo\TraceFinder\2.1\EFS\ExampleReports folder.

Standard Report Types

- Batch Report
- Batch Report Rev 1
- Blank Report
- Breakdown Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- Confirmation Report 2
- High Density Calibration Report
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary Report
- Tune Report

Custom Report Types

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

Target Screening Report Types

Target Screening reports are available only when you install ToxID™ software and enable the Target Screening features. For a detailed procedure for enabling target screening features, see "Target Screening" on page 90.

- 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

Installing the TraceFinder Application

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

❖ **To install the TraceFinder application**

1. Insert the TraceFinder CD, open the TraceFinder launcher, and click **Next**.

   The InstallShield Wizard opens.
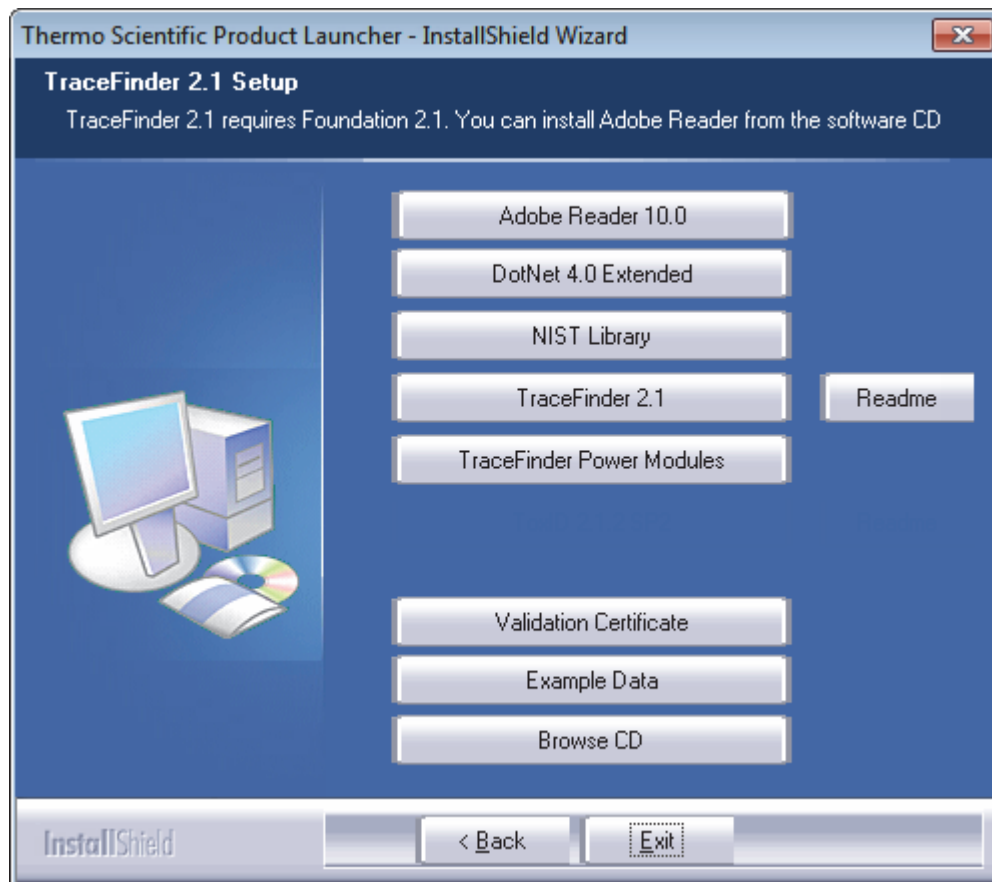
2. Click **TraceFinder 2.1**, and follow the instructions in the InstallShield Wizard.

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

   > **IMPORTANT** If prompted to install Thermo Foundation, click **Yes**, and then when prompted to restart your computer, click **OK**.

   The wizard continues the installation.

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

4. When the installation completes, do not launch the TraceFinder application.

5. Open the TraceFinder launcher again, and click **Next**.

6. Click **NIST Library**, and follow the instructions to install the NIST library (required for ToxID).

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

7. Install the appropriate device drivers, and configure the instruments in the Thermo Foundation Instrument Configuration dialog box.

You can now start your TraceFinder application.

❖ **To install example data**

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

❖ **To start the TraceFinder application**

1. Configure your instruments.

   You cannot configure your instruments while the TraceFinder application is running.

2. Double-click the **TraceFinder** icon on your desktop, or go to **Start > All Programs > Thermo TraceFinder > TraceFinder EFS**.

   By default, user security is not enabled and the application does not require a password. To enable user security, see "User Security" on page 90.

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

1. Enter your assigned user name in the TraceFinder login screen.

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

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

2. Enter your password.

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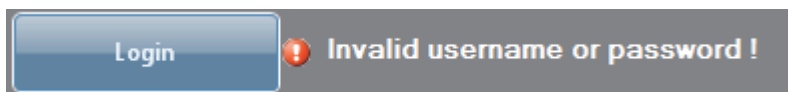
   Correct the user name or password, or contact your system administrator.

3. Click **Login**.

   The TraceFinder dashboard opens. See "TraceFinder Dashboard" on page 35.

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

Figure 2. TraceFinder login screen
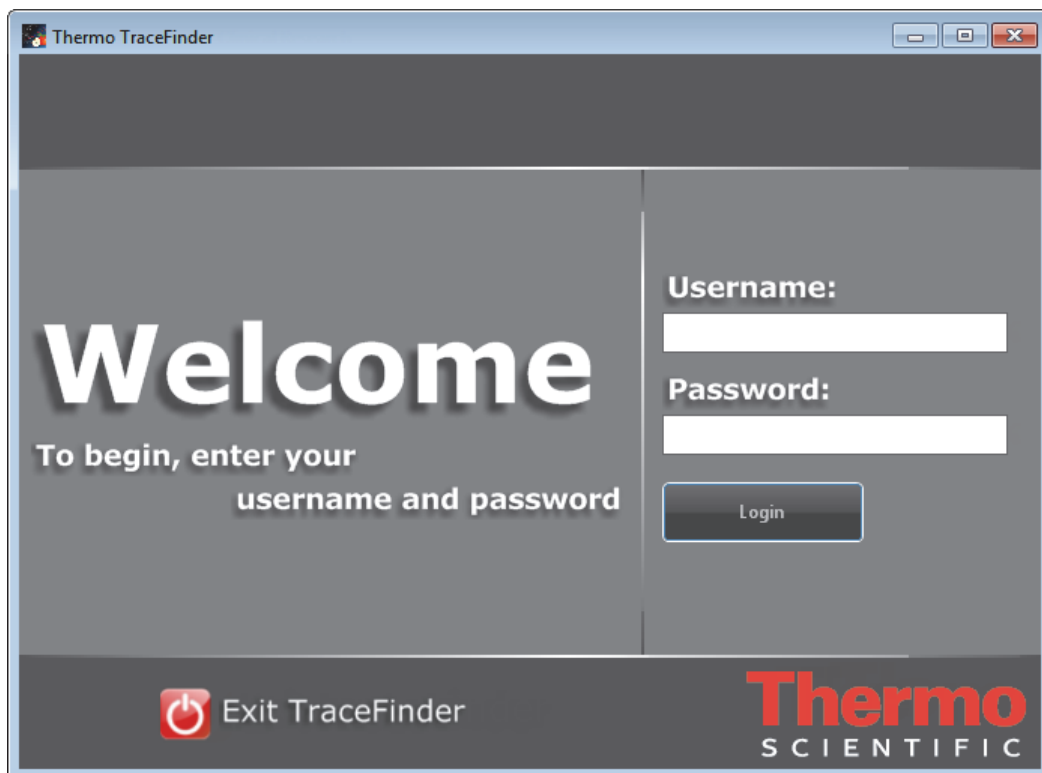
Table 1. Login screen parameters

Parameter	Description
Username	The user's assigned user name.
Password	The assigned password for the user name.
Login	Verifies the user name and password, and displays the dashboard.
Exit TraceFinder	Closes the TraceFinder application without logging in.

Installing the Power Modules

Follow these instructions to install and enable the TraceFinder power modules for multiplexing.

❖ **To install the power modules**

1. Follow the instructions to install the TraceFinder application.

   See "Installing the TraceFinder Application" on page 10.

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

3. Click **TraceFinder Power Modules**, and follow the instructions to install the multiplexing module.

4. License the power modules.

   Licensing for the power modules follows the same procedures as the TraceFinder application licensing. See "System Activation" on page x.

❖ **To enable the power modules**

1. Start the TraceFinder application.

2. Go to the Configuration mode.

3. Click **Application Configuration** in the navigation pane.

4. Click **Optional Features**.

5. On the Optional Features page, select the **Multiplexing** check box.

   For detailed instructions, see "Multiplexing" on page 92.

6. Click **Apply**.

   A message prompts you to restart the TraceFinder application so that your changes can take effect.

7. Click **Yes**.

Installing the NIST and QED Libraries

When you are using triple quadrupole instruments, 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.
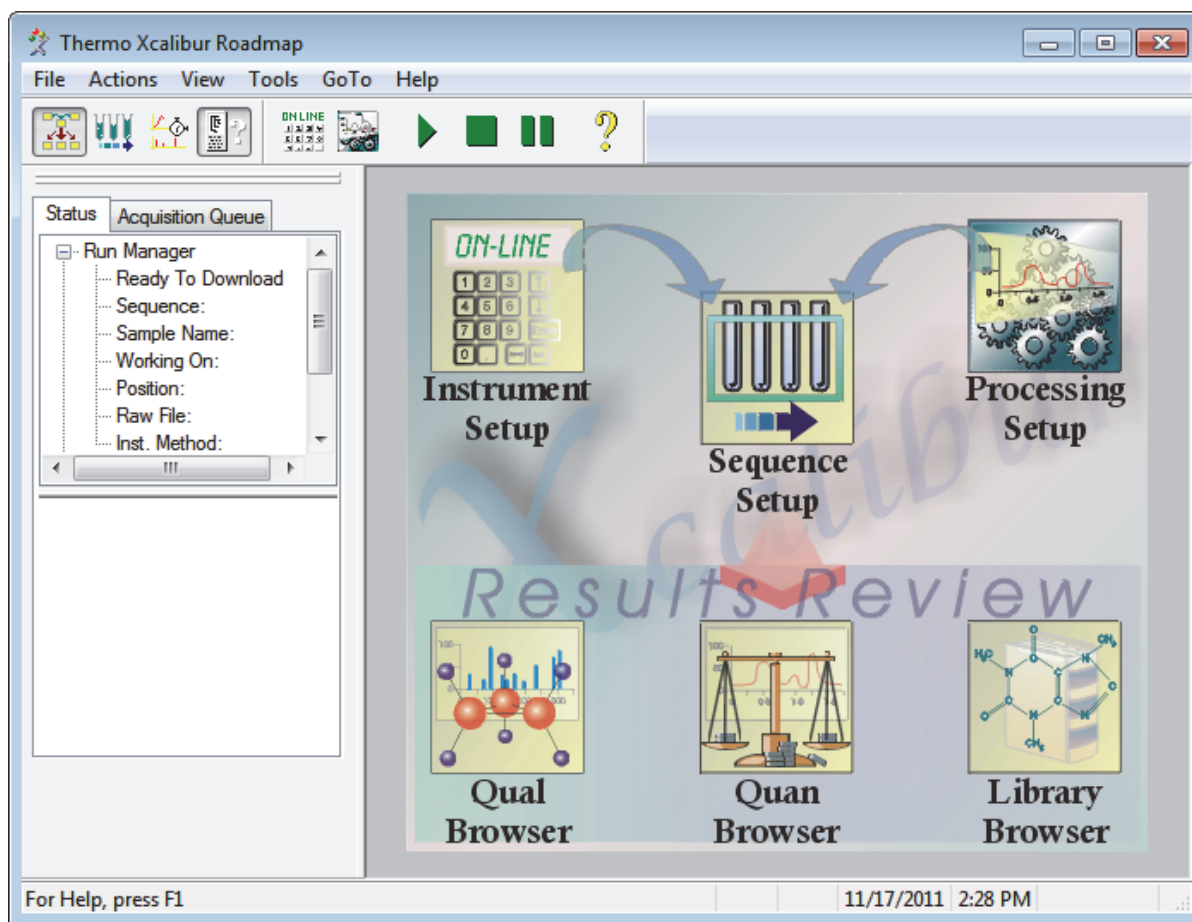
2. Choose **Tools > Library Manager** from the main menu.

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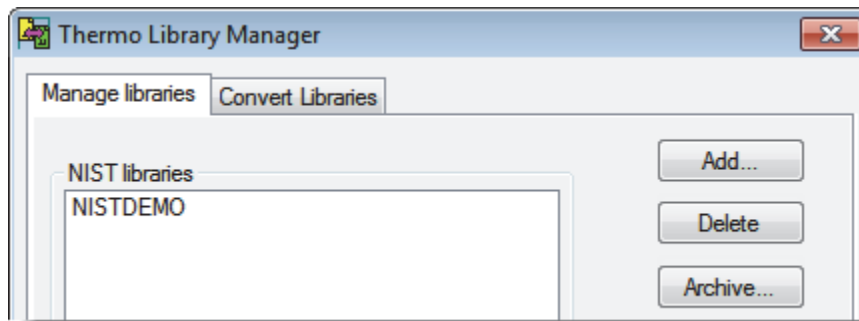
3. Click **Add**.

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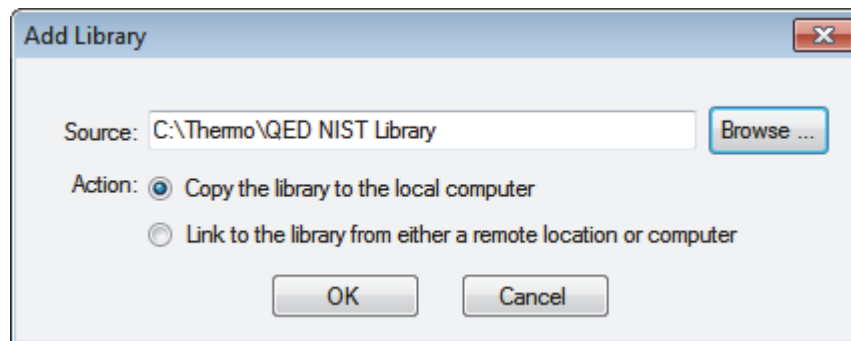
4. Click **Browse**, and locate your QED library in the C:\Thermo folder.

5. Click **OK**.

   The Xcalibur application reports that it has added the library to the NIST 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.
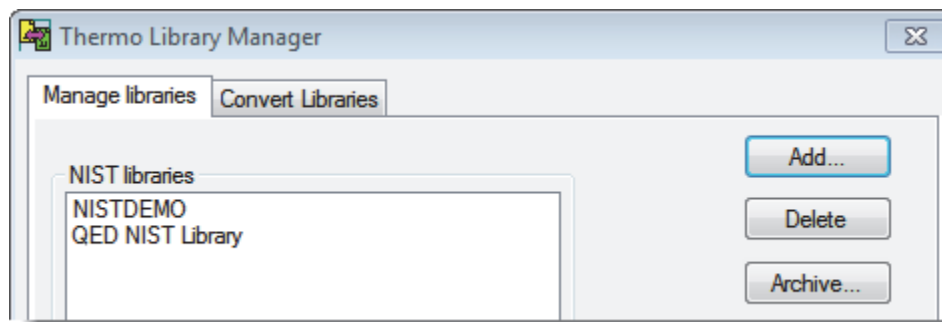
7. Click **Exit** in the Thermo Library Manager dialog box.

8. Start the TraceFinder application.

9. Go to the Method Development mode.

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

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

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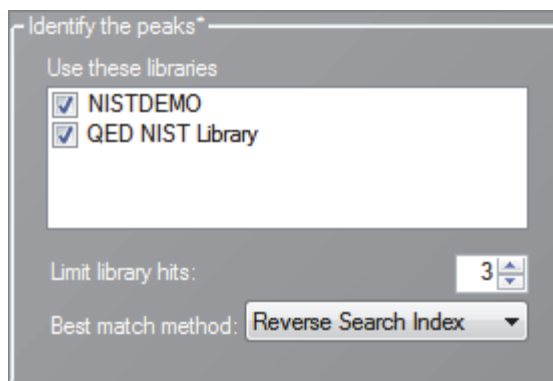
Launching the NIST Library Browser

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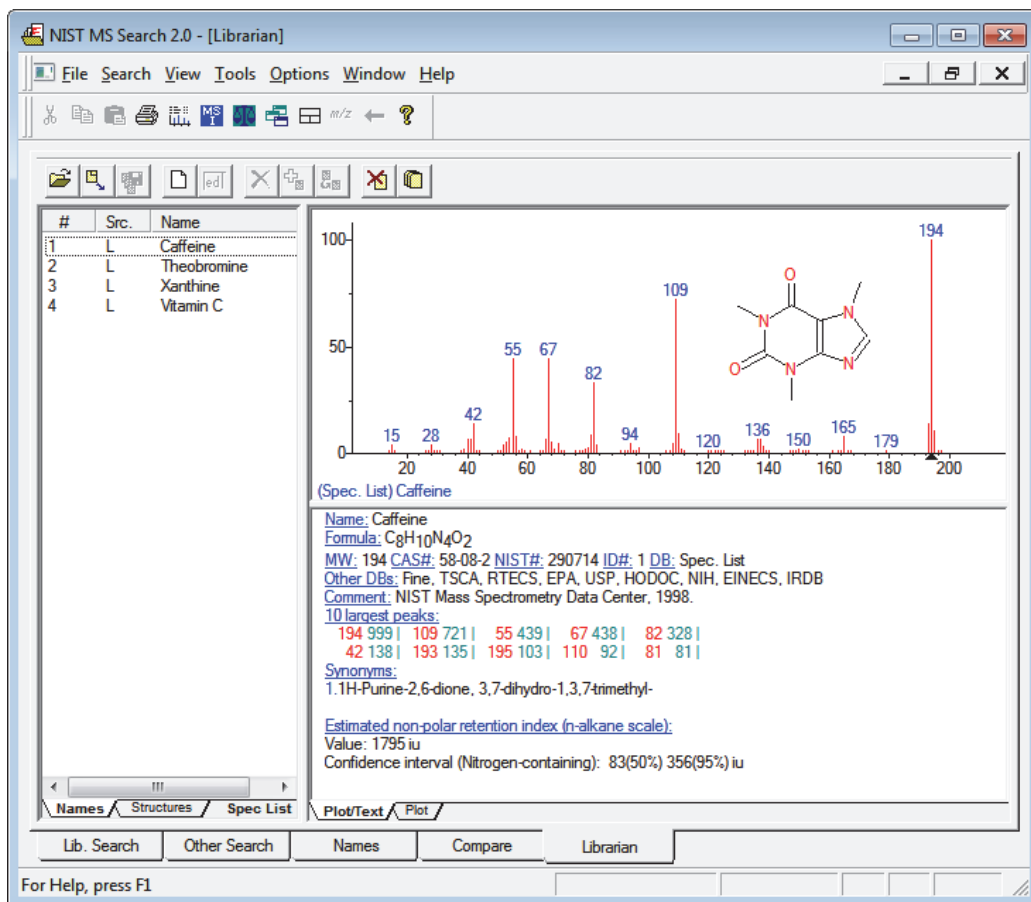
For detailed instructions about using the library browser, refer to the Help in the NIST MS Search window.

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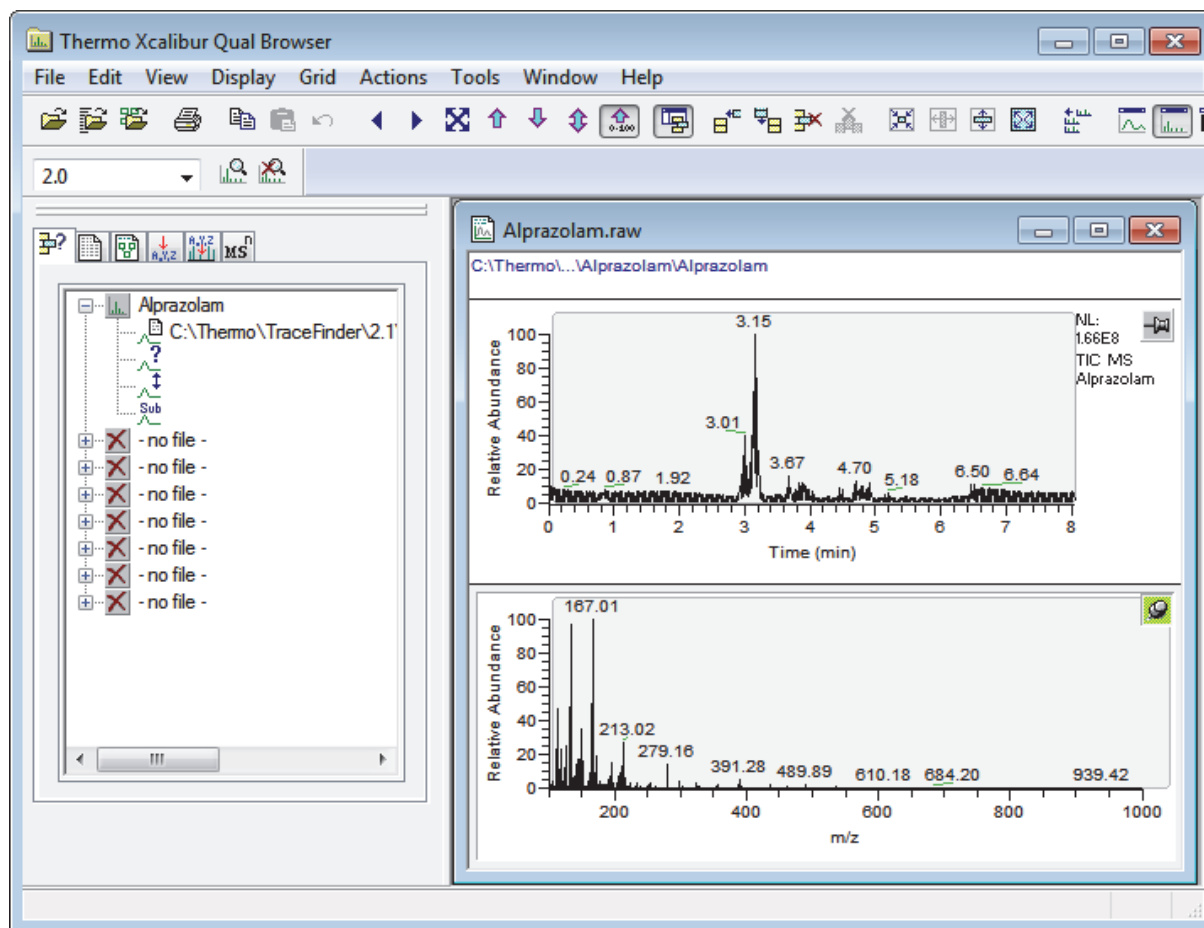
For detailed instructions about using the Qual Browser, refer to the Qual Browser Help.

Converting Legacy Data

Use the TraceFinder Legacy Data Converter to convert methods, batches, method templates, or batch templates from the source versions of TraceFinder 1.0.1/1.1/2.0, EnviroLab Forms, QuanLab Forms, or ToxLab Forms to compatible TraceFinder 2.1 target versions.

Table 2. Version compatibility

Source	TraceFinder 2.1 target			
	General	**EFS**	**Clinical Research**	**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			✓	✓

❖ **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.
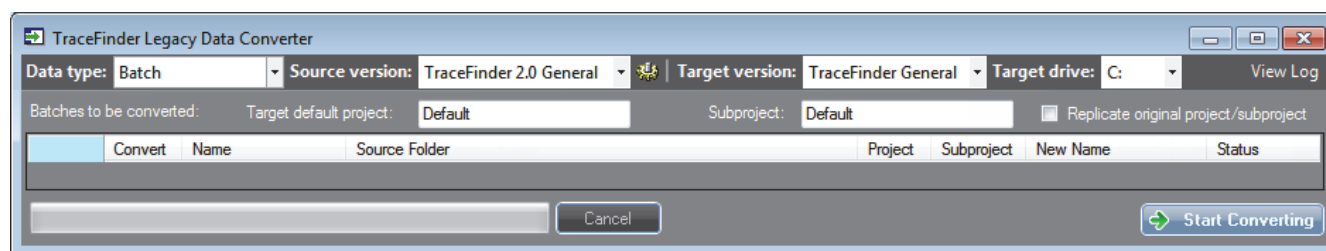
This section includes the following topics:

- Converting Methods

- Converting Batches

- Converting Method Templates

- Converting Batch Templates

Converting Methods

Use the data converter to convert legacy methods to TraceFinder 2.1 methods.

❖ **To convert a method**

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

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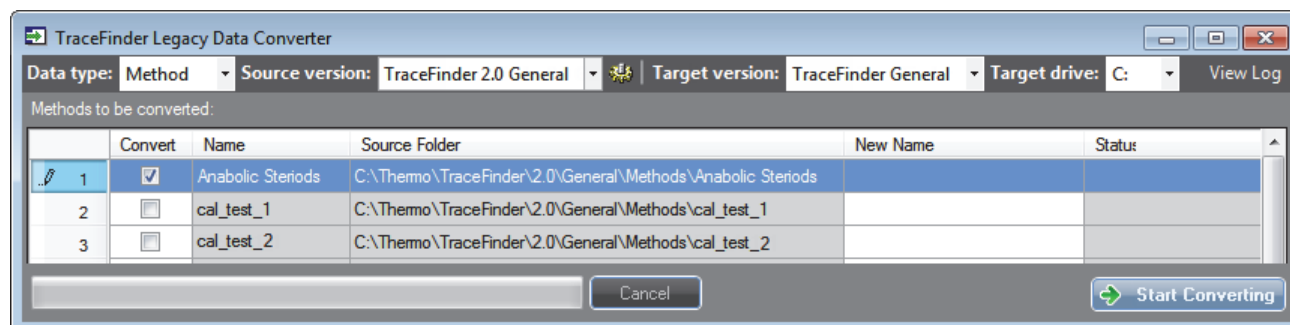
2. In the Source Version list, select the version of the method that you will convert.

   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 **Source Folder** icon, .

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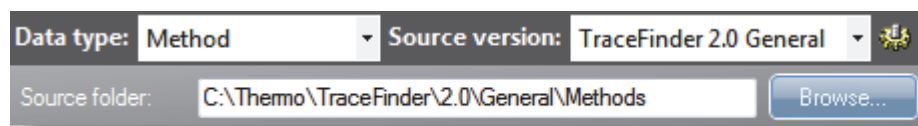
   b. Click **Browse** and locate a method folder.

      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 19.

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 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 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 C:\Thermo*TargetVersion*\Methods folder.

   > **Note** If a method 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 Microsoft Notepad text editor window.

Figure 3. Sample log file for converting a method

```
:======= Start Converting Method from TraceFinder 2.0 to TraceFinder 2.1          ==========
-- Converting master method from
   'C:\Thermo\TraceFinder\2.0\Methods\Sulphonamide Method\Sulphonamide Method.mmx'
-- Creating master method
-- Importing properties of object 'MethodData' from XML file
   'C:\Thermo\TraceFinder\2.0\Methods\Sulphonamide Method\Sulphonamide Method.mmx'
-- Saving master method
-- Copying instrument method
-- Successfully converted master method from
   'C:\Thermo\TraceFinder\2.0\Methods\Sulphonamide Method\Sulphonamide Method.mmx'
   to 'C:\Thermo\TraceFinder\2.1\...\Methods\Sulphonamide Method_1\Sulphonamide Method_1.mmx'
```

Converting Batches

Use the data converter to convert legacy batches to TraceFinder 2.1 batches.

❖ **To convert a batch**

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

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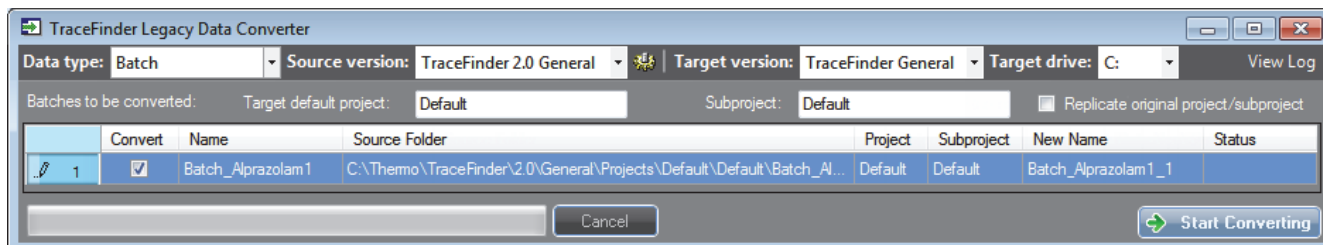
2. In the Source Version list, select the version of the batch that you will convert.

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

   > **IMPORTANT** A valid batch file (.btx) must be inside a folder with the same name. For example:
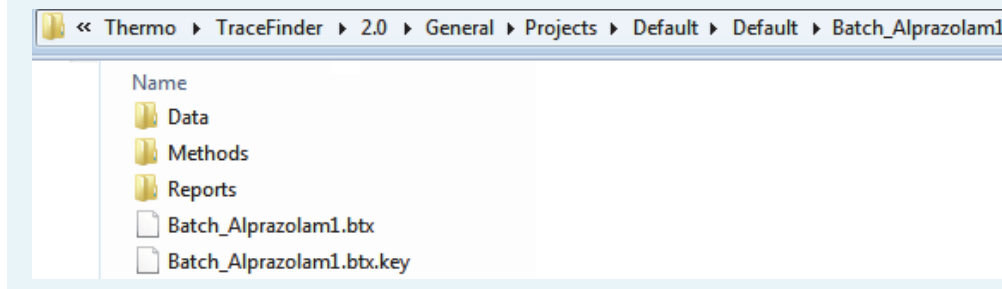
3. To convert a batch that is not in the default list, do the following:

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

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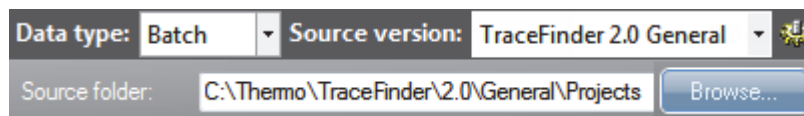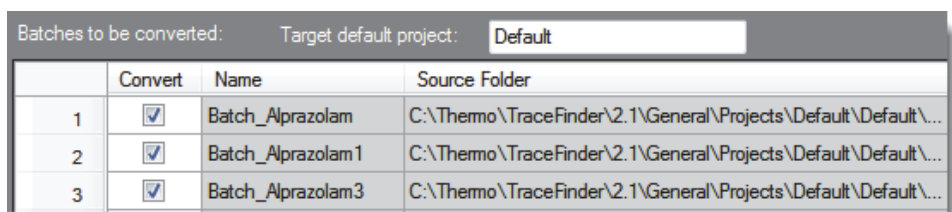
   b. Click **Browse** and locate a batch folder.

      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.

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 19.

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

   You cannot write the converted files to a mapped 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 fail. 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 C:\Thermo*TargetVersion*\Projects folder and uses either the original project and subproject names or the new names that you entered.

> **Note** If a batch conversion fails, 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**.

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

Figure 4. Sample log file for converting a batch

```
:======= Start Converting Batch from TraceFinder2.0 General to TraceFinder General ==========
-- Converting batch from 'C:\Thermo\TraceFinder\1.1\Projects\Default\Default\batch_steroids5\batch_steroi
-- Importing properties of object 'BatchData' from XML file
   'C:\Thermo\TraceFinder\2.0\Projects\Default\Default\batch_steroids5\batch_steroids5.btx'
-- ---------- Importing sample 'steroids01_110504155226' [1/3] ----------
-- Importing properties of object 'SampleData' from XML file
   'C:\Thermo\TraceFinder\2.0\Projects\Default\Default\batch_steroids5\Data\steroids01_110504155226.rsx
-- Saving sample data
-- Copying raw file from 'C:\Thermo\TraceFinder\2.0\Projects\Default\Default\batch_steroids5\Data\steroids
   to 'C:\Thermo\TraceFinder\2.1\General\Projects\Default\Default\batch_steroids5\Data\steroids01_110504
-- ---------- Completed sample import ----------
-- Importing local method for 'batch_steroids5'
-- Importing properties of object 'MethodData' from XML file
   'C:\Thermo\TraceFinder\2.0\Projects\Default\Default\batch_steroids5\Methods\method_steroids\batch_st
-- Saving local method data for 'batch_steroids5_method_steroids'
-- Copying instrument method
-- Saving batch data for 'batch_steroids5'
-- Successfully converted batch from 'C:\Thermo\TraceFinder\2.0\Projects\Default\Default\batch_steroids5\
   to 'C:\Thermo\TraceFinder\2.1\General\Projects\Default\Default\batch_steroids5\batch_steroids5.btx'
```

Converting Method Templates

Use the data converter to convert legacy method templates to TraceFinder 2.1 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.
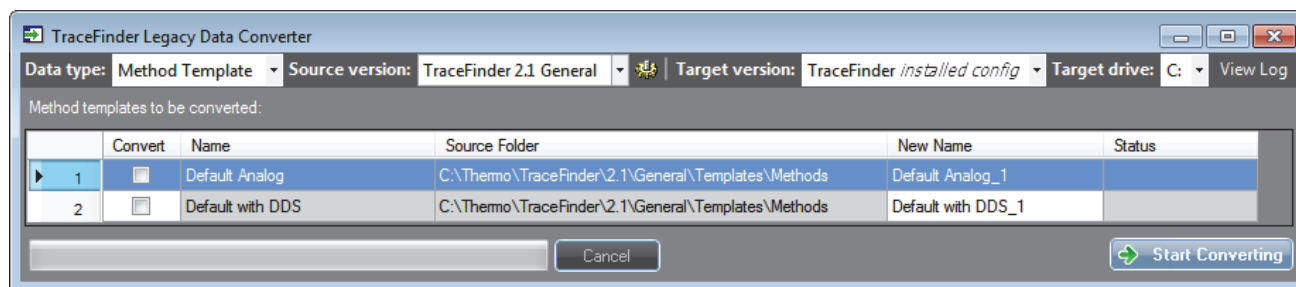
2. In the Source Version list, select the version of the method template that you will convert.

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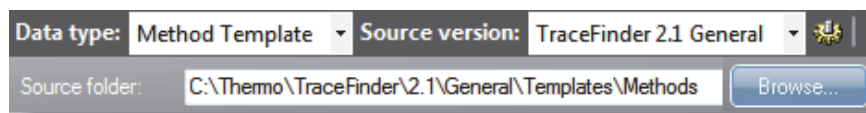
   b. Click **Browse** and locate a template folder.

       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 19.

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 C:\Thermo*TargetVersion*\Templates\Methods 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 5. Sample log file for converting a method template

```
:======= Start Converting Method Template from TraceFinder 2.1 General to TraceFinder EFS ==========
-- Converting method template from 'C:\Thermo\TraceFinder\2.1\General\Templates\Methods\MethodTemplate
-- Importing properties of object 'ProcMethodTemplateData' from XML file
   'C:\Thermo\TraceFinder\2.1\General\Templates\Methods\MethodTemplate4962.pmtx'
-- Saving the method template
-- Successfully converted method template from 'C:\Thermo\TraceFinder\2.1\General\Templates\Methods\Met
   to 'C:\Thermo\TraceFinder\2.1\EFS\Templates\Methods\MethodTemplate4962.pmtx'
```

Converting Batch Templates

Use the data converter to convert legacy batch templates to TraceFinder 2.1 batch templates.

❖ **To convert a batch template**

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

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

2. In the Source Version list, select 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.

   > **IMPORTANT** A valid batch template file (.btx) must be inside a folder with the same name. For example:
   >
   > Thermo ▸ TraceFinder ▸ 2.1 ▸ General ▸ Templates ▸ Batches ▸ Template_Alprazolam
   >
   > Name
   >
   > 📁 Data
   > 📁 Methods
   > 📄 Template_Alprazolam.btx
   > 📄 Template_Alprazolam.btx.key
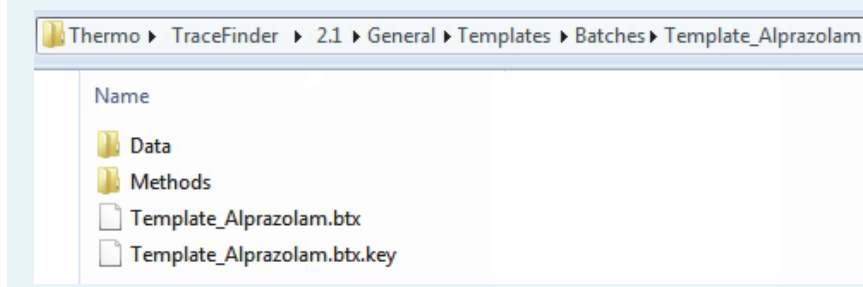
3. To convert a batch template that is not in the default list, do the following:

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

      The application adds a Source Folder box to the window.

      Data type: Batch Template ▾ Source version: TraceFinder 2.1 General ▾ 🔧
      Source folder: C:\Thermo\TraceFinder\2.1\General\Templates\Batches   Browse...
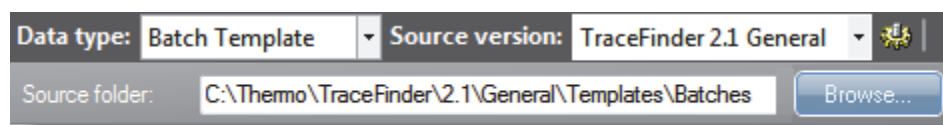
   b. Click **Browse** and locate a template folder.

      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 19.

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.

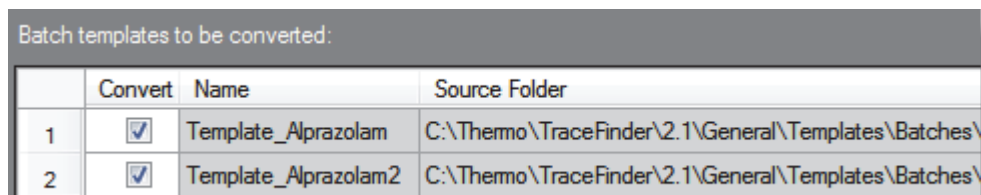   • If the batch template name does not exist in the target folder, the application keeps the original batch template name.

   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 C:\Thermo*TargetVersion*\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 6. Sample log file for converting a batch template

```
======== Start Converting Batch Template from TraceFinder 2.1 General to TraceFinder EFS ==========
-- Converting batch template from 'C:\Thermo\TraceFinder\2.1\General\Projects\ProjectA\SubProjectA1\Batc
-- Importing properties of object 'BatchData' from XML file
   'C:\Thermo\TraceFinder\2.1\General\Projects\ProjectA\SubProjectA1\Batch5247\Batch5247.btx'
-- ---------- Importing sample 'Unknown1' [1/1] ----------
-- Importing properties of object 'SampleData' from XML file
   'C:\Thermo\TraceFinder\2.1\General\Projects\ProjectA\SubProjectA1\Batch5247\Data\Unknown1.rsx'
-- ---------- Completed sample import ----------
-- Importing local method for 'Batch5247'
-- Importing properties of object 'MethodData' from XML file
   'C:\Thermo\TraceFinder\2.1\General\Projects\ProjectA\SubProjectA1\Batch5247\Methods\Method2\Batch
-- Saving local method data for 'Batch5247_Method2'
   Successfully converted batch template from
   'C:\Thermo\TraceFinder\2.1\General\Projects\ProjectA\SubProjectA1\Batch5247\Batch5247.btx'
    to 'C:\Thermo\TraceFinder\2.1\EFS\Templates\Batches\Batch5247\Batch5247.btx'
```

Choosing a Mode

When user security is enabled, the dashboard displays the options applicable to the current user's assigned role. The following table shows the available modes for each user role.

Table 3. User roles and mode access

User role	Method Development	Acquisition	Analysis	Configuration
LabDirector	✓	✓	✓	✓
ITAdmin				✓
Supervisor	✓	✓	✓	
Technician		✓	✓	
QAQC			✓	

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

Follow these procedures:

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

❖ **To choose a mode**

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

   The dashboard shows only the modes that you have permission to use. See "TraceFinder Dashboard" on page 35.

2. To change modes from within any of the TraceFinder application modes, click a mode button in the navigation pane.
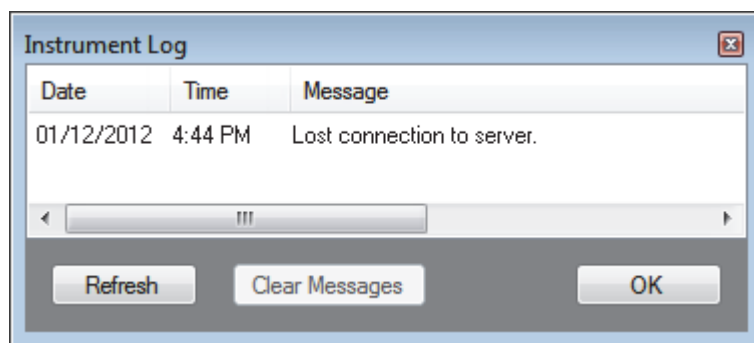
❖ **To display a log of instrument errors**

1. Right-click the status light in the lower right corner of any mode.
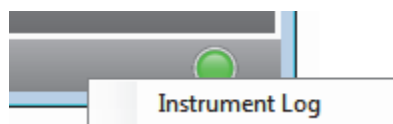
2. Choose **Instrument Log**.

   The Instrument Log dialog box opens.

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

3. Do any of the following:

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

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

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

         C:\Thermo\TraceFinder\2.1\EFS\Logs\TraceFinder.log

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

❖ **To monitor instrument status**

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

     Green indicates that the instrument is ready.

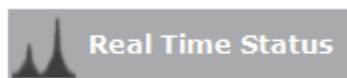   Yellow indicates that the instrument is in standby mode.
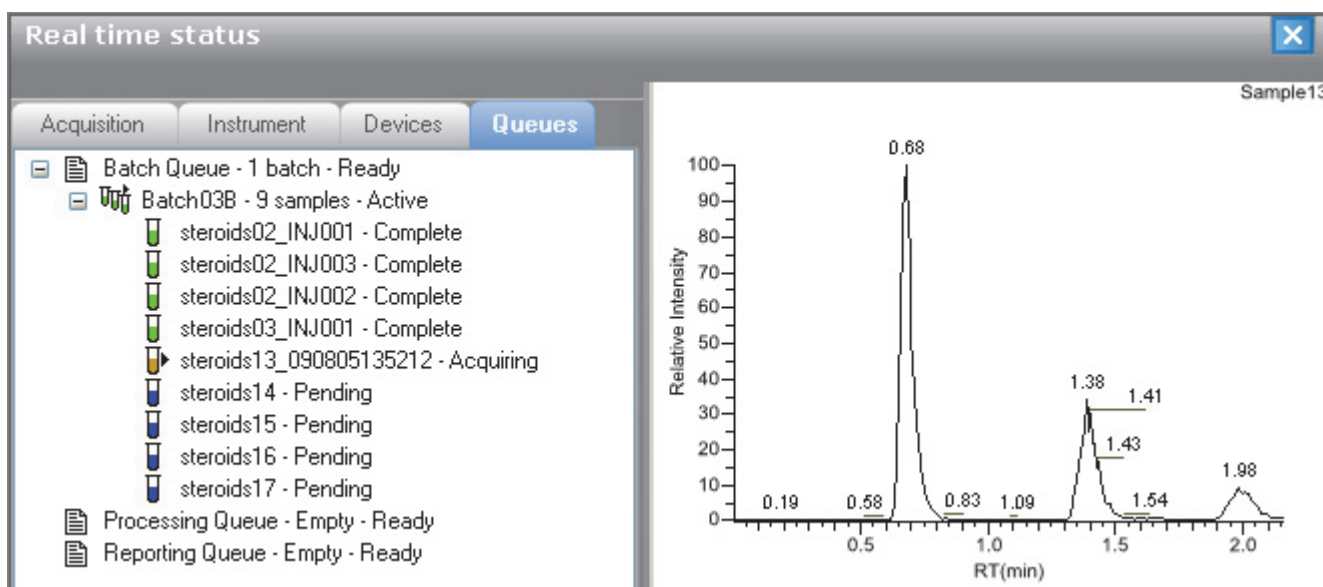
     Red indicates that the instrument is turned off or no device is configured.

❖ **To watch the real-time display from the dashboard**

Click **Real Time Status**.

The real-time status is displayed at the bottom of the dashboard.

For descriptions of all the features of the real-time display, see "Real-Time Display" on page 279.

TraceFinder Dashboard

A dashboard without user security or for a user in the LabDirector role looks like this.

Table 4. TraceFinder dashboard screen parameters (Sheet 1 of 2)

Parameter	Description
Real Time Status	Opens the real-time display for the current acquisition. The acquisition progress is displayed within the current mode window.
Help	Opens the TraceFinder Help.
Log Off	Logs off the current user and displays the login screen. This function is available only when user security is enabled. See "User Security" on page 90.
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 94.

Table 4. TraceFinder dashboard screen parameters (Sheet 2 of 2)

Parameter	Description
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."
Configuration	Opens the Configuration mode where you can set permissions, assign users to roles, configure available reports and import new reports, and maintain the various databases, including the Compound Datastore. See Chapter 3, "Using the Configuration Mode."

Using the Configuration Mode

This chapter discusses the configuration tasks assigned to the ITAdmin and LabDirector roles when user security is enabled. When user security is not enabled, all users have access to all features in the Configuration mode except the User Administration tasks.

Contents

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

Users in the ITAdmin or LabDirector role are responsible for the following:

- Handling the databases
- Applying roles to users
- Understanding security, users, and groups
- Creating local users and network groups
- Creating projects and subprojects
- Maintaining compounds in the compounds datastore

❖ **To access the Configuration mode**

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

The Configuration mode navigation pane opens.
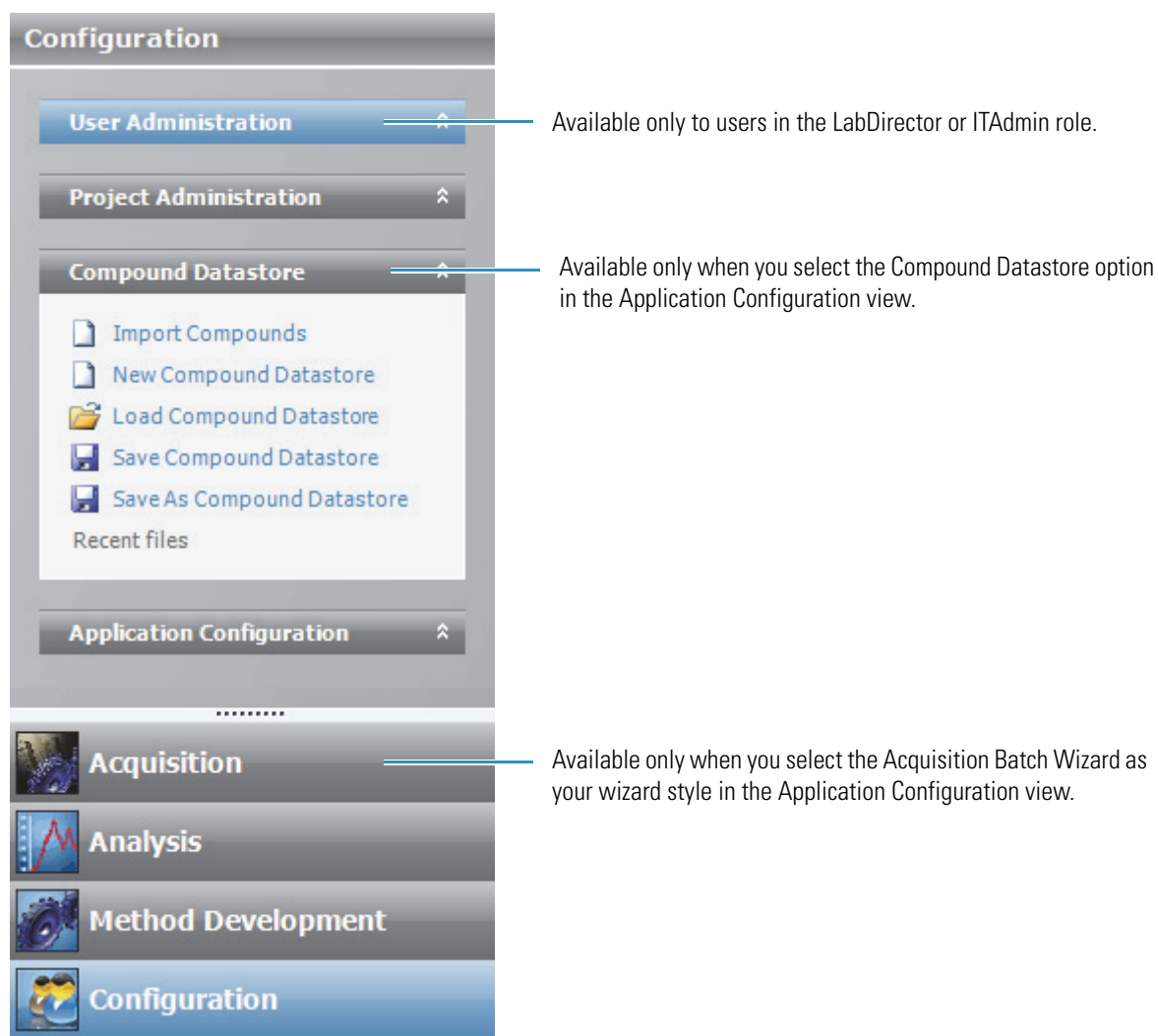
Figure 7. Configuration mode navigation pane

Available only to users in the LabDirector or ITAdmin role.

Available only when you select the Compound Datastore option in the Application Configuration view.

Available only when you select the Acquisition Batch Wizard as your wizard style in the Application Configuration view.

Table 5. Configuration mode navigation pane functions (Sheet 1 of 2)

Function	Description
User Administration	Opens the User Administration view where you can add, remove, or edit user accounts and permissions. See "User Administration" on page 40.
	When user security is not enabled, this task pane is not available. When user security is enabled, this task pane is available only to users in the LabDirector or ITAdmin role. See "Application Configuration" on page 67.
Project Administration	Opens the Project Administration view where you can create and manage projects and subprojects. See "Project Administration" on page 49.

Table 5. Configuration mode navigation pane functions (Sheet 2 of 2)

Function	Description
Compound Datastore	Opens the Compound Datastore view where you can manage the definition of compounds in the current datastore. See "Compound Datastore" on page 55. This task pane is available only when you have selected the Compound Datastore option on the Optional Features page of the Application Configuration view. See "Application Configuration" on page 67.
Application Configuration	Opens the Application Configuration view where you can specify available reports, application defaults, and detection algorithms. You can also enable the user security, target screening, compound datastore, multiplexing, and batch wizard features. See "Application Configuration" on page 67.

User Administration

In the User Administration view of the Configuration mode (when user security is enabled), users in the LabDirector or ITAdmin role can add, remove, or edit user accounts and permissions.

For detailed descriptions of each user role and the permissions and responsibilities for each role, see "Choosing User Roles" on page 46.

❖ **To open the User Administration view**

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

The Configuration navigation pane opens.

> **Note** The User Administration view is available only when you enable user security. Follow the instructions "To turn on user security" on page 90.

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

The User Administration view opens. See "User Administration view" on page 44.
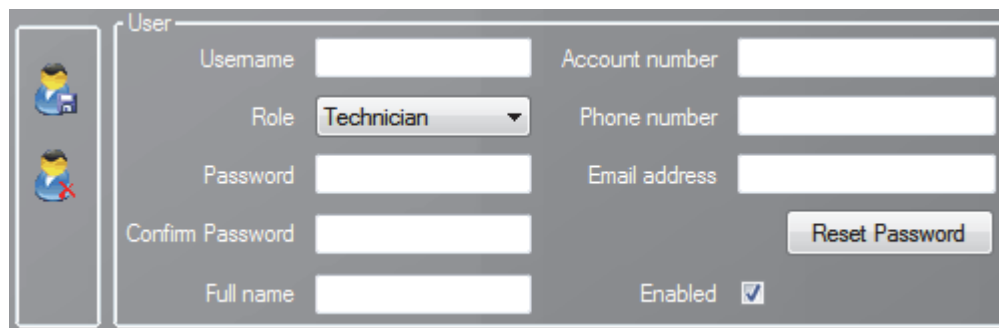
Editing User Information

Follow these procedures:

- To add a user
- To edit user information
- To change a user password
- To remove a user

❖ **To add a user**

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

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

2. Type a unique name in the Username field.

3. Select a role from the Role list.

    A user in the LabDirector or ITAdmin role must assign each user to one of these defined roles. For detailed information about the permissions allowed for each role, see "Choosing User Roles" on page 46.

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

    Make sure to communicate the password to the user.

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

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

    You can disable a user login without deleting the user's information. Follow the instructions "To edit user information" on page 42.

7. Do one of the following:

When all the user information is correct, click the **Save Changes** icon, .

The TraceFinder application adds the new user to the User Listing table, and the parameters in the User area are unavailable.

–or–

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

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

❖ **To edit user information**

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

> **Note** Clicking anywhere in the row selects the user.

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

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

The application enables the parameters in the User area.

3. Edit any of the parameter values.

If you are editing your own user name, the Enabled check box is unavailable because you cannot make your own account unavailable.

4. Do one of the following:

When all the user information is correct, click the **Save Changes** icon, .

The TraceFinder application adds the new parameter values to the User Listing, and the parameters in the User area are unavailable.
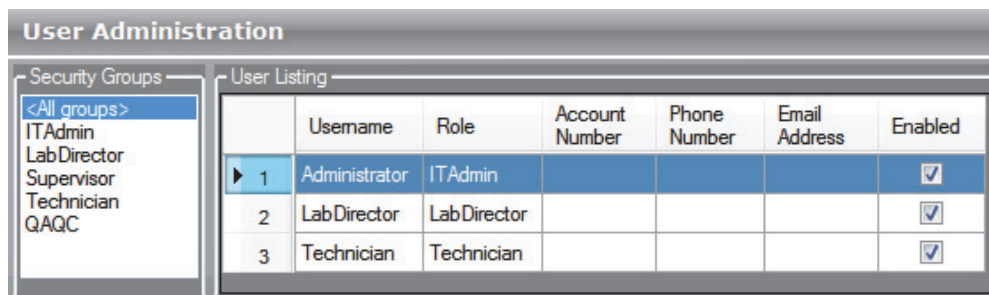
–or–

To discard all changes and not save the edits, click the **Cancel Changes** icon, .

All changes are discarded, and the parameters in the User area are unavailable.
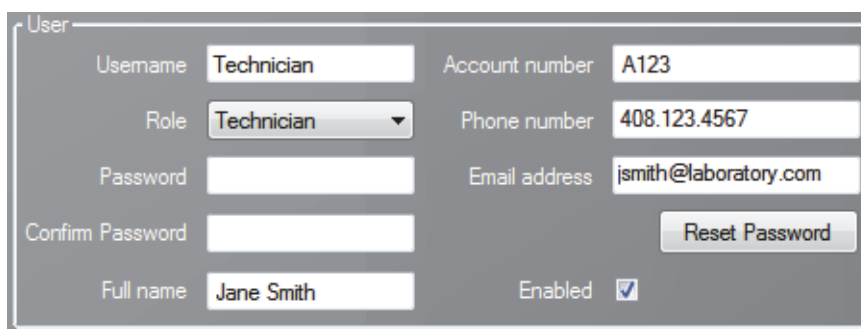
❖ **To change a user password**

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

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

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

The parameters in the User area are enabled.

3. Click **Reset Password**.

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

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

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

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

Make sure to communicate the new password to the user.

❖ **To remove a user**

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

> **Note** Clicking anywhere in the row selects the user.

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

2. Click the **Remove User** icon, ![icon].

If you select your current user name, the Remove User icon is unavailable. You cannot remove yourself.

3. When prompted, confirm that you want to remove this user.

If the user is currently logged in to the TraceFinder application, the user's current session is not affected.

4. Click **OK**.

> **Note** Rather than completely removing the user, you can disable a user login without removing all the user information from the system. Follow the instructions .

Figure 8. User Administration view

Table 6. User Administration view parameters

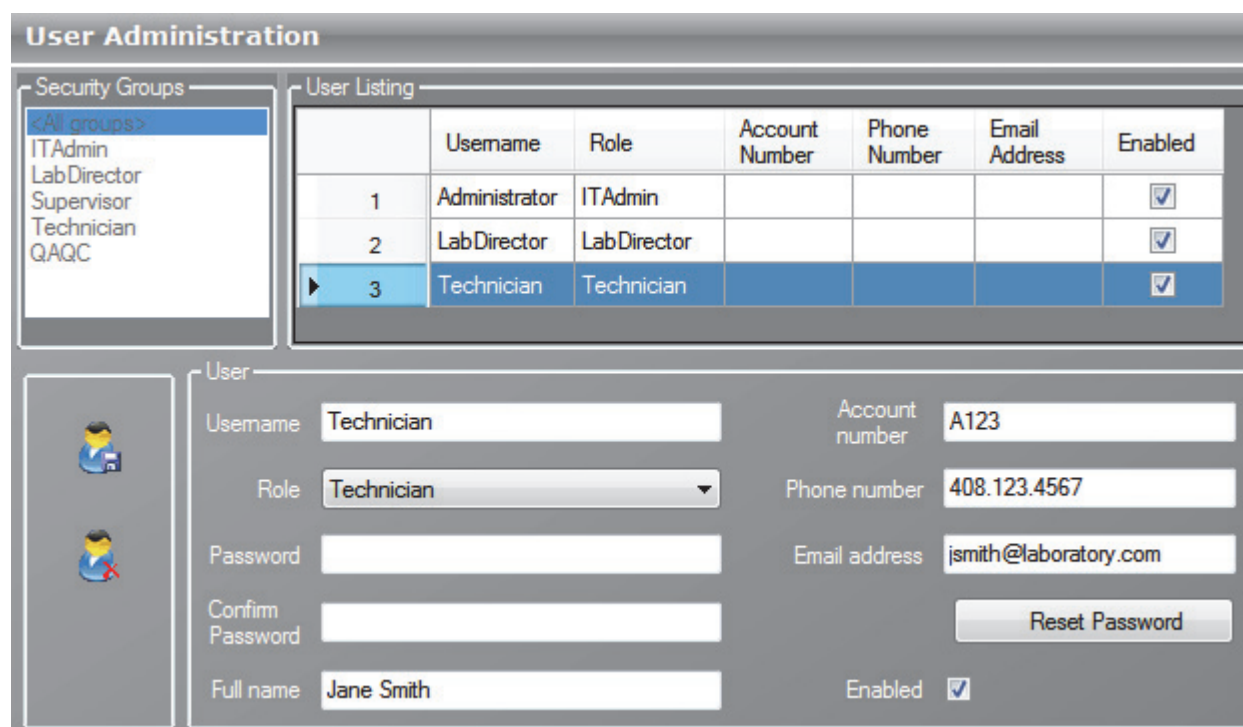| Parameter		Description
Security Groups		All permission levels defined in the TraceFinder application. For detailed descriptions of user permissions, see "Choosing User Roles" on page 46.
User Listing		
Username		User login name.
Role		Security group that defines user permissions.
Account Number		User account number.
Phone Number		User telephone number.
Email Address		User e-mail address.
Reset Password		Enables the Password and Confirm Password parameters so that you can change them.
Enabled		Available or unavailable status for the user account.
User		
Username		Login name for the current user.
Role		Security group that defines the current user's permissions.
Password		Login password for the current user.
Full Name		The current user's actual name.
Account Number		Optional account number for the current user.
Phone Number		Optional telephone number for the current user.
Email Address		E-mail address for the current user. Used to notify user of a randomly generated password.
Enabled		Allows or disallows access for this user. When this user is currently logged in, disallowing takes effect after the user logs off.
Reset Password		Makes the password visible as a string of asterisks that you can select and change.
Icon	**Function**	
	Add User	Enables the fields in the User area where you can enter information for a new user.
	Remove User	Deletes all information for the selected user.
	Edit User	Enables the User area where you can edit any of the parameters for the selected user.
	Save Changes	Adds the new parameter values to the User Listing table and disables the parameters in the User area.
	Cancel Changes	Discards all new or edited information.

Choosing User Roles

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

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

TraceFinder Mode Access

A laboratory director or an IT administrator assigns you to a role that gives you access to specific modes of the TraceFinder application. When you log in, the dashboard displays links to only the modes that you can access.

Table 7. User roles and mode access

User role	Method Development	Acquisition	Analysis	Configuration
LabDirector	✓	✓	✓	✓
ITAdmin				✓
Supervisor	✓	✓	✓	
Technician		✓	✓	
QAQC			✓	

LabDirector

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

A laboratory director is responsible for these tasks:

- Creating or editing methods for new levels of detection or adding new compounds to the existing database
- Reviewing data from the mass spectrometer
- Running samples and reviewing data collected by others
- Reporting the data
- Understanding the results and giving final approval of the released data before archiving

ITAdmin

In the ITAdmin role, you set security, manage users into roles, and manipulate the various databases. You are responsible for adding compounds into the various compound databases.

An IT administrator is responsible for these tasks:

- Handling the databases
- Applying roles to users
- Understanding security, users, and groups
- Creating local users and network groups

Supervisor

In the Supervisor role, you are responsible for setting up the instrument samples and using previously built sequences and methods for processing and acquiring data. You also develop and edit methods for processing and acquiring data, review the data, and distinguish between the need to rerun samples or pass reports up to the lab manager for final review. On a daily basis, you establish the priority for a list of samples to run and create the sequence of events.

A supervisor is responsible for these tasks:

- Submitting samples

- Creating and submitting batches

- Reporting the data to management

- Creating or editing methods for new levels of detection or adding new compounds to the existing database

- Reviewing data from the mass spectrometer

- Understanding the results, who ran the batch, and who passed along the results before giving intermediate approval and sending the data to management

- Modifying new compounds or adjusting methods for specific result sets

Technician

In the Technician role, you are responsible for setting up the instrument samples and using previously built sequences and methods for processing and acquiring data. You also edit existing methods for processing and acquiring data, review collected data, and distinguish between the need to rerun samples or pass reports up to the supervisor. On a daily basis, you are responsible for gathering the list of samples to run and creating the sequence of events.

A technician is responsible for these tasks:

- Submitting samples

- Creating and submitting batches

- Creating data to be reviewed by management

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

- Reviewing data from the mass spectrometer

- Understanding the resulting data, making integration changes, and passing those changes up for further approval

QAQC

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

A QAQC technician is responsible for these tasks:

- Reviewing data from the mass spectrometer

- Understanding the results and who ran and passed along the results before giving intermediate approval and sending the data to management

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

> **Note** In the QAQC role, you have access only to the Analysis mode.

Project Administration

When user security is enabled, users in the LabDirector or ITAdmin role can create and manage projects and subprojects on fixed or network drives in the Project Administration view of the Configuration mode.

This section includes the following topics:

- Working with Drives

- Working with Projects

❖ **To open the Project Administration view**

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

The Configuration navigation pane opens. See "Configuration mode navigation pane" on page 38.

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

The Project Administration view opens.

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

C:\Thermo\TraceFinder\2.1\EFS\Projects

Working with Drives

Drives can be any of the following:

- Fixed: Directly connected to your computer.

- Network: Either a remote box or a mapped drive. A shared folder that is mapped to a drive letter might physically exist on your computer, but because it is mapped, it is considered to be a Network drive.

- Removable: Temporary drives such as a 3.5-inch disk or a USB drive.

Follow these procedures:

- To choose a drive

- To change the default drive

- To hide a drive from the display

- To refresh the display

❖ **To choose a drive**

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

   If you have not created a Projects directory on this drive, you see this message:
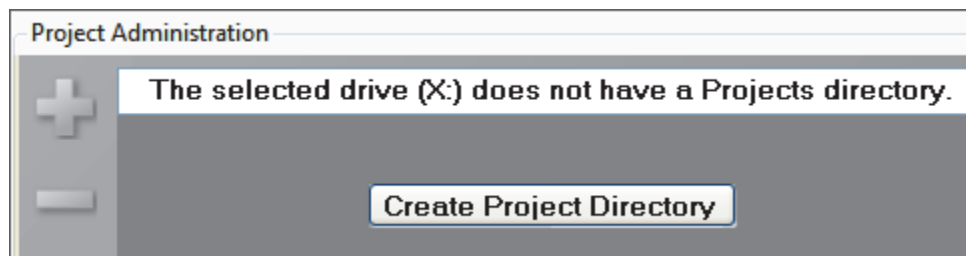
2. Click **Create Projects Directory**.

   The TraceFinder application adds a new Projects directory to the selected drive. To create projects and subprojects on this drive, see "To create projects or subprojects" on page 52.

❖ **To change the default drive**

Select the check box in the Default column.

You can set only fixed drives as the default drive. The default drive is the only drive that you can use to acquire data.

❖ **To hide a drive from the display**

Clear the check box in the Show column.

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

❖ **To refresh the display**

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

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

Working with Projects

When you create a batch, the application stores the data files, local method, and reports in a project and subproject that you create in the C:\Thermo\TraceFinder\2.1\EFS\Projects folder.

If you installed the TraceFinder example data, the main Projects folder includes an Example project folder that contains subprojects with example batches that you can use to experiment. To install the example data from the InstallShield Wizard, see the instructions "To install example data" on page 11.

Follow these procedures:

- To create projects or subprojects

- To delete projects or subprojects

- To remove all empty folders

- To copy the folder hierarchy from another drive

❖ **To create projects or subprojects**

1. Select the top-level project.

   You can select the main Projects folder and create a new project under it, or you can select one of the existing projects and create a subproject under it.

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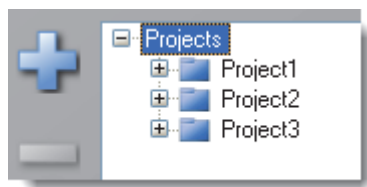
2. Click the plus sign.

   The TraceFinder application creates a new, unnamed project folder under the selected project.

3. While the new project is still highlighted, type a new name.

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

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

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

❖ **To delete projects or subprojects**

1. Select the project or subproject that you want to delete.
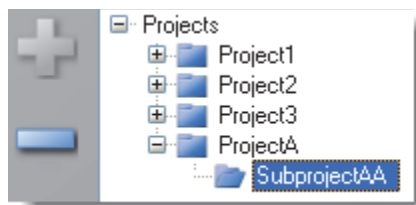
You can delete projects that do not have subprojects. You can delete subprojects that do not have batches. When the selected project or subproject is available for deletion, the application enables the minus sign icon, [image] .

2. Click the minus sign, or right-click and choose **Remove Project** from the shortcut menu.

3. At the prompt, click **Yes** to remove the selected project or subproject.

❖ **To remove all empty folders**

1. Select the project or subproject that contains empty folders.

2. Right-click and choose **Remove All Empty Child Folders** from the shortcut menu.

   A dialog box asks if you want to remove all empty folders.

3. Click **OK**.

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

❖ **To copy the folder hierarchy from another drive**

1. Select the top-level Projects directory in the Project Administration area.

   When you copy the hierarchy *from* the drive *to* your Projects folder, the application will add new folders to the current hierarchy, but it will not remove folders.

2. Right-click and choose **Copy Folder Hierarchy from Drive** from the shortcut menu.

3. Choose a drive from the list of available drives.
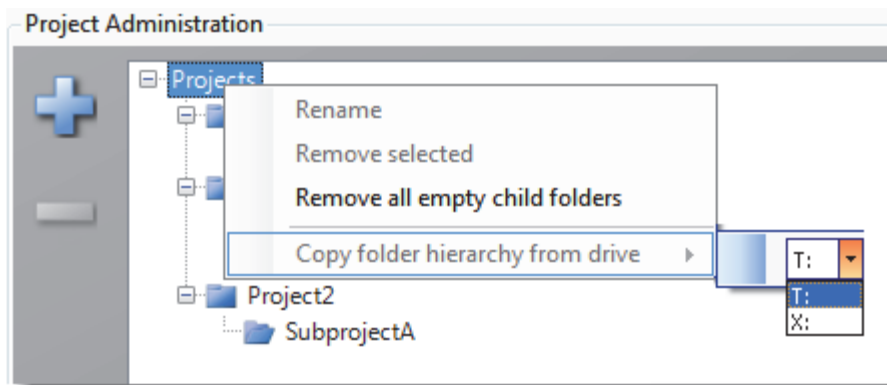
   At the prompt, you must confirm that you want to create a folder hierarchy that matches that of the specified drive.

4. Click **OK**.

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

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

Compound Datastore

When user security is enabled, users in the LabDirector or ITAdmin role can manage compound definitions in the current datastore in the Compound Datastore view.

This section includes the following topics:

- Opening and Saving a Datastore

- Adding Compounds, Quantitative Peaks, and Confirming Ions to a Datastore

- Choosing Experiment Types

For a description of all the parameters in the Compound Datastore view, "Compound Datastore view" on page 59.

Opening and Saving a Datastore

You can use the default datastore or you can create your own datastore. The Compound Datastore task pane is available only when the Compound Datastore feature is enabled. See "Enabling Optional Features" on page 88.

Follow these procedures:

- To open the Compound Datastore editor

- To open a compound datastore

- To create a new compound datastore

- To save a datastore

- To save a datastore to a new name

❖ **To open the Compound Datastore editor**

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

The Configuration navigation pane opens. See "Configuration mode navigation pane" on page 38.

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

The current datastore opens in the Compound Datastore view. For a detailed list of all parameters and functions in the Compound Datastore view, see "Compound Datastore view" on page 59.

❖ **To open a compound datastore**

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

   The Open Compound Datastore dialog box opens.
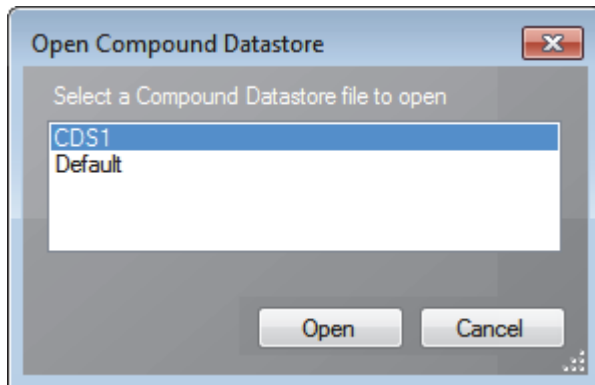
2. Double-click the name of the datastore that you want to open.

   The selected datastore opens in the Compound Datastore view. See "Compound Datastore view" on page 59.

❖ **To create a new compound datastore**

Click **New Compound Datastore** in the Compound Datastore task pane.

A new, empty datastore opens in the Compound Datastore view.
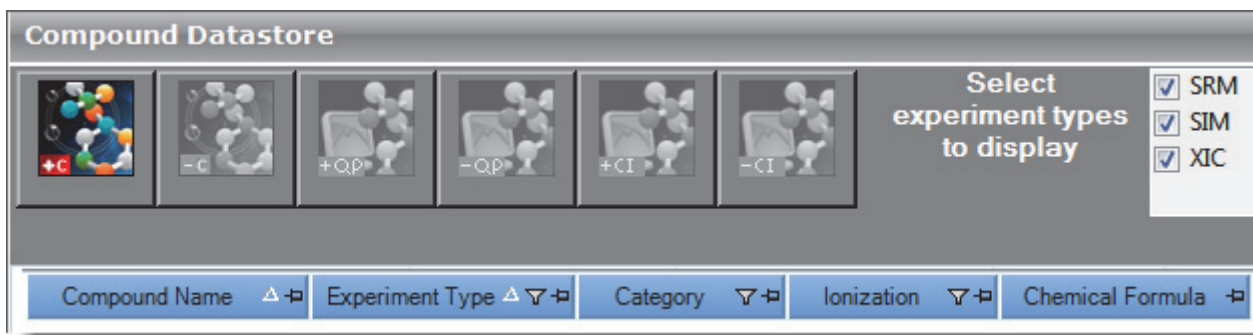
You can import a file of compounds into the new datastore (by following the instructions, To import compounds), or you can manually add compounds one at a time (by following the instructions, To add a compound to the datastore).

❖ **To save a datastore**

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

   The application stores the database as

   …\Thermo\TraceFinder\2.1\EFS\Databases*filename*.xml

If the datastore contains any compounds that do not have associated quantitative peaks, the Invalid Compound Datastore Not Saved dialog box opens, listing the compounds.
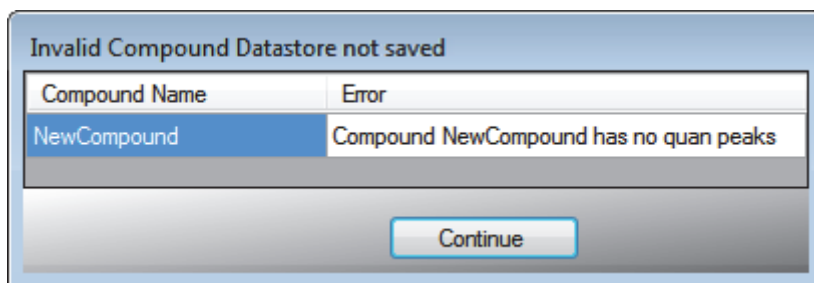
2. To add a quantitative peak row to the listed compounds, click **Continue**.

   The application returns you to the Compound Datastore view.

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

   See "To add a quantitative peak to a compound" on page 64.

❖ **To save a datastore to a new name**

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

   The Save Compound Datastore dialog box opens.
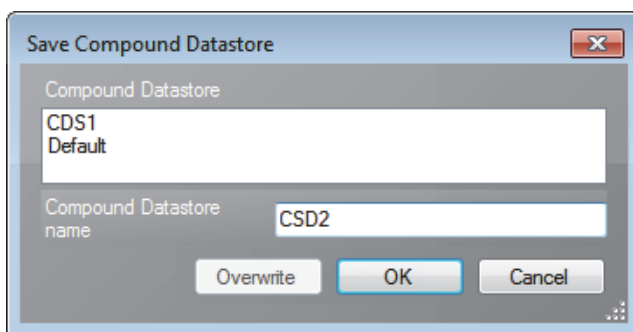
2. Type a file name for the new compound datastore.

3. Click **OK**.

   The application stores the database as

   …\Thermo\TraceFinder\2.1\EFS\Databases*filename*.xml

Table 8. Save Compound Datastore dialog box parameters

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

Figure 9.   Compound Datastore view

Table 9.   Compound Datastore view parameters (Sheet 1 of 3)

Parameter	Description
Function icons	
	Adds a new compound row.
	Removes the selected row and all quantitative peak and confirming ion rows within it.
	Adds a new quantitative peak row to the compound. Each compound requires at least one quantitative peak.
	Removes the selected row and all confirming ion rows within it.
	Adds a new confirming ion row to the quantitative peak.
	Removes the selected confirming ion row.
Select Experiment Types To Display	Specifies one of these experiment types that each use a different structure for the mass filter. See "Choosing Experiment Types" on page 66. • SRM: Selected Reaction Monitoring • XIC: Extracted Ion Chromatogram • SIM: Single Ion Monitoring
Compound parameters	
Compound Name	Alphanumeric name assigned to the compound.
Experiment Type	Experiment type: SRM, XIC, or SIM.
Category	(Optional) Alphanumeric identifier.

Table 9. Compound Datastore view parameters (Sheet 2 of 3)

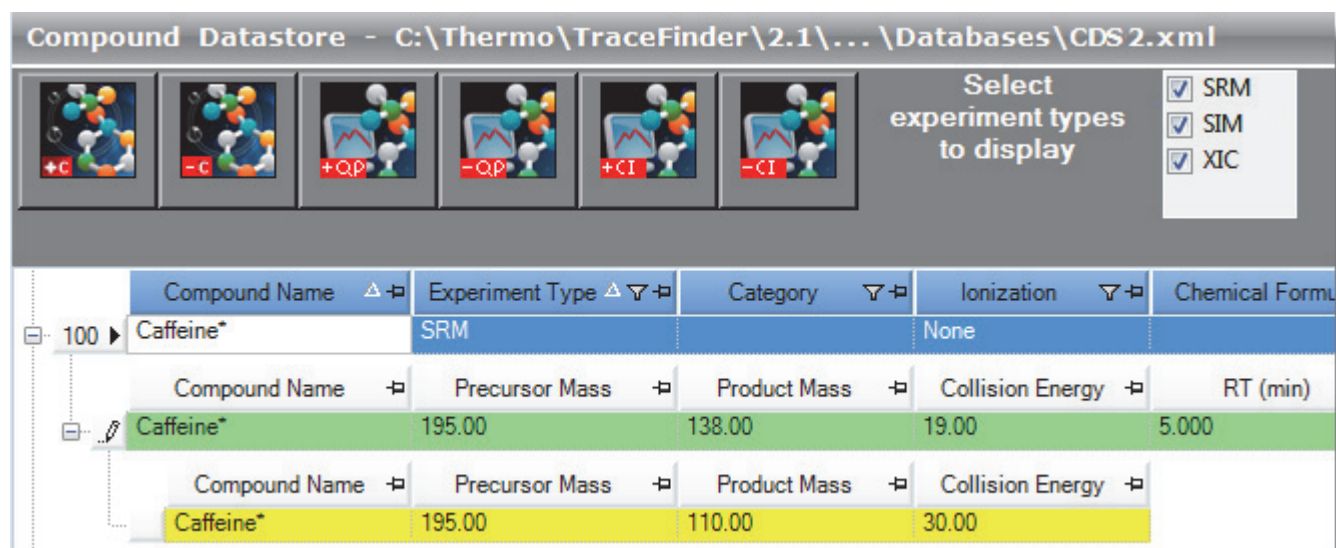| Parameter	Description
Ionization	(Optional) Alphanumeric identifier. Valid values: None, ESI, APCI, EI, CI, or APPI Default: None
Chemical Formula	(Optional) Alphanumeric chemical identifier.
Quantitative peak parameters	
Precursor Mass	The mass-to-charge ratio (*m/z*) of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio units. In confirming ion rows, the precursor mass is a noneditable copy of the quantitative peak precursor mass. Available only for SRM experiments. Default: 0.0 Range: 10.000 to 2999.999
Product Mass	The mass-to-charge ratio of the 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
Mass	The mass-to-charge ratio of the quantitation ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (*m/z*) units. Available only for XIC and SIM experiments. Default: 0.0 Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00
RT (min)	Retention time. The application uses RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Window (sec)	The application uses RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 499.50 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Polarity	**+** (positive) or **–** (negative)
Lens	(Optional) Range: –400 to 400

Table 9. Compound Datastore view parameters (Sheet 3 of 3)

Parameter	Description
Energy Ramp	(Optional) Available only for SRM experiments. Range: 0.00 to 200.00
Confirming ion parameters	
Precursor Mass	The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio (*m/z*) units. Available as a noneditible field only for SRM experiments. Default: 0.0 Range: 10.000 to 2999.999
Product Mass	The mass-to-charge ratio of the quantitation ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (*m/z*) units. Available only for SRM experiments. Default: 0.0 Range: 10.000 to 2999.999
Mass	The mass-to-charge ratio of the quantitation ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (*m/z*) units. Available only for XIC and SIM experiments. Default: 0.0 Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00

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

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

Follow these procedures:

- To import compounds

- To add a compound to the datastore

- To remove a compound

- To add a quantitative peak to a compound

- To remove a quantitative peak

- To add a confirming ion to a quantitative peak

- To remove a confirming ion

❖ **To import compounds**

1. Click **Import Compounds** in the Compound Datastore task pane.

2. Browse to a .csv or .xml compounds file and click **Open**.

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

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

Compound Name	ExperimentType	Category	Ionization	Ch
Monuron	SRM	Class 1	ESI	

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

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

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

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

❖ **To add a compound to the datastore**

1. Click the **Add Compound** icon, , or right-click the compounds list

   and choose **Add Compound** from the shortcut menu.

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

2. Click the first table cell, and type the required Compound Name parameter.

3. (Optional) Change the value for the Experiment Type.

   The default is SRM. For descriptions of available experiment types, see "Choosing Experiment Types" on page 66.

   After you add a quantitative peak to the compound, you cannot change the experiment type, even if you cancel the quantitative peak.

4. (Optional) Type a value or select a value from the Category list.

   You can use any alphanumeric string. After you type a new Category value, that value is available from the list.

5. (Optional) Change the values for Ionization.

   The default is None.

6. (Optional) Type a value for the Chemical Formula.

   You can use any alphanumeric string.

Each compound requires at least one quantitative peak.

❖ **To remove a compound**

1. Select the compound row that you want to delete.

2. Click the **Remove Compound** icon, , or right-click

   and choose **Remove Compound** from the shortcut menu.

3. If you are sure you want to delete the selected row, at the prompt, click **OK**.

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

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

❖ **To add a quantitative peak to a compound**

1. Select the compound.

2. Click the **Add Quan Peak** icon, , or right-click

   and choose **Add Quan Peak** from the shortcut menu.

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

Quantitative peak row

3. Enter all required parameters.

   For a list of required and optional parameters, see the list of "Compound Datastore view parameters" on page 59.

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

4. Repeat steps 2 through 3 to add as many as six quantitative peaks to the compound.

❖ **To remove a quantitative peak**

1. Select the row of the quantitative peak that you want to delete.

2. Click the **Remove Quan Peak** icon, , or right-click

   and choose **Remove Quan Peak** from the shortcut menu.

3. If you are sure you want to delete the selected row, at the prompt, click **OK**.

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

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

❖ **To add a confirming ion to a quantitative peak**

1. Click the **Add Confirming Ion** icon, , or right-click the quantitative peak row

   and choose **Add Confirming Ion** from the shortcut menu.

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

Confirming ion row

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

   The required confirming ion values differ for each experiment type. See "Choosing Experiment Types" on page 66.

3. Repeat steps 1 through 2 to add as many as 10 confirming ions to the quantitative peak.

❖ **To remove a confirming ion**

1. Select the confirming ion row that you want to delete.

2. Click the **Remove Confirming Ion** icon, , or right-click

   and choose **Remove Confirming Ion** from the shortcut menu.

3. If you are sure you want to delete the selected row, at the prompt, click **OK**.

   The application removes the selected confirming ion row.

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

❖ **To filter a list**

Click the funnel icon, , in the column header.

For each column, the application displays filterable criteria (compound names, experiment types, categories, or ionization methods) in a list. In all lists, you can choose to view all criteria or a specific type of criterion for that column.

Choosing Experiment Types

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

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

SRM: Selected Reaction Monitoring

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

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

XIC: Extracted Ion Chromatogram

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

Confirming ions include a single mass value.

SIM: Single Ion Monitoring

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

Confirming ions include a single mass value.

Application Configuration

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

This section includes the following tasks:

- Specifying the Reports Configuration

- Specifying Configuration Defaults

- Specifying Detection Parameters

- Enabling Optional Features

❖ **To open the Application Configuration view**

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

   The Configuration navigation pane opens. See "Configuration mode navigation pane" on page 38.

2. Click **Application Configuration**.

   The Application Configuration view opens.
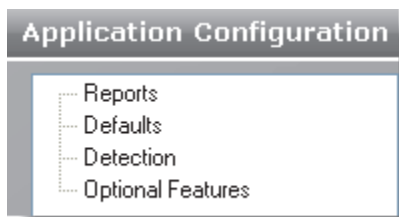
Table 10. Application Configuration pages

Page	
Reports	See "Specifying the Reports Configuration."
Defaults	See "Specifying Configuration Defaults" on page 73.
Detection	See "Specifying Detection Parameters" on page 76.
Optional Features	See "Enabling Optional Features" on page 88.

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

Specifying the Reports Configuration

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

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

C:\Thermo\TraceFinder\2.1\EFS\ExampleReports

Follow these procedures:

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

❖ **To open the Reports page**

In the Application Configuration view, click **Reports**.
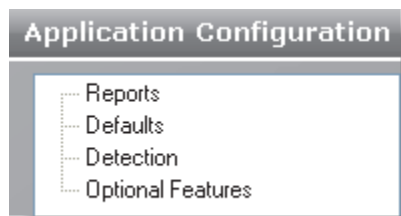
The Reports page of the Application Configuration view opens. For a list of reports, see "Reports" on page 70.

❖ **To specify which reports are available**

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

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

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

2. To create a single composite report for an entire batch (rather than 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. Batch-level reports are prepended with a **B** to differentiate them.

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

3. Do one of the following:

Apply the current selections as follows:

a. Click **Apply**.

A message prompts you to restart the TraceFinder application so that a user can access the reports you selected for the Method Development, Analysis, and Acquisition modes.

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

–or–

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

❖ **To import new reports**

1. Click **Import**.

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

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

Reports

The application uses the following standard, custom, and target screening reports (see Figure 10, Figure 11, and Figure 12, respectively). For descriptions of the parameters on the Reports page, see "Reports page parameters" on page 72.

Figure 10. Reports page showing standard reports

Figure 11. Reports page showing custom reports

Figure 12. Reports page showing target screening reports
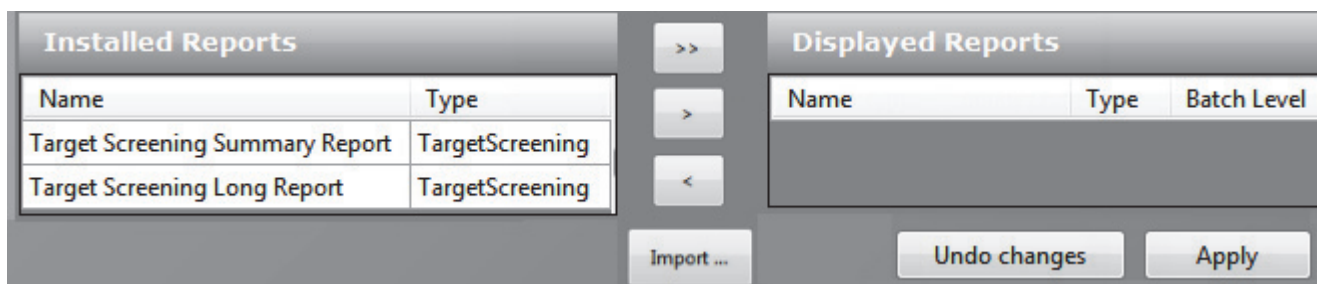
> **Note** Target screening reports are available only when you install the ToxID software and enable the target screening features. See "Enabling Optional Features" on page 88.

Table 11. Reports page parameters

Parameter	Description
Installed Reports	All reports listed in this pane are potentially available but are not selected for use in the application.
Displayed Reports	All reports listed in this pane are selected for use in the application.
>>	Moves all reports from the Installed Reports list to the Displayed Reports list.
>	Moves the selected reports from the Installed Reports list to the Displayed Reports list.
<	Moves the selected reports from the Displayed Reports list to the Installed Reports list.
<<	Moves all reports from the Displayed Reports list to the Installed Reports list.
Import	Opens a browser where you can select a report file to add to the Installed Reports list.
Undo Changes	Returns the report selections to their original state (when you first opened this page).
Apply	Applies the current selections, and prompts you to restart the TraceFinder application so that a user can access the reports you selected for the Method Development, Analysis, and Acquisition modes.

Specifying Configuration Defaults

Use the Application Configuration view of the Configuration mode to specify the default laboratory and instrument names, the displayed mass precision, and the intensity scale to use for reporting. When user security is enabled, only users in the LabDirector or ITAdmin role can access these features.

Follow these procedures:

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

❖ **To open the Application Defaults page**

In the Application Configuration view, click **Defaults**.
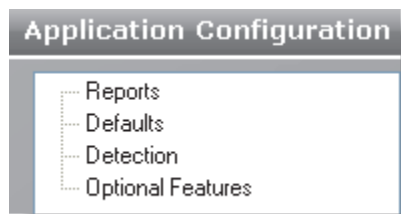
The Application Defaults page of the Application Configuration view opens.
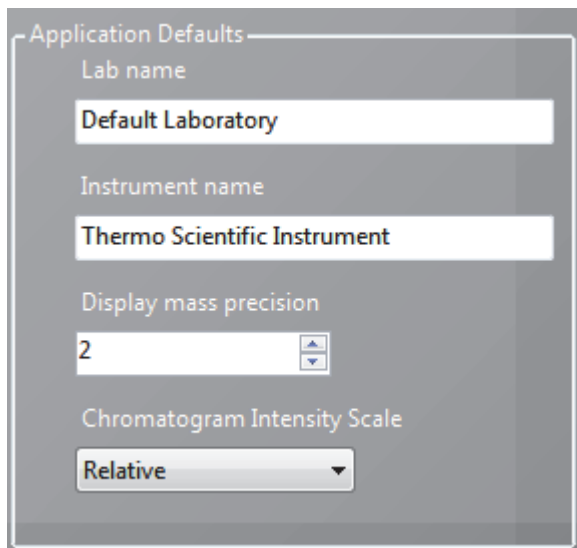
❖ **To specify a default laboratory name and instrument name**

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

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

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

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

4. Click **Yes**.

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

1. In the Display Mass Precision box, set the mass precision decimal places value to an integer from 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 **Relative** or **Absolute** from the Chromatogram Intensity Scale list.

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

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

4. Click **Yes**.

Specifying Detection Parameters

When user security is enabled, users in the LabDirector or ITAdmin role can specify detection parameters for the Genesis, ICIS, or Avalon detection algorithms. Use the Peak Detection Defaults page to specify a peak detection algorithm and its options and to determine the area under a curve.

This section includes procedures for specifying the following detection algorithms:

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

❖ **To specify common detection parameters**

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

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

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

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

   a. Select the unit of measure that you want to use.

   b. In the Value box, specify the number of millimass units or parts per million to use as the upper limit.

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

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

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

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

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

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

   b. In the Window (+/-%) box, select the acceptable ion ratio range.

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

6. In the Peak Detection Parameters area, select one of the detection algorithms: **Genesis**, **ICIS**, or **Avalon**.
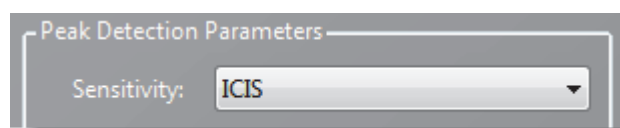
Figure 13. Common peak detection areas
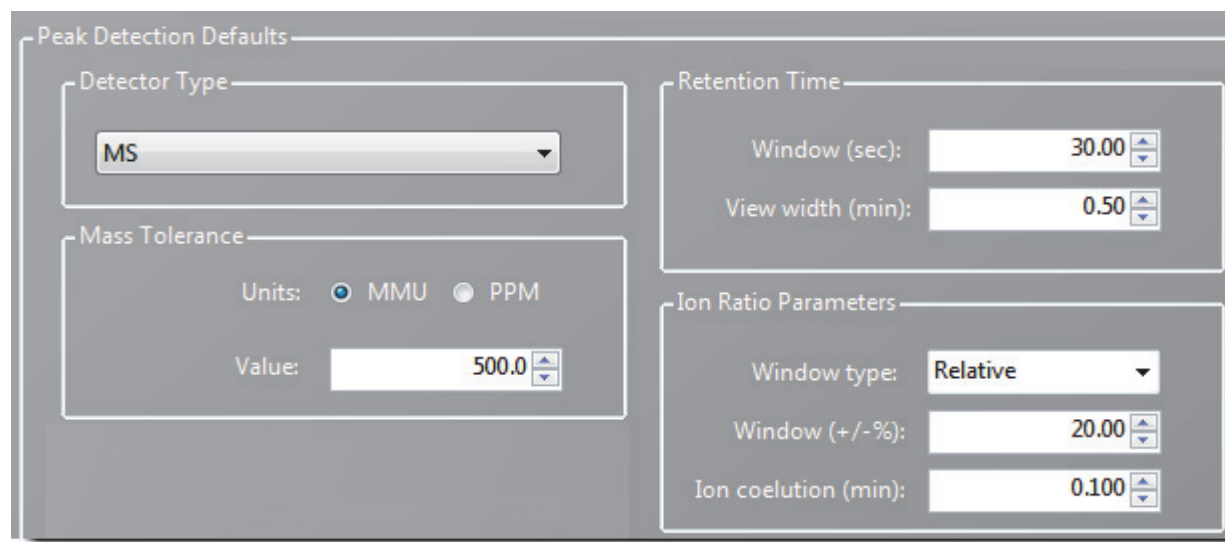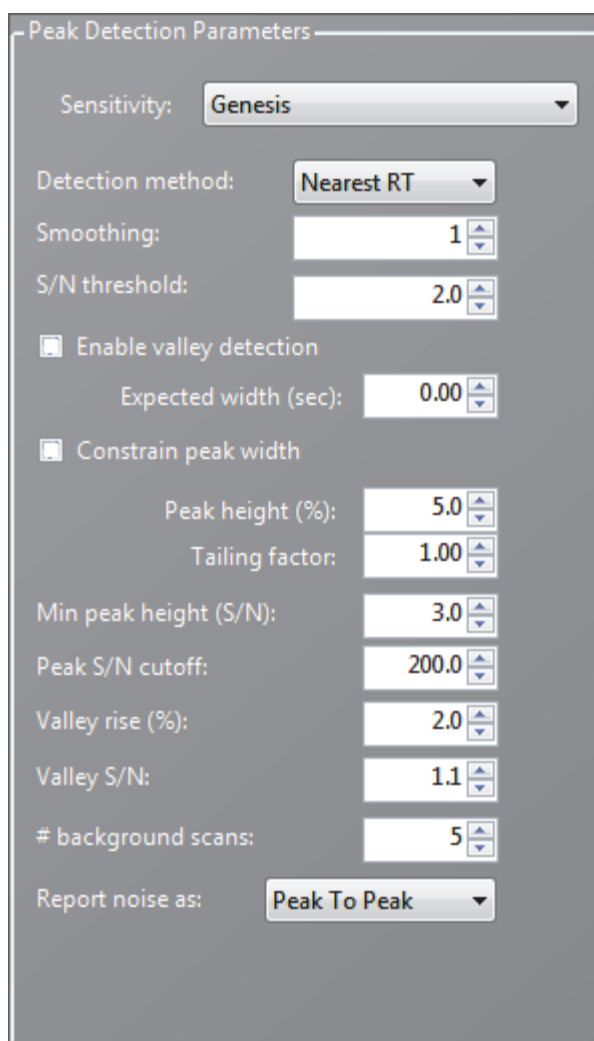
Table 12. Common peak detection parameters

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

Genesis Detection Method

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

Figure 14. Genesis peak detection page

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

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

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

Parameter	Description
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value. Default: 1 Range: Any odd integer from 1 through 15 points
S/N threshold	Current signal-to-noise threshold for peak integration. Peaks with signal-to-noise values less than this value are not integrated. Peaks with signal-to-noise values greater than this value are integrated. Range: 0.0 to 999.0
Enable Valley Detection	Uses the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Expected Width (sec)	The expected peak width parameter (in seconds). This parameter controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the *expected width*/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the TraceFinder application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. Range: 0.0 to 999.0
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a threshold and a tailing factor. Selecting the Constrain Peak Width check box enables the Peak Height (%) and Tailing Factor options.
Peak Height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when you select the Constrain Peak Width check box. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0
Min Peak Height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0

Table 13. Genesis peak detection page 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 15. ICIS peak detection page

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

Parameter	Description
Sensitivity	Specifies the ICIS peak detection algorithm.
Detection Method	Highest peak: Uses the highest peak in the chromatogram for component identification.
	Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value.

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

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

Parameter	Description
Area Noise Factor	The noise level multiplier used to determine the peak edge after the location of the possible peak. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 5
Peak Noise Factor	The noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value. Range: 1 through 1000 Default: 10
Baseline Window	The TraceFinder application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 40
Constrain Peak Width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box enables the Peak Height (%) and Tailing Factor options.
Peak Height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when you select the Constrain Peak Width check box. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0
Min Peak Height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0
Noise Method	The options are INCOS or Repetitive. INCOS: Uses a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. Repetitive: Uses a multiple pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but the analysis takes longer.

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

Parameter	Description
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 16. Avalon peak detection page

Table 15. Avalon peak detection page parameters

Parameter	Description
Sensitivity	Specifies the Avalon peak detection algorithm.
Detection Method	Highest peak: Uses the highest peak in the chromatogram for component identification. Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value. 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.
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 17. Avalon Event List dialog box
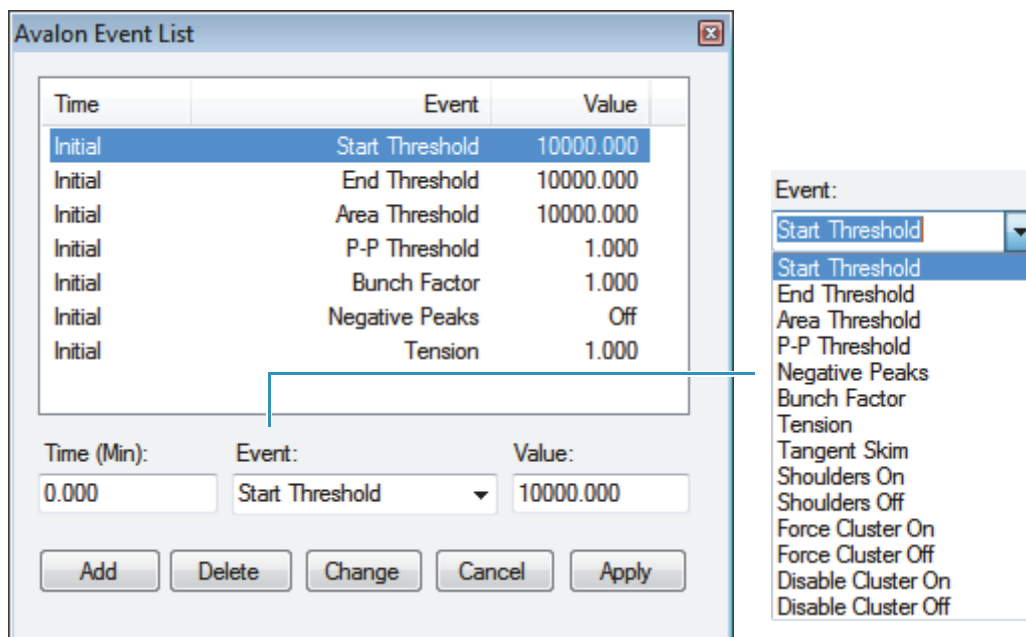
Table 16. Avalon Event List dialog box parameters

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

Figure 18. Event types

Table 17. Event type descriptions (Sheet 1 of 2)
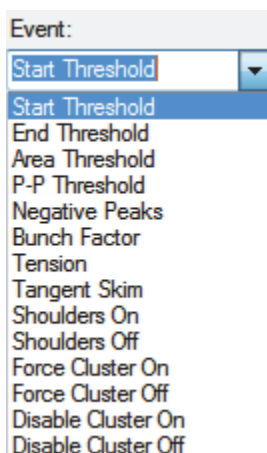
Event type	Description
Start Threshold	Specifies the threshold at the start of a peak. The Start Threshold is directly related to the RMS noise in the chromatogram. Range: 0 to 999 999 999
End Threshold	Specifies the threshold at the end of a peak. The End Threshold is directly related to the RMS noise 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 17. 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.

Enabling Optional Features

In the Application Configuration view of the Configuration mode, you can enable the
following features:

- User Security

- Target Screening

- Quick Acquisition

- EPA Tune Criteria

- Compound Datastore

- Multiplexing

- Delay Calibration Calculation

- Batch Wizard Style

- Acquisition Submission Options

❖ **To open the Optional Features page**

In the Application Configuration view, click **Optional Features**.
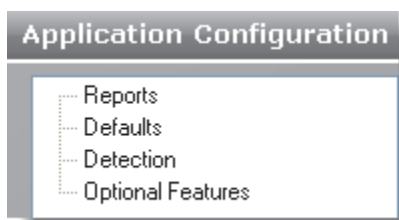
The Optional Features page of the Application Configuration view opens.
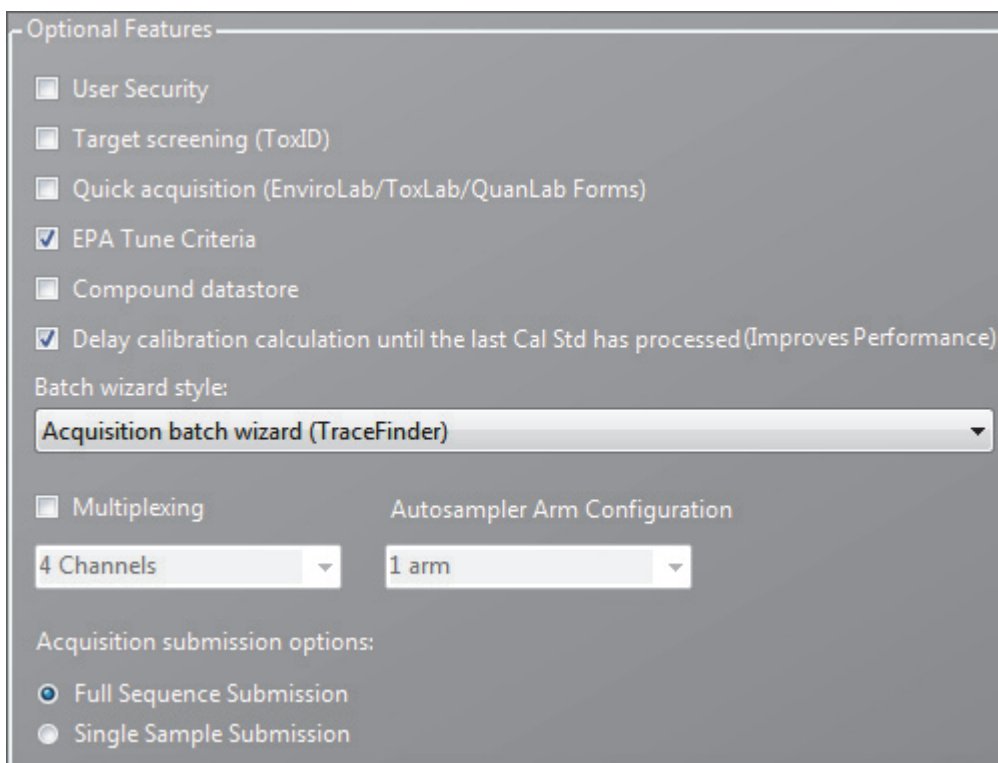
User Security

When user security is enabled, all users must log in to the TraceFinder application for access to only those modes assigned to their user role. See "Choosing User Roles" on page 46.

❖ **To turn on user security**

1. Select the **User Security** check box.

   When this check box is selected, all users must log in to the TraceFinder application for access to the modes assigned to their user role. See "Choosing User Roles" on page 46. When user security is enabled, only users in the LabDirector or ITAdmin roles can access the Configuration mode.

   When this check box is cleared, users are not required to log in to the TraceFinder application. When they start the application, the dashboard is the first screen that users see and all modes are available to them. The User Administration view in the Configuration mode is hidden from all users except those assigned the LabDirector or ITAdmin role.

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

2. Click **Apply**.

   A message prompts you to restart the TraceFinder application so that your changes can take effect.

3. Click **Yes**.

Target Screening

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

❖ **To enable target screening**

1. Select the **Target Screening (ToxID)** check box.

2. Click **Apply**.

   A message prompts you to restart the TraceFinder application so that your changes can take effect.

3. Click **Yes**.

For a list of available target screening reports, see "Reports" on page 70.

Quick Acquisition

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

> **Note** The Quick Acquisition feature is not available when you enable multiplexing. See "Multiplexing" on page 92.

❖ **To enable quick acquisition**

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

2. Click **Apply**.

   A message prompts you to restart the TraceFinder application so that your changes can take effect.

3. Click **Yes**.

For a description of the Quick Acquisition features, see "Working with Master Methods" on page 100.

EPA Tune Criteria

When you select the EPA Tune Criteria option, the application supports Tune, Breakdown, and Tune/Breakdown sample types and MSTune and Breakdown compound types. This option changes the Breakdown method to a Tune/Breakdown method on the General page of the Master Method View and adds the Tune tab to the QAQC page of the Master Method View.

❖ **To enable the tune criteria**

1. Select the **EPA Tune Criteria** check box.

   By default, the EPA Tune Criteria option is selected.

2. Click **Apply**.

   A message prompts you to restart the TraceFinder application so that your changes can take effect.

3. Click **Yes**.

For a description of the Tune/Breakdown method on the General page of the Master Method View, see "Editing the General Page" on page 121.

For a description of the Tune page on the QAQC page of the Master Method View, see "Editing the QAQC Page" on page 183.

Compound Datastore

❖ **To enable the compound datastore**

1. Select the **Compound Datastore** check box.

   By default, the Compound Datastore option is not selected.

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

3. Click **Yes**.

   The application implements the following changes:

   • Displays the Acquisition List page on the Compounds page in the Master Method View. See "Editing the Compounds Page" on page 129.

   • Displays the Compound Datastore task pane on the Configuration mode navigation pane. See "Compound Datastore" on page 55.

   • Enables the Export SRM Data command in the Method Development mode. See "Exporting SRM Data" on page 227.

Multiplexing

The Multiplexing options are available only when you have installed the Power Modules. See "Installing the Power Modules" on page 13.

❖ **To specify multiplexing features**

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

2. Choose **2 Channels** or **4 Channels**.

3. When you are using 2 channels, select a 1- or 2-arm autosampler configuration.

   The **1 arm** configuration enables channels 1 and 3; the **2 arm** configuration enables channels 2 and 4.
   When you use a 4-channel configuration, autosampler 1 uses channels 1 and 3 and autosampler 2 uses channels 2 and 4.

4. Click **Apply**.

   A message prompts you to restart the TraceFinder application so that your changes can take effect.

5. Click **Yes**.

When you enable multiplexing, the following optional features are not available:
   • Quick Acquisition
   • Batch Template Wizard
   • Single Sample Submission (Intelligent Sequencing)

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 255) or monitor an acquisition (see "Devices Page" on page 282).

Delay Calibration Calculation

Use the Delay Calibration Calculation… option to make the application wait until it processes the last calibration sample in a batch before it calculates the calibration curve (faster) instead of recalculating the calibration curve after each calibration sample (more responsive).

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

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

   By default, this option is selected.

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

3. Click **Yes**.

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 enable multiplexing, the application automatically enables 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 331.

   > **Note** The Batch Template Wizard feature is not available when you enable multiplexing. See Multiplexing.

2. Click **Apply**.

   A message prompts you to restart the TraceFinder application so that your changes can take effect.

3. Click **Yes**.

Acquisition Submission Options

To control acquisitions, you can enable full-sequence or single-sample submission options. 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 are using Full Sequence Submission, priority batches always run immediately after the currently acquiring batch completes.

• When you are using Single Sample Submission, priority batches always run immediately after the currently acquiring sample completes.

❖ **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 preparation for all sample injections when the pre-run condition begins. All samples in the batch must complete before other batches (even higher priority batches) can begin.

- 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 enable multiplexing. See "Multiplexing" on page 92.

2. Click **Apply**.

A message prompts you to restart the TraceFinder application so that your changes can take effect.

3. Click **Yes**.

Using the Method Development Mode

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

> **Contents**
>
> - Working with Master Methods
> - Working with Instrument Methods
> - Working with Development Batches
> - Using Quick Acquisition

From the Method Development mode, you can create a 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** from the dashboard or the navigation pane.

The Method Development navigation pane opens. For detailed descriptions of all the features on the Method Development navigation pane, see "Method Development navigation pane."

Figure 19. Method Development navigation pane

Available only when you enable the Compound Datastore feature in the Configuration mode.

Available only when you select the Acquisition Batch Wizard as your wizard style in the Configuration mode.
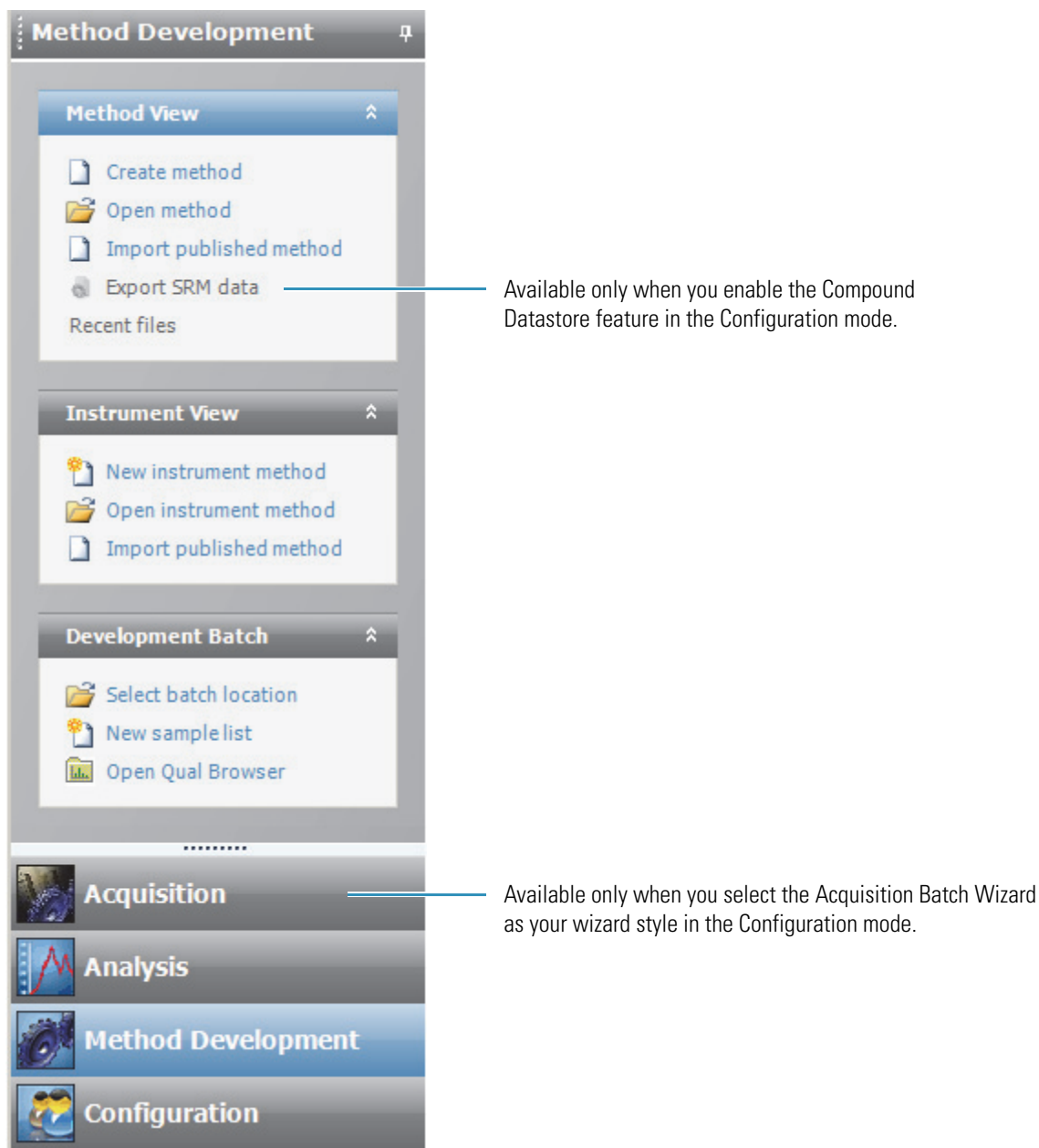
Table 18. Method Development navigation pane commands (Sheet 1 of 2)

Command	Description
Method View	See "Working with Master Methods" on page 100.
Create Method	Opens the Create Master Method dialog box where you can choose the process that you want to use to start your master method.
Open Method	Opens the Open Master Method dialog box where you can choose a master method to open.

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

Command	Description
Import Published Method	Opens the Import Published Method dialog box where you can select a published method to import.
Export SRM Data	Writes the selected reaction monitoring (SRM) table to the following file:
	…\Thermo\TraceFinder\2.1\EFS\Methods*methodname*.xml
	You can use this data in the instrument method editor when you open the TSQ 2.1 application. This command is displayed only when you enable the Compound Datastore option in the Configuration mode. See "Compound Datastore" on page 92.
	The compounds in the Acquisition List must contain at least one SRM experiment type.
Recent Files	Displays recently saved master methods.
Instrument View	See "Working with Instrument Methods" on page 228.
New Instrument Method	Opens the Instrument View where you can specify instrument settings for your configured instruments.
	If the instrument that you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the application. You cannot configure an instrument while the TraceFinder application is running.
Open Instrument Method	Opens a browser where you can choose an instrument method to open.
Development Batch	See "Working with Development Batches" on page 235.
Select Batch Location	Specifies a location to store temporary development batch raw data files.
New Sample List	Removes acquired samples from your development batch so that you can start a new sample list.
Open Qual Browser	Opens the Thermo Xcalibur Qual Browser where you can view the acquired raw data files.

Working with Master Methods

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

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

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

This section includes instructions for the following tasks:

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

Creating a New Master Method

To begin a master method, follow any of four different procedures in the Create Master Method dialog box:

- Creating a New Method with Method Forge

- Importing an Xcalibur Master Method

- Associating a Raw Data File

- Selecting Compounds from the Compound Datastore

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

Figure 20. Create Master Method dialog box
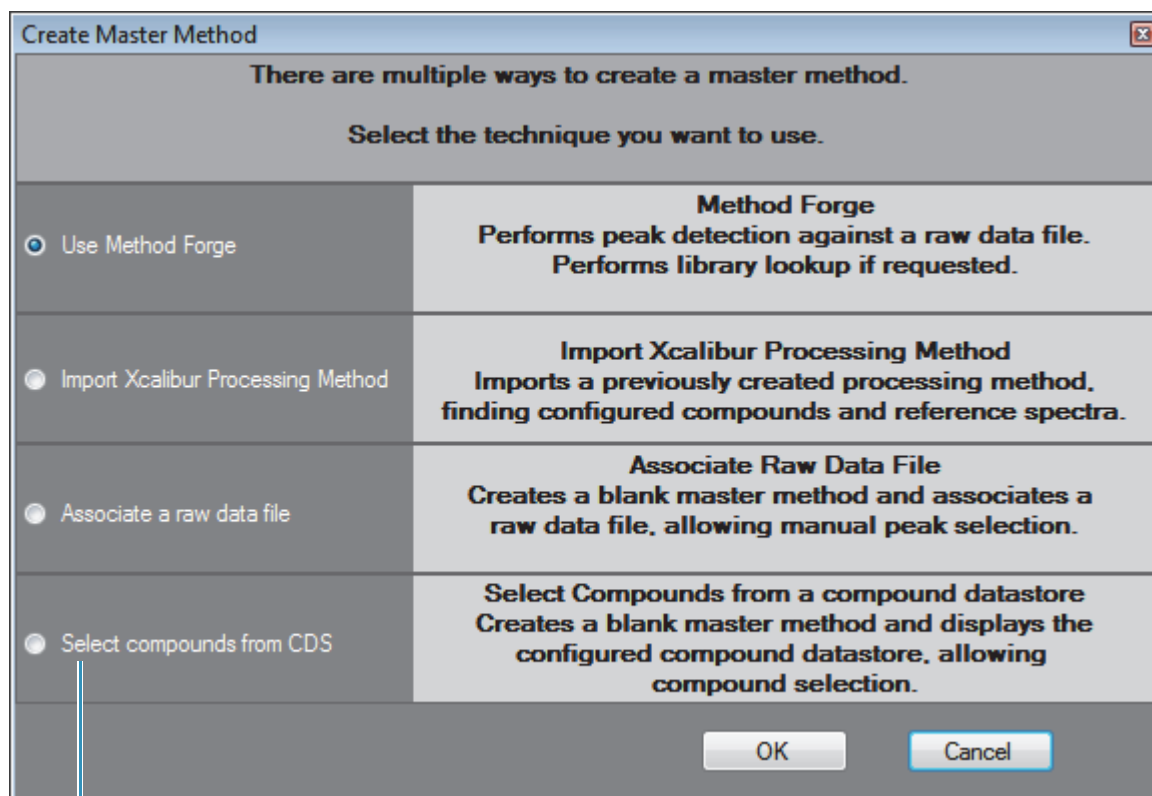
Available only when you enable the Compound Datastore feature in the Configuration mode.

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 parameters" on page 108.

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 Method View task pane, click **Create Method**.
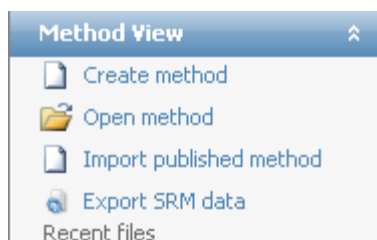
The Create Master Method dialog box opens. See "Create Master Method dialog box" on page 101.

2. Select the **Use Method Forge** option and click **OK**.
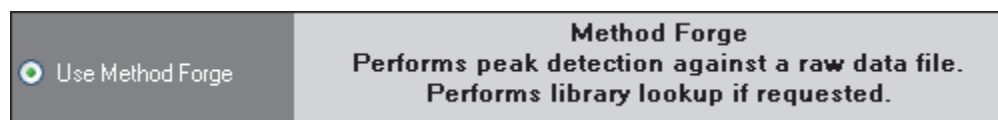
The Method Forge dialog box opens. For detailed descriptions of all the features on the Method Forge dialog box, see "Method Forge dialog box" on page 108.

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.

3. In the Method Forge dialog box, do one of the following:

Select the **Use the Default Template** option.

–or–

Select the **Select a Custom Template** option and highlight your custom template in the Method template table.

For detailed instructions on creating a custom method template, see "Creating a Method Template" on page 216.

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

You can enter an existing method name and overwrite it when you create the method. If you do not specify a name, the application names the method for the raw data file used to create the method.

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

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

Choose **Manual Injection**.

–or–

Specify the autosampler settings:

   a. Choose **Use Autosampler**.

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

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

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

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

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

- 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 NIST library and displays the identified compound names instead of the peak times.

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

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

9. (Optional) Select the compounds that you want to add to the compound datastore and click **Add to CDS**.

The selected compounds are added to the current compound datastore.

> **Note** You must click **Add to CDS** before you continue to the method.

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

    The TraceFinder application uses all compounds found in the raw data file in your method and displays the General page of the Master Method View. For detailed descriptions of all the features on the General page, see "General page" on page 126.

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

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

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

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

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

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

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

    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 119.

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

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

   Method View
   - Create method
   - Open method
   - Import published method
   - Export SRM data
   - Recent files

   The Create Master Method dialog box opens. See "Create Master Method dialog box" on page 101.

2. Select the **Use Method Forge** option and click **OK**.
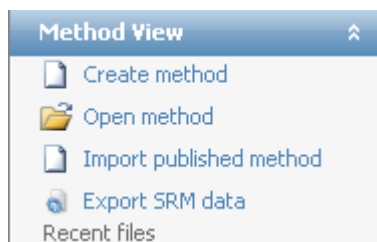
   ⦿ Use Method Forge
   Method Forge
   Performs peak detection against a raw data file.
   Performs library lookup if requested.
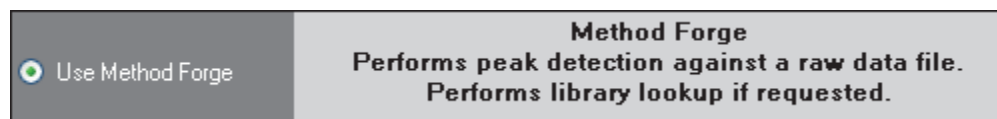
   The Method Forge dialog box opens. For detailed descriptions of all the features on the Method Forge dialog box, see "Importing an Xcalibur Master Method" on page 110.

3. Do one of the following:

   Select the **Use the Default Template** option.

   –or–

   Select the **Select a Custom Template** option and highlight your custom template in the Method Template table.

   For detailed instructions about creating a custom method template, see "Creating a Method Template" on page 216.

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

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

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

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

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

   The Master Method View displays a list of possible matches in the Library Results pane. The TraceFinder application displays the best match in the Compound Name list and displays the peak spectrum for that compound.
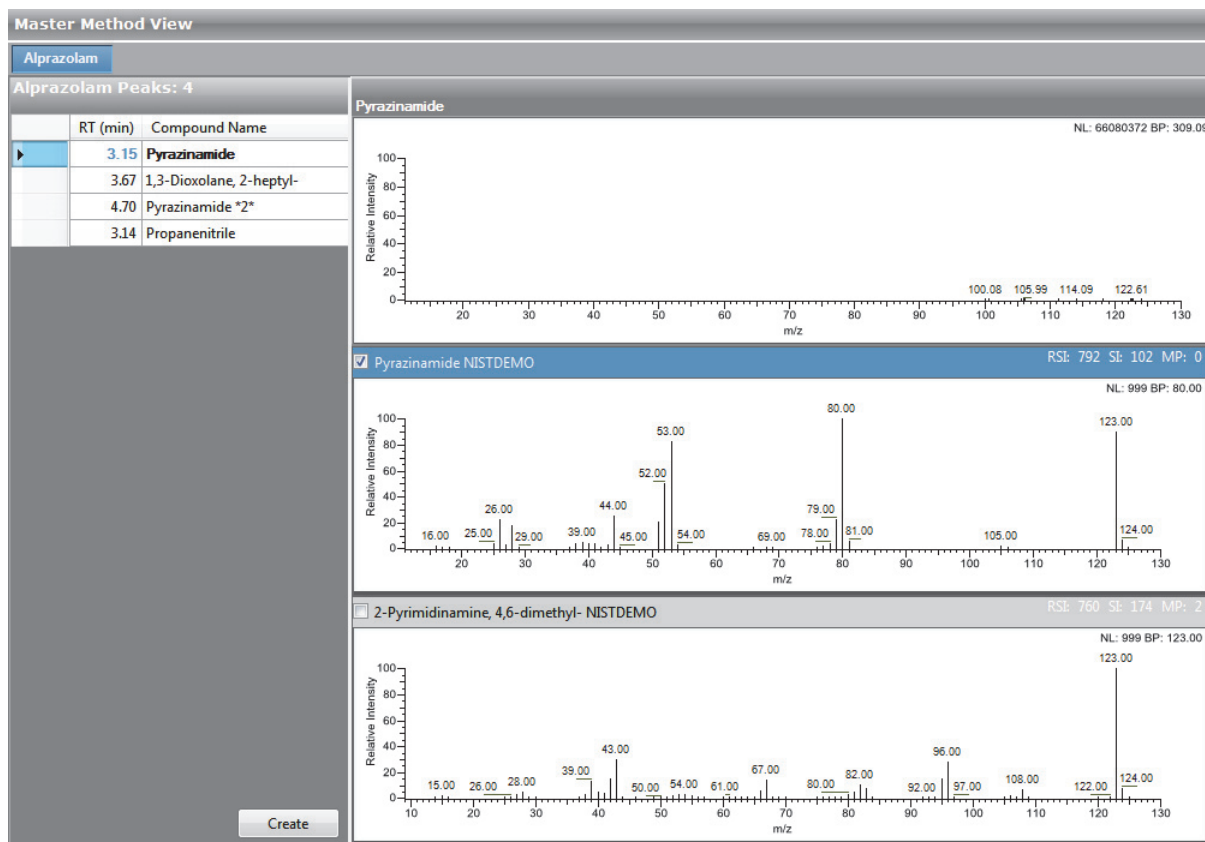
8. To use a compound other than the compound chosen by the TraceFinder application, scroll to the spectrum for that compound and select the compound name in the header of the spectrum pane.
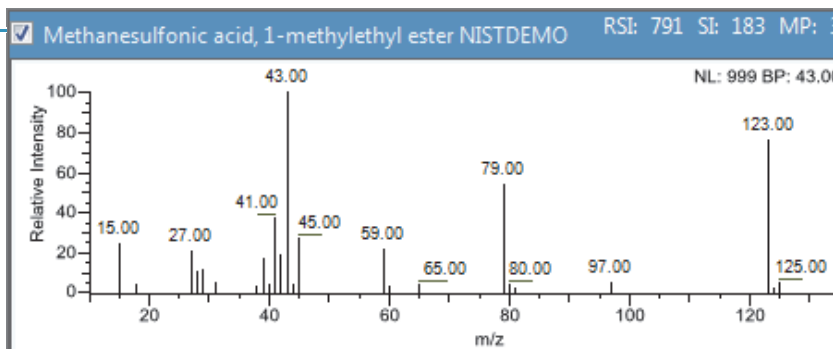
Selected compound

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

   The TraceFinder application uses all compounds found in the raw data file in your method and displays the General page of the Master Method View. For detailed descriptions of all the features on the General page, see "General page" on page 126.

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

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

    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 119.

Figure 21. Method Forge dialog box
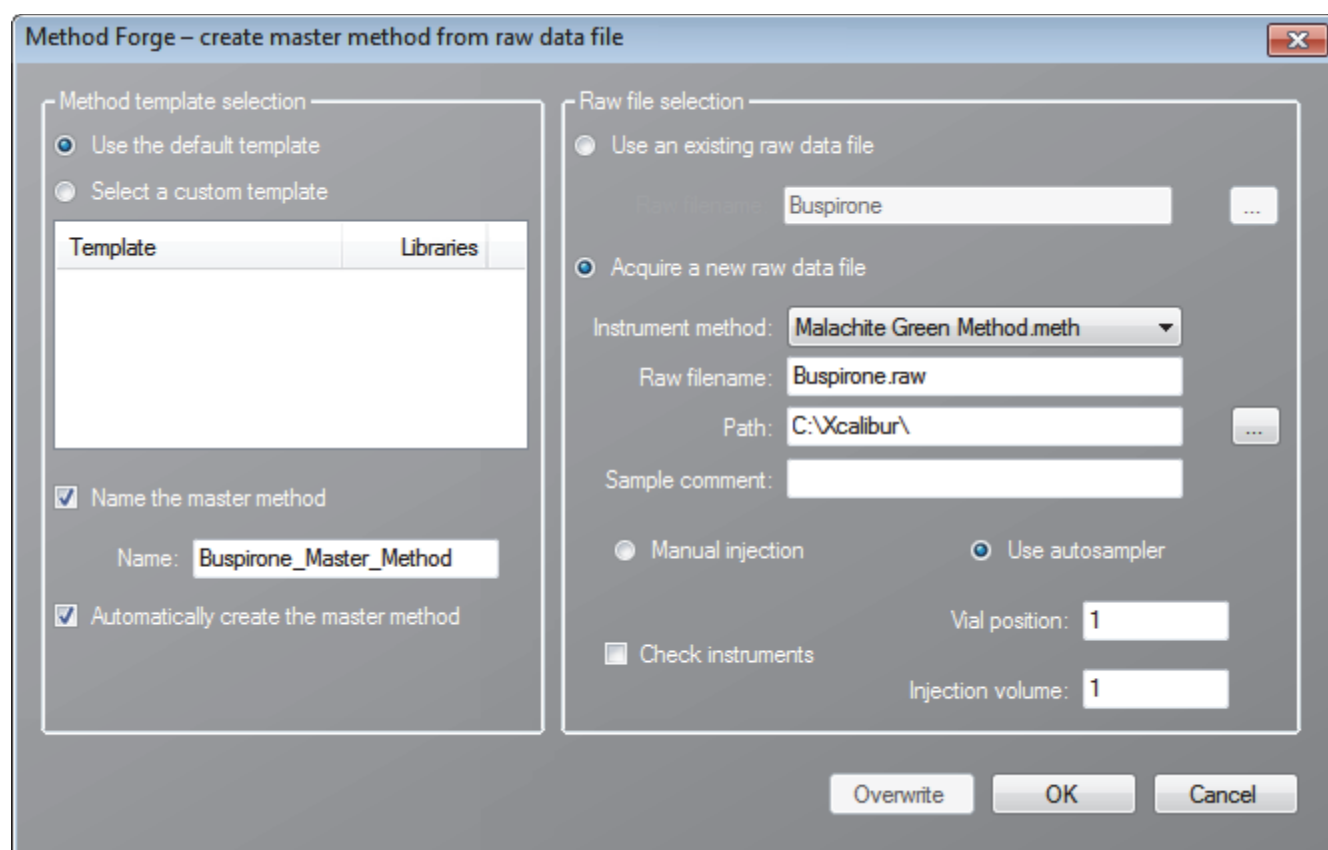
Table 19. Method Forge dialog box parameters (Sheet 1 of 2)

Parameter	Description
Method template selection	
Use the Default Template	Creates a new method with the default template.
Select a Custom Template	Lists all the available method templates.
	For detailed instructions about creating a custom method template, see "Creating a Method Template" on page 216.

Table 19. Method Forge dialog box parameters (Sheet 2 of 2)

Parameter	Description
Name the Master Method	The name for the new master method.
Automatically Create the Master Method	When the acquisition completes, Method Forge performs peak detection, library searching, and identification of characteristic ion and reference spectrum. This information is loaded into a new master method. This process occurs immediately when you specify an existing raw data file.
Raw file selection	
Use an Existing Raw Data File	Enables the Raw Filename box where you can select a raw data file used in creating the master method.
Acquire a New Raw Data File	Enables 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.
Function button	
Overwrite	Overwrites the specified master method name. This function is enabled only when the specified master method name already exists.
OK	Creates a master method using the data and parameters 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. From the Method View task pane, click **Create Method**.
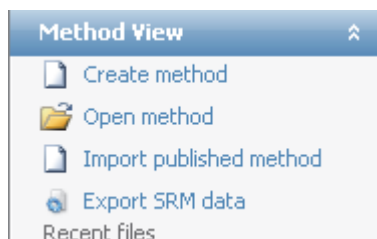
The Create Master Method dialog box opens. See "Create Master Method dialog box" on page 101.

2. Select the **Import Xcalibur Processing Method** option and click **OK**.

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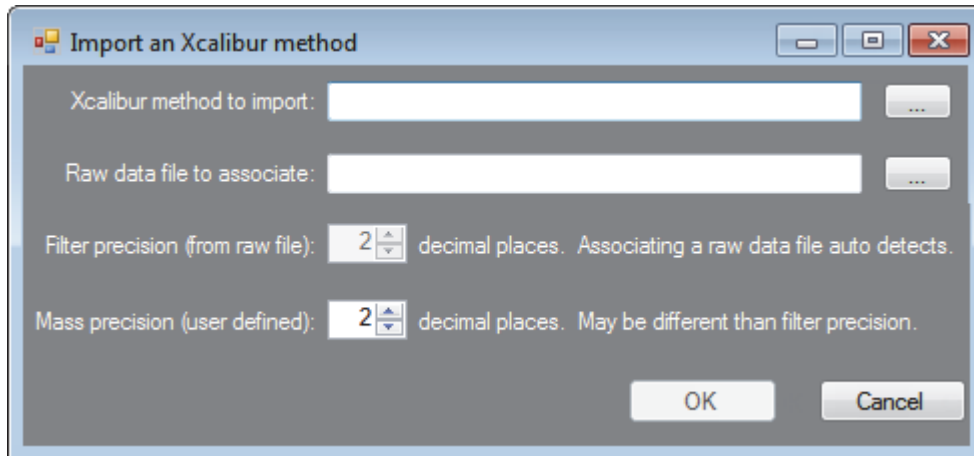
3. Click the browse button for the Xcalibur Method to Import box, browse to the Xcalibur processing method file, and open the file.

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

4. (Optional) Click the browse button for the Raw Data File to Associate box, browse to 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:

C:\Thermo\TraceFinder\2.1\EFS\Methods*MethodName*

5. (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.
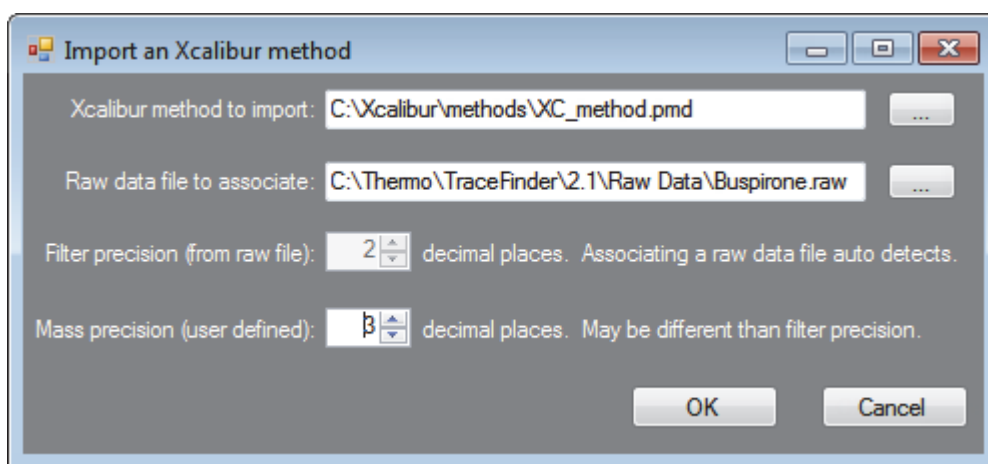
> **Note** When you associate a raw data file, the application reads the filter precision from the associated file so that you cannot change the Filter Precision value.

6. Click **OK**.

If the compounds in the imported Xcalibur method file are not in the Compound Datastore, the TraceFinder application displays the compounds in the Edit Compound Dependent Parameters dialog box.
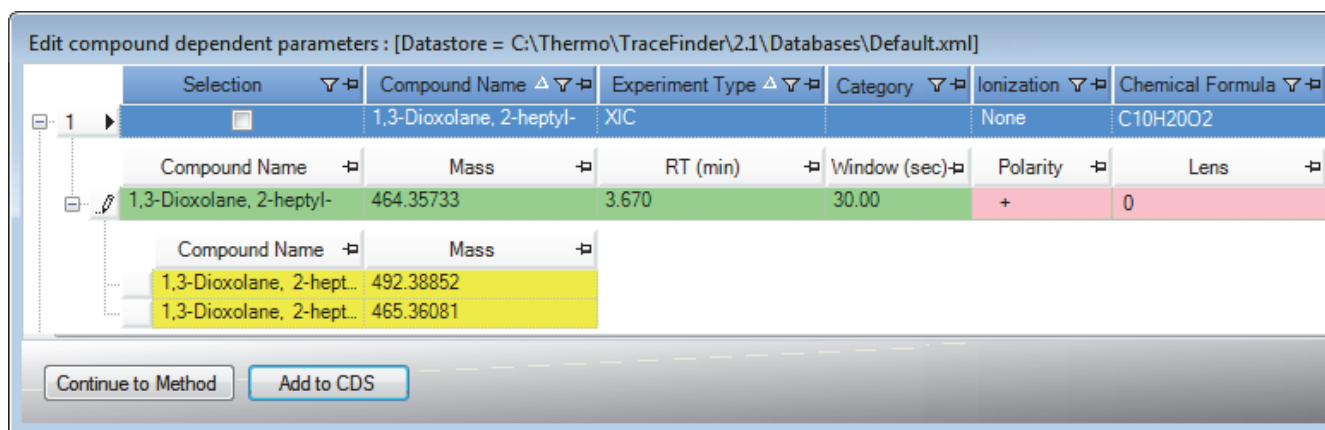
7. (Optional) Select the compounds that you want to add to the Compound Datastore and click **Add to CDS**.

    The selected compounds are added to the current compound datastore.

    To add these compounds to the datastore, you must click Add to CDS before you continue to the method. When you click Continue to Method, the Edit Compound Dependent Parameters dialog box closes and you cannot return to add the compounds.

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

    The TraceFinder application adds all compounds found in the imported Xcalibur method and displays the General page of the Master Method View. For detailed descriptions of all the features on the General page, see "General page" on page 126.

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

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

    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 119.

Working with Master Methods

Associating a Raw Data File

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

Follow these procedures:

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

❖ **To associate a raw data file with the method**

1. From the Method View task pane, click **Create Method**.
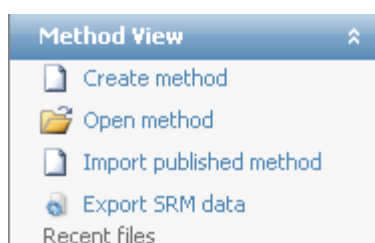
The Create Master Method dialog box opens. See "Create Master Method dialog box" on page 101.

2. Select the **Associate a Raw Data File** option and click **OK**.
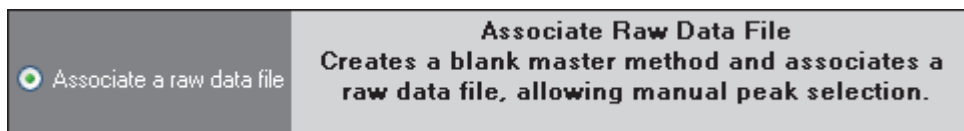
The Associate a Raw Data File dialog box opens.
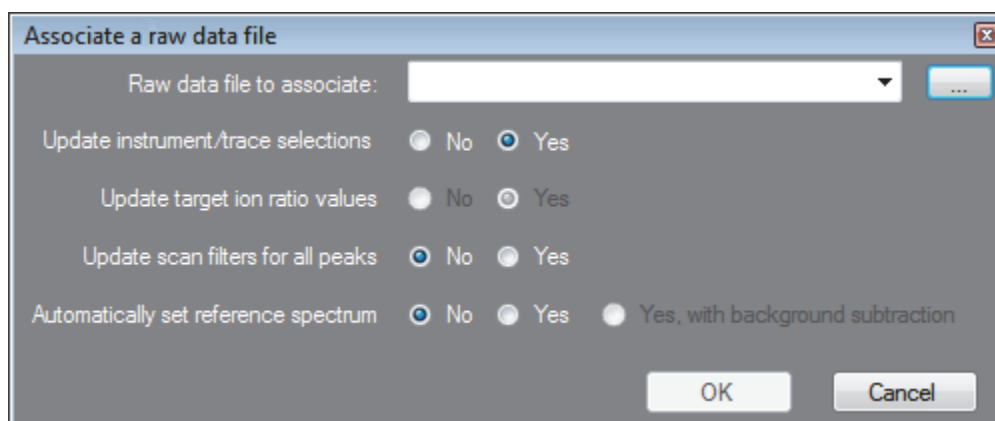
3. Browse to a raw data file to associate with the method (or select from the list of previously associated raw data files) and open the file.

   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:

   C:\Thermo\TraceFinder\2.1\EFS\Methods

4. 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 150.

   - **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.

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

5. Click **OK**.

   The TraceFinder application displays the General page of the Master Method View. For detailed descriptions of all the features on the General page, see "General page" on page 126.

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

7. To add compounds to the method, follow the instructions "To add compounds to the method" on page 115.

   To save the method, it must include at least one compound.

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

   For a detailed description of how to modify a master method, see "Editing a Master Method" on page 119.

❖ **To add compounds to the method**

1. Click the **Compounds** tab.

   The Detection page is selected by default.

General	Compounds	QAQC	Groups	Reports
Identification	Detection	Calibration		Calibration levels
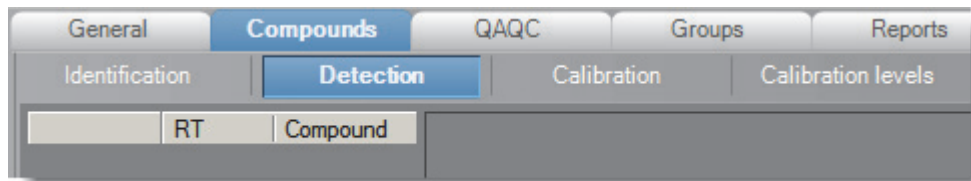
	RT	Compound	

   > **Note** When the Compound Datastore is enabled, the Compounds page includes an Acquisition List tab. See "Enabling Optional Features" on page 88.

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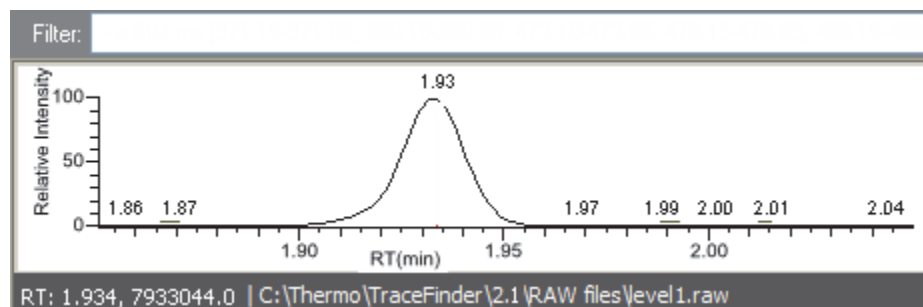
2. Select a filter from the Filter list.

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

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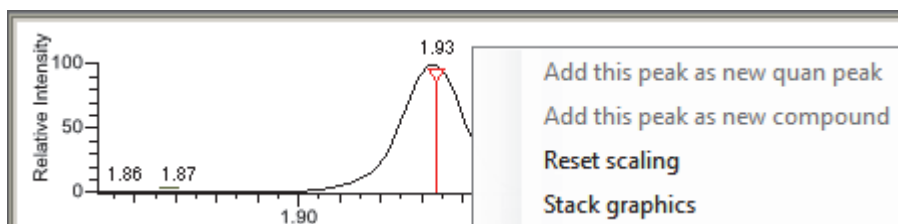
   The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quantitative peak, and the second and third largest ions as the confirming ion peaks.

   > **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.

5. (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.

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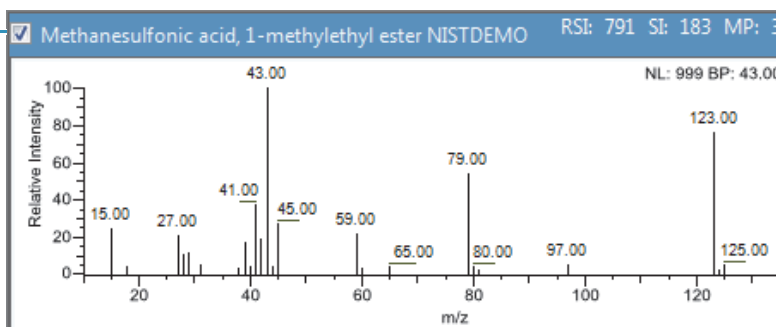
b. In the Type of Compound to Add list, select a compound type.

c. Click **OK**.

6. 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 129.

For detailed descriptions of how to modify a master method, see "Editing a Master Method" on page 119.

Selecting Compounds from the Compound Datastore

You can select compounds from the compound datastore to create a new master method. This method for creating a master method is available only when the compound datastore is enabled. See "Compound Datastore" on page 92.

❖ **To select compounds from the datastore**

1. From the Method View task pane, click **Create Method**.
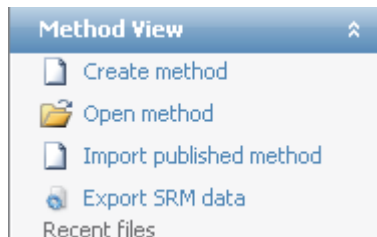
The Create Master Method dialog box opens.

2. Select the **Select Compounds from CDS** option and click **OK**.
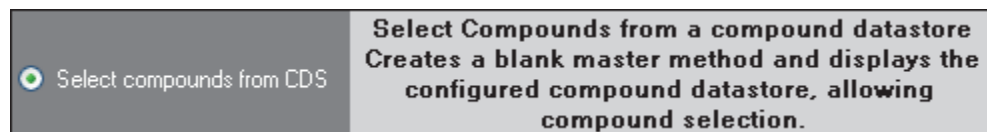
The Select Compounds to Add dialog box opens, listing all the compounds defined in the compound datastore.
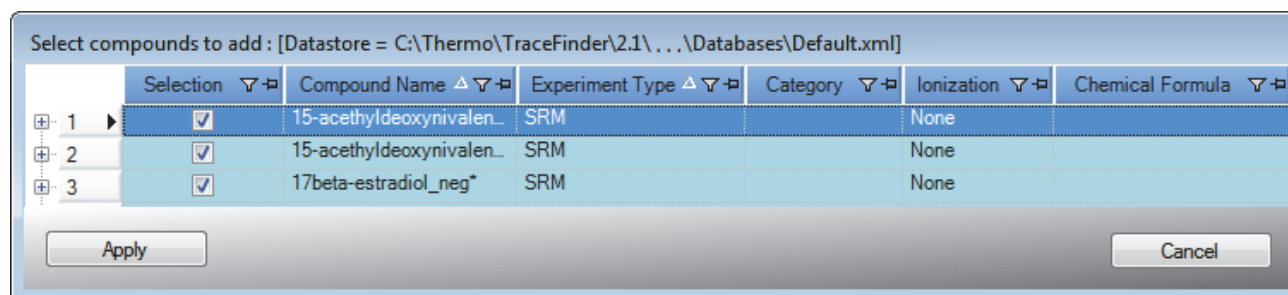
3. Select the check box for each of the compounds that you want to add to the method.

4. To quickly select multiple compounds, right-click and use any of the commands on the shortcut menu.

Table 20. Select Compounds to Add shortcut menu commands

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

5. Click **Apply**.

   The TraceFinder application adds the selected compounds to the method.

   Note After you add a compound to a method, the compound is no longer enabled in the Select Compounds to Add dialog box. You cannot remove the applied compounds from the method by returning to this dialog box. To remove a compound from a method, see "Acquisition List" on page 129.

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

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

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

Editing a Master Method

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

This section includes instructions for the following tasks:

- Opening a Master Method

- Editing the General Page

- Editing the Compounds Page

- Editing the QAQC Page

- Editing the Groups Page

- Editing the Reports Page

Opening a Master Method

Use the TraceFinder application to open a master method that was created and saved in the current TraceFinder application or converted from these legacy applications: TraceFinder, EnviroLab Forms, QuanLab Forms, or ToxLab Forms. To convert legacy methods, see "Converting Legacy Data" on page 19.

❖ **To open a saved master method**

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

The Method Development navigation pane opens.
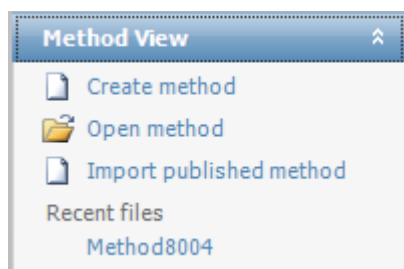
2. In the Method View task pane, do one of the following:

Click **Open Method.**

–or–

Click a method name in the Recent Files list.

When you save a method, the application adds it to the Recent Files list. The Recent Files list displays a list of your most recently saved master method files.

The Open Master Method dialog box opens, displaying all available methods.
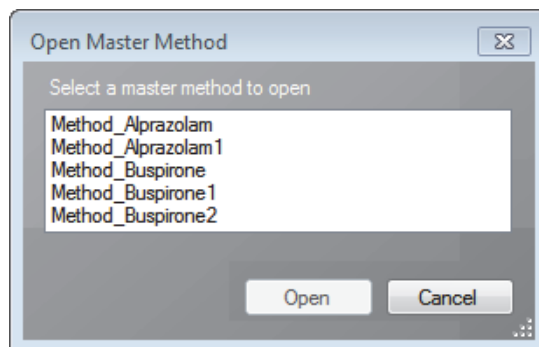
3. Select a master method and click **Open**.

The TraceFinder application copies all components of the selected method including its associated instrument method.

The General page for the selected method opens in the Method View. For detailed descriptions of all the features on the General page, see "General page" on page 126.

Editing the General Page

The General page defines basic information about the master method. For detailed descriptions of all the features on the General page, see "General page" on page 126.

Follow these procedures:

- To specify general information for a master method

- To edit the instrument method parameters

- To select a qualitative peak processing template

- To set automated background subtraction options

- To specify a chromatogram reference sample

- To specify mass tolerance

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

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

   The default name is Default Laboratory.
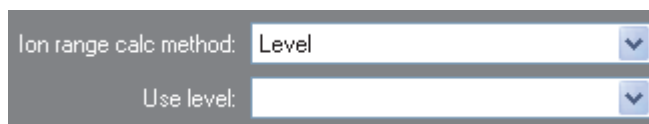
2. In the Assay Type box, type the assay type to be targeted by the method.

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

   Use 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 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 calibration levels on the Compounds page, see "Editing the Compounds Page" on page 129.

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

❖ **To edit the instrument method parameters**

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

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

   The Thermo Xcalibur Instrument Setup dialog box opens. This example of an instrument setup shows multiple configured instruments.
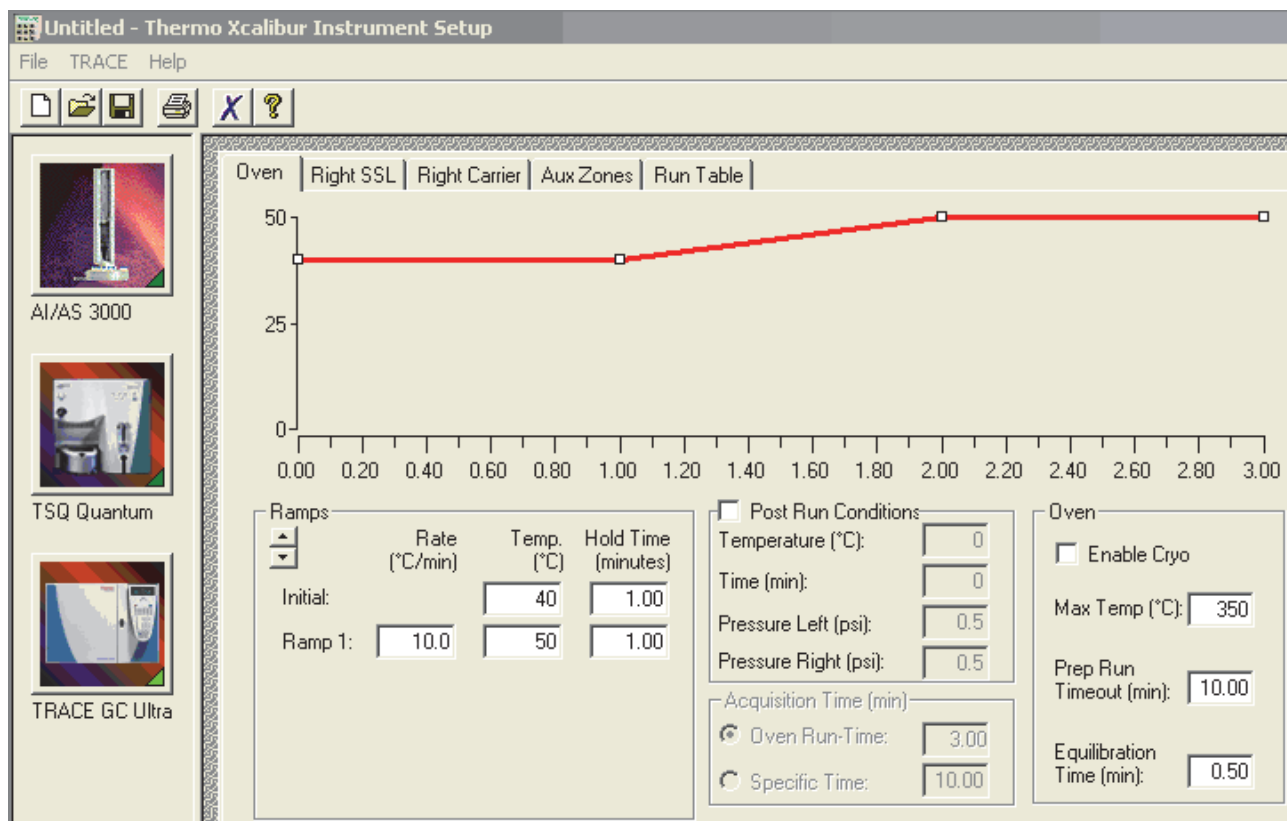
3. Edit the values on the instrument page for your instrument.

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" on page 126.

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.
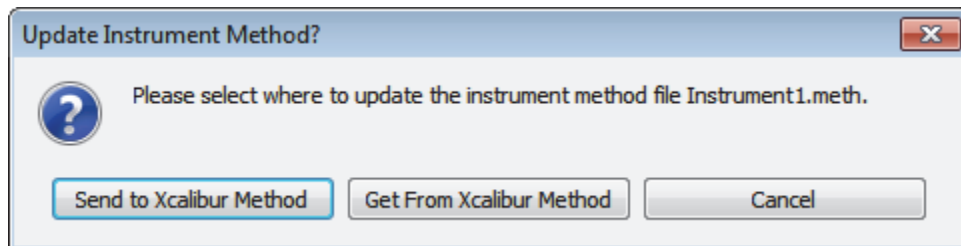
6. Choose one of the following options:

   • **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:

   C:\Thermo\TraceFinder\2.1\EFSTemplates\Methods

❖ **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.

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

This is the number of scans that the TraceFinder application subtracts from the background after averaging. If you selected 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 ⬍

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.

❖ **To specify a chromatogram reference sample**

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

Set chromatogram reference sample:	External ▾	
Set Reference sample:		Select

2. Click **Select**.

The Open Chromatograph Reference Sample dialog box opens.

Open Chromatogram Reference Sample	

⊟ 🔲 Default
  ⊟ 📁 Default
    ▥ Batch_Alprazolam1
    ▥ Batch_Alprazolam2
	cal_1
	solvent
	UnknownA1

Select a reference sample from the right panel and click "Open".	Open Cancel

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 Master Method View.

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

❖ **To specify mass tolerance**

1. Select the units of measure 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.

Figure 22. General page

Table 21. 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 Configuration Defaults" on page 73.
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 through 5000 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 129.
Instrument Method	Instrument method used for acquiring samples.
Tune/Breakdown	Breakdown or tune method used for processing 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

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

Parameter	Description
Number of Scans to Subtract	Valid values: Even numbered integers Default: 0
Stepoff Value	Offset from the selected peak to the first subtracted peak.
Set Chromatogram Reference Sample	Valid values: None, External Default: None
Set Reference Sample	This parameter is enabled only when you set Set Chromatogram Reference Sample to External. Click Select to choose a reference sample from the project folders.
Mass Tolerance	Upper limit of MMU or PPM. Default: 500 Range: 0.1 through 50 000 • (Default) MMU (millimass units): MMU is a static calculation to the extracted mass. • PPM (parts per million): PPM is a variable calculation dependent on the actual mass. The smaller the mass, the narrower the tolerance range. The larger the mass, the wider the tolerance range.
Notes	Optional notes about the method.

Editing the Compounds Page

Use the Compounds page to set all parameters used to identify, detect, and quantify the target compound list.

From the Compounds page of the Master Method View, you can access the following pages:

Acquisition List   See also "Acquisition List page parameters" on page 131.

Identification   See also "Identification page parameters" on page 134.

Detection   See also "Detection page panes" on page 147.

Calibration   See also "Calibration page parameters" on page 173.

Calibration Levels   See also "Calibration levels page parameters" on page 176.

QC Levels   See also "QC levels page parameters" on page 178.

Real Time Viewer   See also "Real Time Viewer page parameters" on page 179.

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 181.

Acquisition List

The Acquisition List page displays all compounds defined for the current method. From this page, you can add or delete compounds from the method. For detailed descriptions of all the features on the Acquisition List page, see "Acquisition List page parameters" on page 131.

The Acquisition List page is displayed only when you enable the Compound Datastore option in the Configuration mode. See "Compound Datastore" on page 92.

Follow these procedures:

- To filter the compound list

- To delete a compound from the list

- To add a compound to the list

❖ **To filter the compound list**

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

   The application displays a list of filterable criteria. In all lists, you can choose to filter by All, Blanks, NonBlanks, or by custom filter criteria. Other filter criteria are specific to the individual columns.

2. To create a custom filter based on compound values in a specific column, choose **Custom** from the column list.

   For detailed instructions about creating a custom filter, see Appendix C, "Using Filter Criteria."

❖ **To delete a compound from the list**

1. Select the compound to remove from the list.

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

   A confirmation dialog box opens, listing the compound to be removed.

3. To confirm the deletion, click **Yes**.

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

❖ **To add a compound to the list**

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

   The Select Compounds to Add dialog box opens, listing all the compounds defined in the compound datastore.
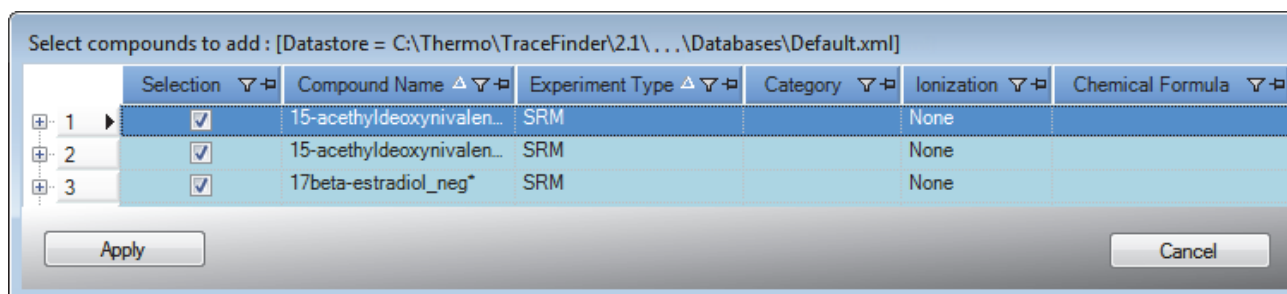
2. Select the check box for each of the compounds that you want to add to the method.

3. To quickly select multiple compounds, right-click and use any of the commands on the shortcut menu.

Table 22. Select Compounds to Add shortcut menu commands

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

4. Click **Apply**.

   The TraceFinder application adds the compounds to the Acquisition List page of the Master Method View. See "Acquisition List page."

Figure 23. Acquisition List page

Table 23. Acquisition List page parameters (Sheet 1 of 2)

Parameter	Description
Function Icons	
	Opens the Select Compounds to Add dialog box that lists all the compounds defined in the compound datastore.
	Deletes the selected compound. The icon is unavailable when no row is selected. If you used the filters to display a subset of compounds, the selected compound might not be visible on the Acquisition List page.
Compound parameters	
Compound Name	Alphanumeric name assigned to the compound.
Experiment Type	Experiment type: SRM, XIC, or SIM.
Category	(Optional) Alphanumeric identifier.
Ionization	(Optional) Alphanumeric identifier. Valid values: ESI, APCI, EI, CI, or APPI
Chemical Formula	(Optional) Alphanumeric chemical identifier.
Quantitative peak parameters	
Precursor Mass	The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio (m/z) units. Available only for SRM experiments. Range: 10.000 to 2999.999
Product Mass	The mass-to-charge ratio of the 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. Range: 10.000 to 2999.999
Mass	The mass-to-charge ratio of the quantitation ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (m/z) units. Available only for XIC and SIM experiments. Range: 10.000 to 2999.999

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

Parameter	Description
Collision Energy	The energy used when ions collide with the collision gas. Range: –250 to 250
Lens	(Optional) Range: –400 to 400
Polarity	**+** (positive) or **–** (negative)
RT (min)	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column. The TraceFinder application uses the RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Window (sec)	Acquisition window. The TraceFinder application uses the RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 499.50 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Energy Ramp	Available only for SRM experiments. Range: 0.00 to 200.00
Confirming ion parameters	
Precursor Mass	The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio (m/z) units. Available as a read-only field for SRM experiments only. Range: 10.000 to 2999.999
Product Mass	The mass-to-charge ratio of the 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. Range: 10.000 to 2999.999
Mass	The mass-to-charge ratio of the quantitation ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (m/z) units. Available only for XIC and SIM experiments. Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00

Identification

The Identification page lists the compounds that are targeted for analysis, reporting, and other compound-specific values. 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, internal standards, and surrogates.
Non Quan Compounds	Displays only non-quantitation compounds, such as native, breakdown, and tune compounds.
Target Compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.
Surrogates	Displays only surrogate compounds.

Figure 24. Identification page

Table 24. Identification page parameters

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, Internal Standard, Surrogate, MSTune, Native, and Breakdown. The TraceFinder application uses target compounds, internal standards, and surrogates in quantitative analysis.
Active	Identifies each compound to be included in data review and reporting. By default, all added compounds are set to active. This active or inactive setting populates 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 181.

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 148.
Signal	See also "Signal page parameters" on page 154.
Detect	See also "Detect page parameters for Genesis" on page 158. See also "Detect page parameters for ICIS" on page 162. See also "Detect page parameters for Avalon" on page 164.
Spectrum	See also "Spectrum shortcut menu commands" on page 170.
Ratios	See also "Ratios page parameters" on page 172.

On the Detection page (see "Detection page" on page 146), 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 use the cut-and-paste feature on confirming ion peaks
- To add a trace to the real-time viewer
- To replace a confirming ion peak
- To add a mass as a new confirming ion peak
- 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.
Non Quan Compounds	Displays only non-quantitation compounds, such as native, breakdown, and tune compounds.
Target Compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.
Surrogates	Displays only surrogate compounds.

❖ **To change the displayed information for detected peaks**

1. Right-click the chromatogram plot for any of the 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.
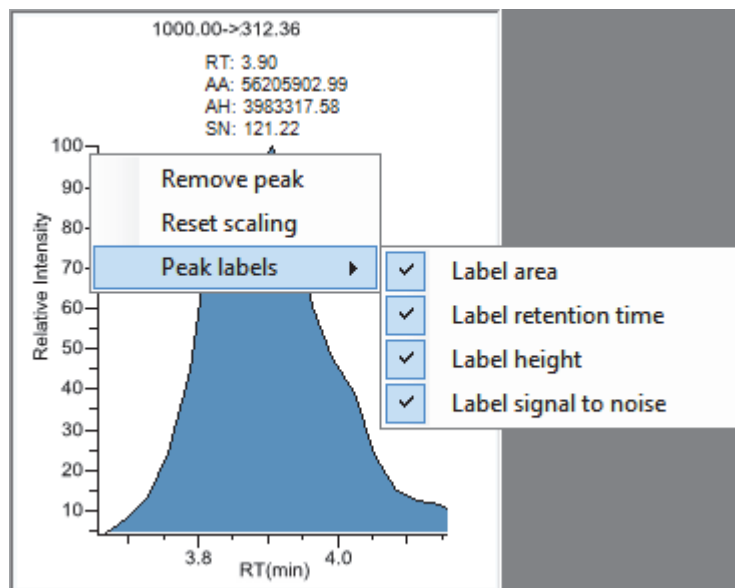
3. To remove a label, select the label type again and clear it.

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**

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

   The Associate a Raw Data File dialog box opens.

Associate a raw data file	⊠

   Raw data file to associate: [   ] ▼ [...]

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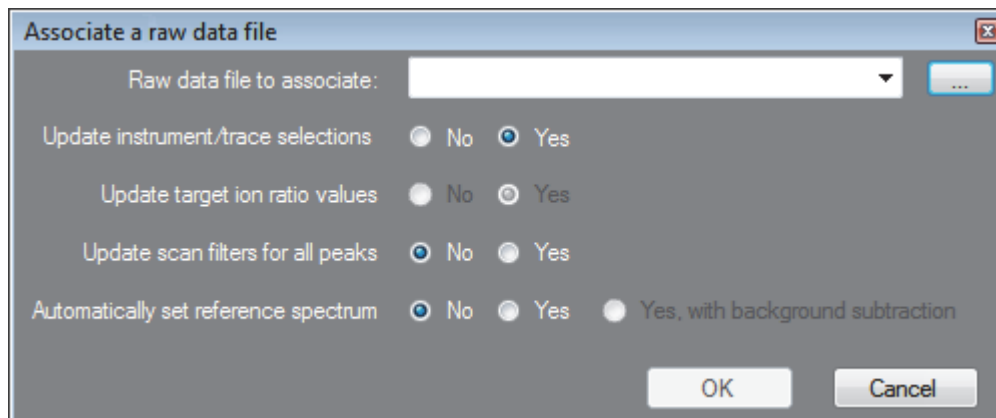
2. Browse to a raw data file to associate with the method (or select from the list of previously associated raw data files) and open the file.

   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:

   C:\Thermo\TraceFinder\2.1\EFS\Methods

3. To update the target ion ratio values when you associate this raw data file, select the **Yes** option.

4. To update the scan filters when you associate this raw data file, select the **Yes** option.

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

   Select the **Yes** option.

   –or–

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

   This feature is available only when you have set background subtraction values on the General page of the Master Method View. See "Editing the General Page" on page 121.

6. Click **OK**.

The TraceFinder application displays the chromatographic and spectrum data for the compounds in the selected raw data file.
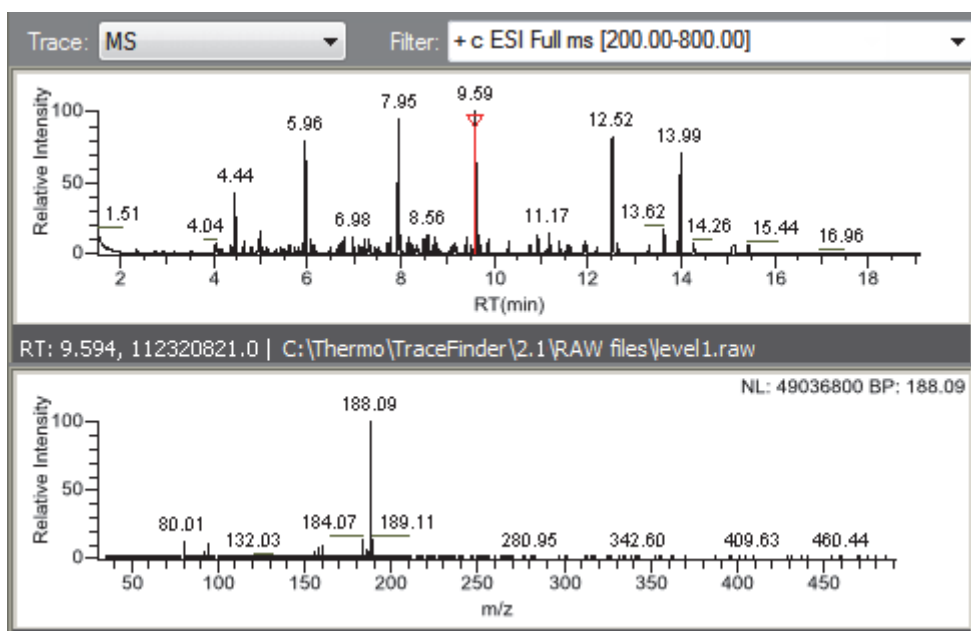
7. Select a filter from the Filter list.

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

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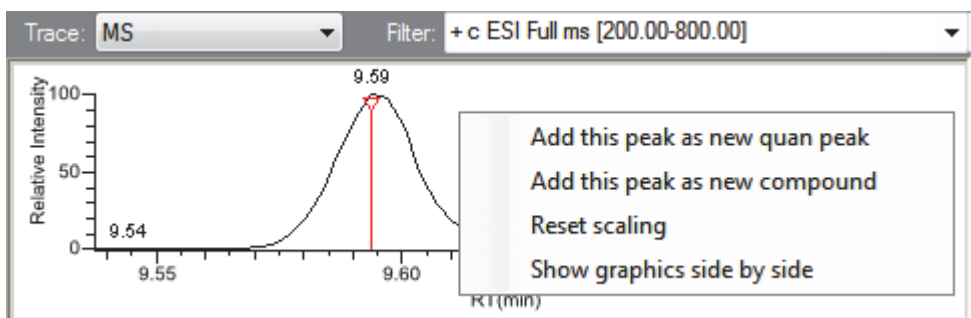
The TraceFinder application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quantitative peak, and the second and third largest ions as the confirming ion peaks.

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

Figure 25. Add New Compound dialog box
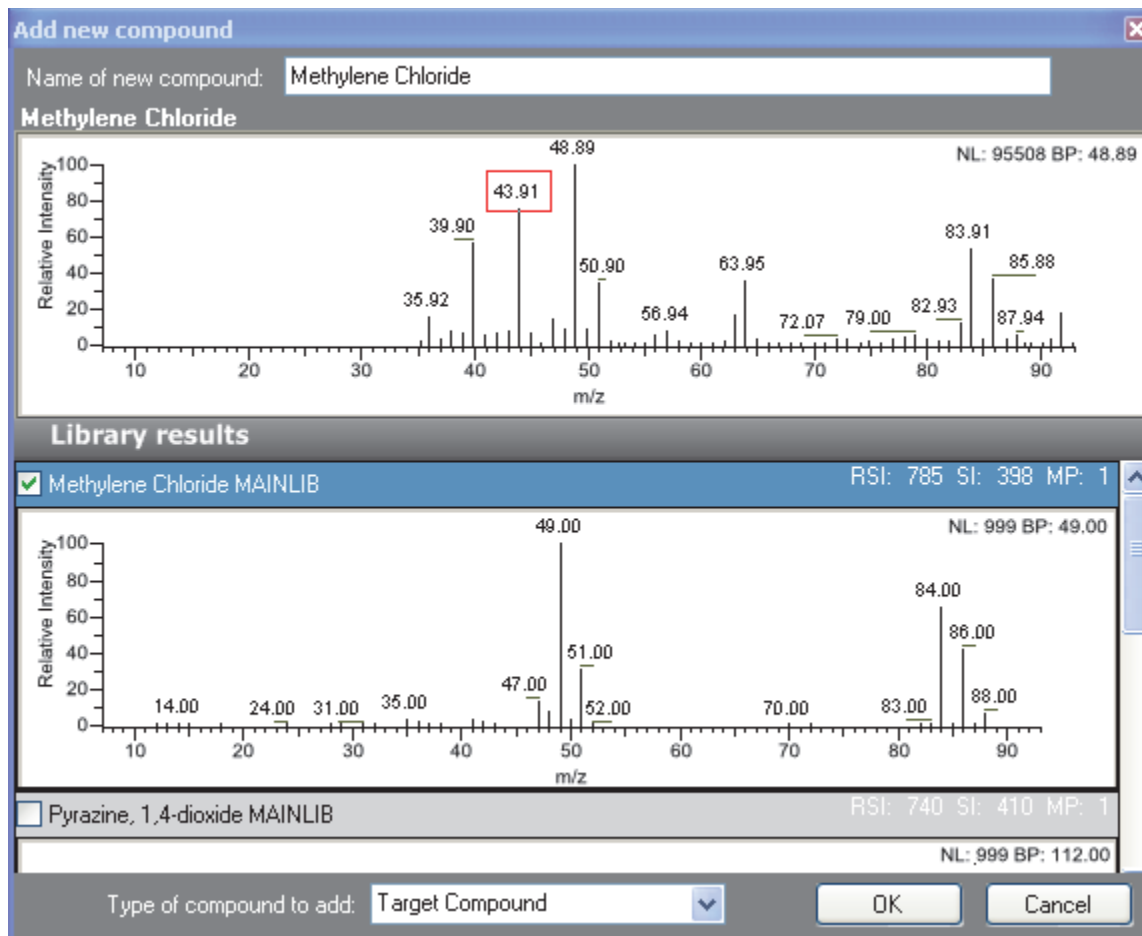
10. (Optional) To use a compound other than the compound already in the library, scroll to the spectrum for that compound and select the compound name in the title bar of the spectrum pane.
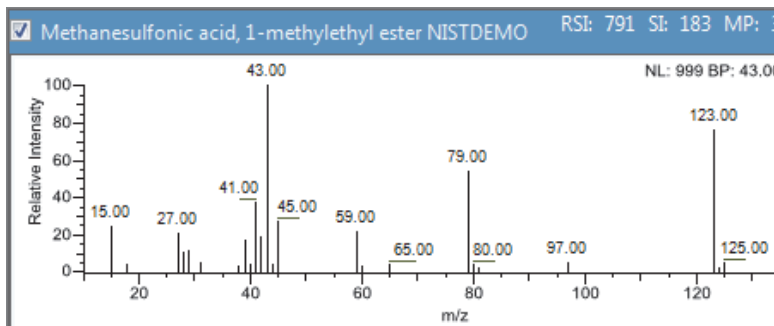
11. In the Type of Compound to Add list, select a compound type.

12. Click **OK**.

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

❖ **To change the compound reference spectrum**

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

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

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

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

❖ **To replace a quantitation mass**

1. Click the pane for the quantitation mass that you want to replace.

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

   The red box indicates the selected peak.
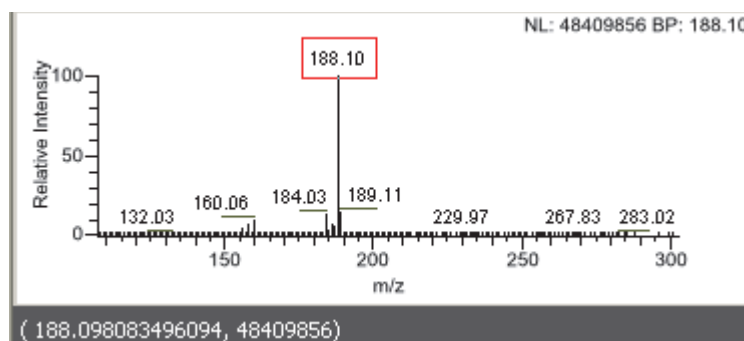
3. Right-click and choose **Set This Spectral Peak as Quan Value** from the shortcut menu.

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 171.

❖ **To add a mass to the existing quantitation mass ranges**

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

   The red box indicates the selected peak.

2. Right-click and choose **Add This 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 171.

❖ **To add a quantitative peak**

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

   The red box indicates the selected peak.

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

   The application adds a new quantitative peak to the compound.
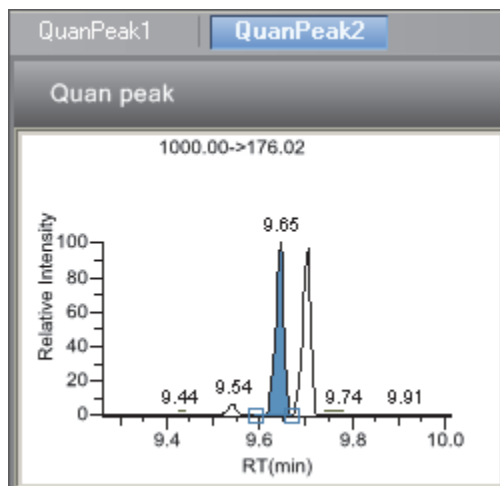
   You can use the shortcut menu in the spectrum pane for this new quantitative peak to perform any of the tasks that you would perform on the original quantitative peak.

❖ **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. See "Add New Compound dialog box" on page 142. If the name of the first match is already in the library, the dialog box opens with the matching compound selected.

Figure 26. Add New Compound dialog box
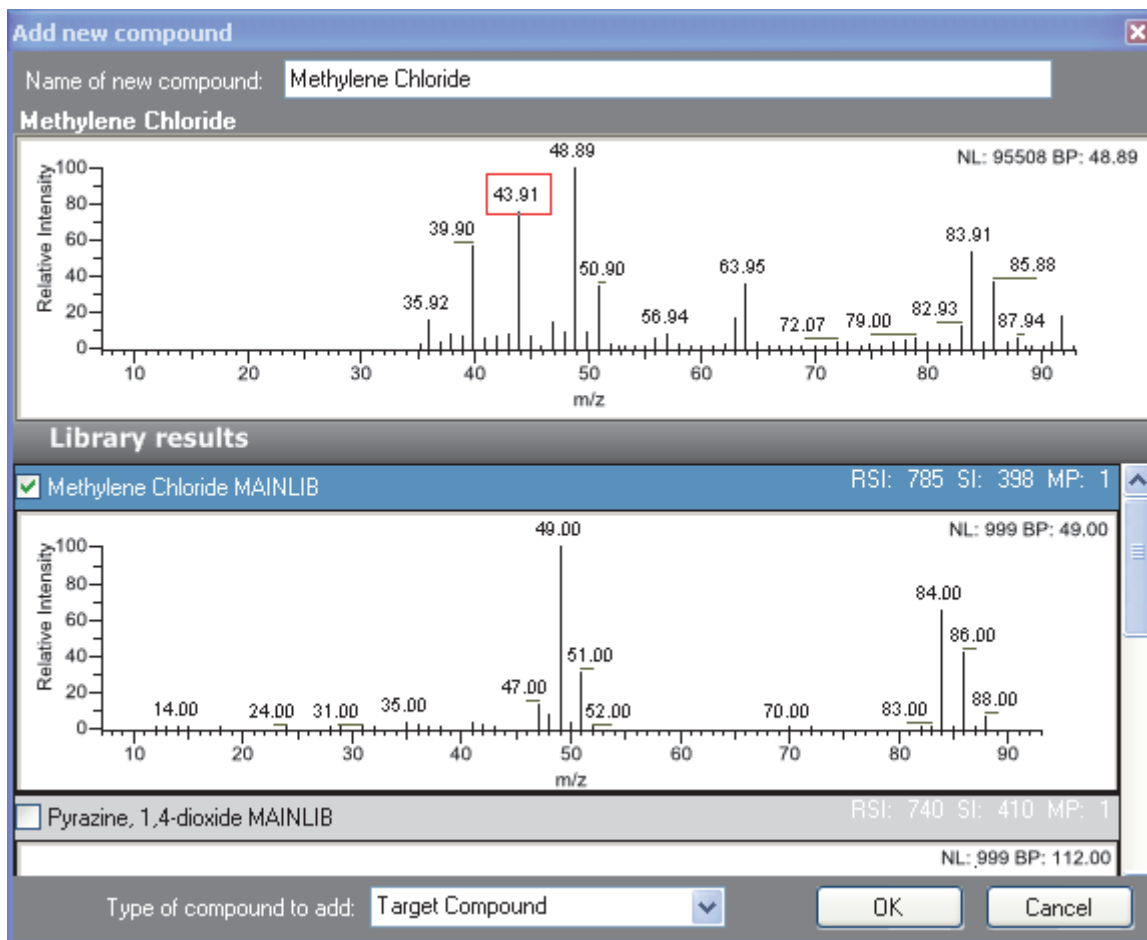
3. (Optional) Make any of the following changes:

    a.   Change the name for the compound in the Name of New Compound box.

    b.   Use a compound other than the compound chosen by the TraceFinder application by scrolling to the spectrum for that compound and selecting the compound name in the title bar of the spectrum pane.
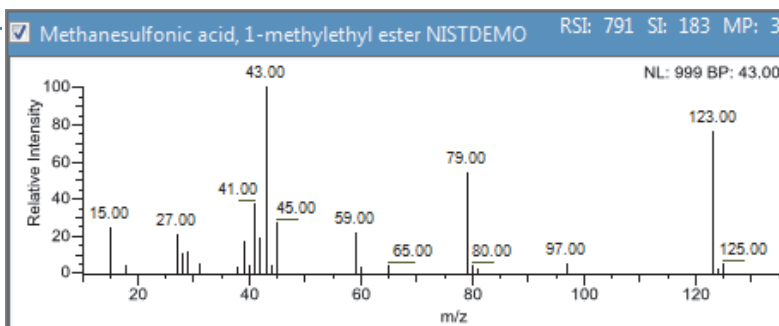
    c.   In the Type of Compound to Add list, select a compound type.

4. Click **OK**.

❖ **To replace a 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 use the cut-and-paste feature on confirming ion peaks**

Right-click the header bar for the confirming ion peak that you want to remove and choose **Cut Confirming Peak** from the shortcut menu.

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 add a trace to the real-time viewer**

Right-click the header bar for the quantitative peak or confirming ion peak that you want to add to the real-time viewer display and choose **Display in Real Time Viewer** from the shortcut menu.
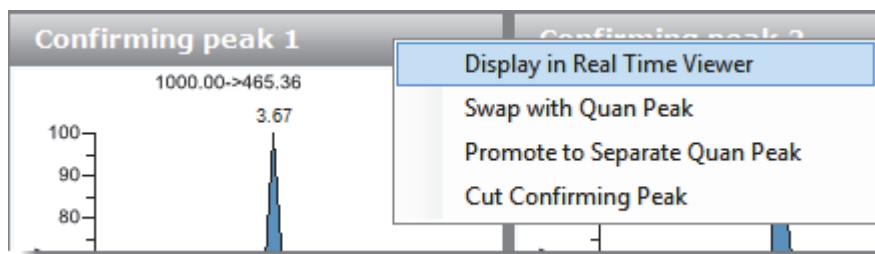
The application moves the peak to the Traces to Display in Real Time Viewer pane on the Real Time Viewer page. See .

Trace *m/z* 465.36 added to Real Time Viewer

When you acquire samples with this method, the application displays the *m/z* 465.36 trace in addition to the TIC in the Real Time Status pane.
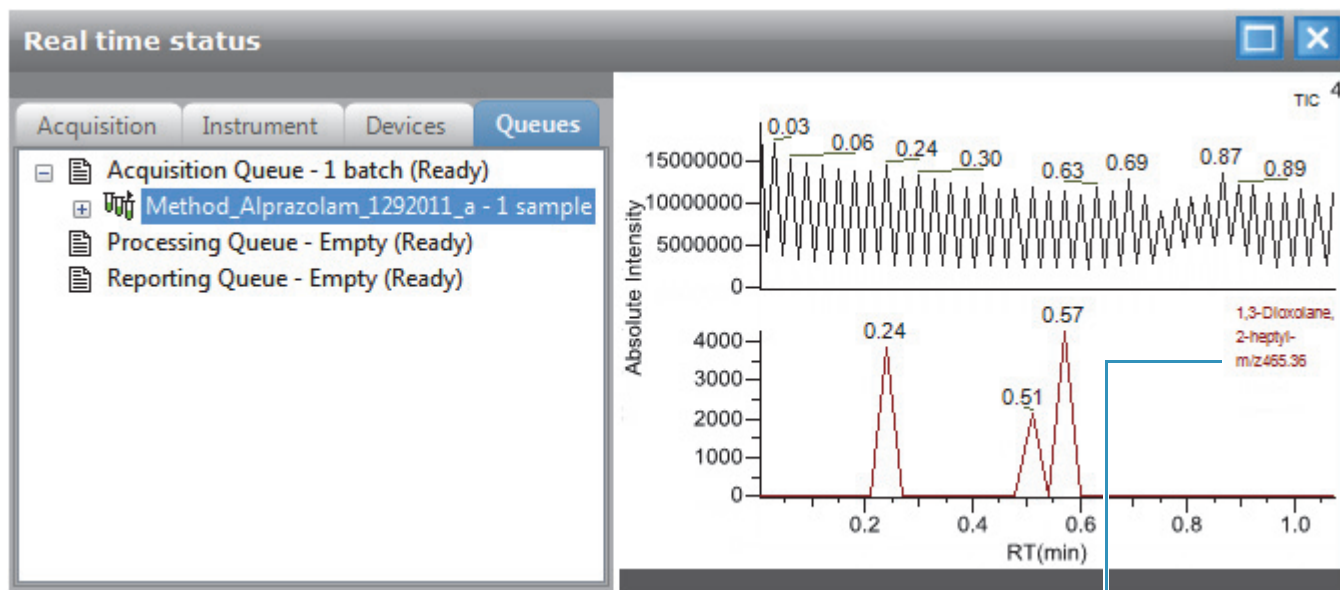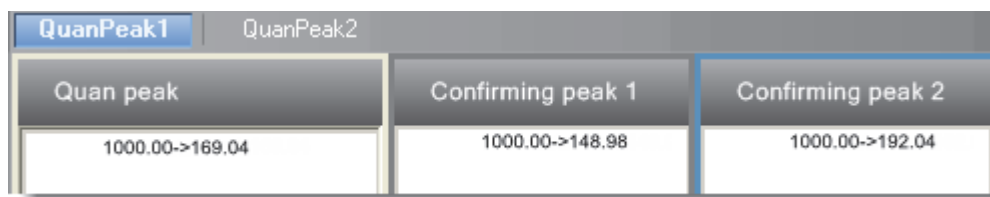
Trace *m/z* 465.36 added to Real Time Status display

❖ **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 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 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 save the new method**

1. Choose **File > Save**.

   The Save Master Method dialog box opens.

2. Do one of the following:

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

   –or–

   Select a method name to overwrite and click **Overwrite**.

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

   …\Thermo\TraceFinder\2.1\EFS\Methods

Figure 27. Detection page

Table 25. 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 181.
Quan Peak	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.
Trace	Displays a combination of the Detector and Trace values used for the raw data file.
Filter	Displays the filter used for the raw data file.
Reference Chromatogram and Spectra	Displays a reference chromatogram and spectra for the raw data file. 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 the collapse icon, ▶.
Additional pages	
Times	Defines the retention time and window for a quantitative peak. See "Times" on page 148.
Signal	Defines the detector and detection parameters used to display each chromatogram trace. See "Signal" on page 150.
Detect	Defines the peak detection algorithm and its options. See "Detect" on page 156.
Spectrum	Defines a reference mass spectrum for a quantitative peak or compound. See "Spectrum" on page 166.
Ratios	Defines the criteria for evaluating, confirming, or qualifying ions. See "Ratios" on page 171.

Times

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

Figure 28. Times page

Parameters for single RT detection types

Parameters for RT range detection types

Table 26. 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 26. 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 (see "Signal page" on page 154) 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 parameters" on page 154.

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 Ranges area is 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 29. Edit Mass Ranges dialog box
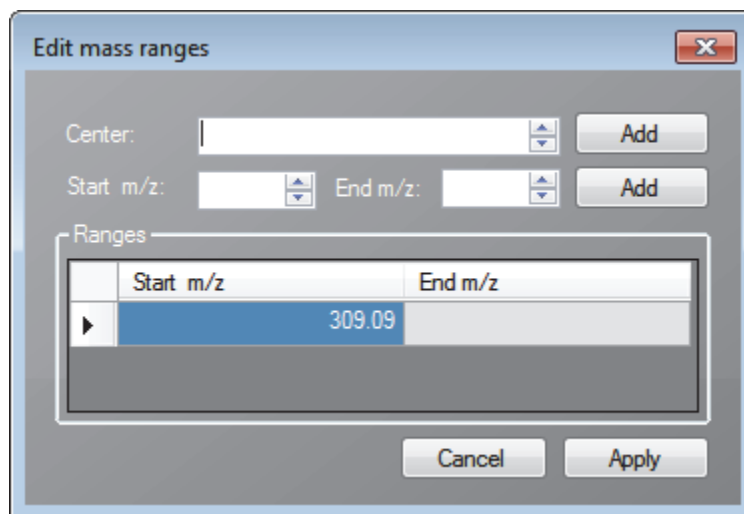
4. Enter a value in the Center Mass box and click **Add**.

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.

   Figure 30. XIC Filter dialog box
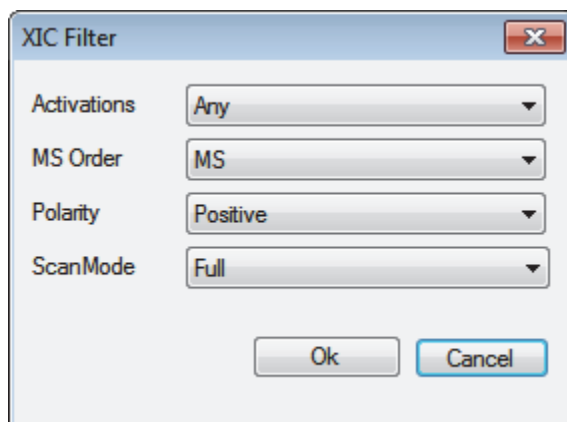
5. Select an Activation type:

CID	Collision-induced dissociation
MPD	Multiple photo dissociation
ECD	Electron capture dissociation
PQD	Pulsed dissociation
ETD	Electron transfer dissociation
HCD	Higher energy collision-induced dissociation
Any	Allows any activation method.
SAactivation	
PTRactivation	
NETDactivation	Negative electron-transfer dissociation activation
NPTRactivation	

6. Select an MS Order:

Any	Allows any MS order.
MS	Single mass spec stage
MS2-MS10	Multiple mass spec stages
Ng	Nano gram
N1	Nano liter
Par	

7. Select a value for the polarity.

    Valid values: **Positive**, **Negative**, or **Any**.

8. Select a Scan Mode:

Full	
Zoom	
SIM	Selective ion monitoring
SRM	Selective reaction monitoring
CRM	Consecutive reaction monitoring
Any	Allows any scan mode.
Q1MS	MS using quadrupole 1
Q3MS	MS using quadrupole 3

9. Click **OK**.

    The application updates the chromatogram data using the specified XIC filter options.

❖ **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.
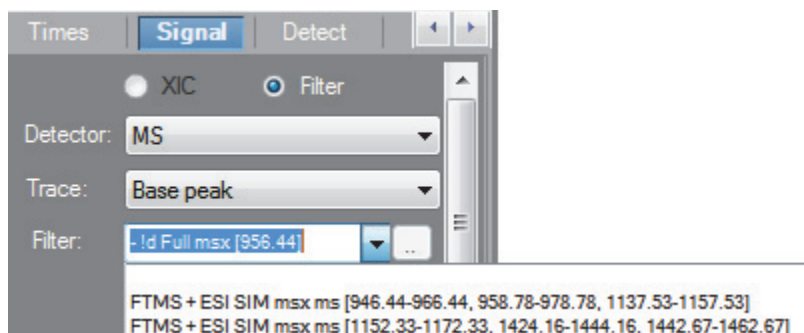
The application applies the selected filter to the quantitative or confirming ion peak.

5. To apply this same filter to other peaks, right-click and choose one of the following from the shortcut menu:

   • **Set This Filter on All Peaks in This Compound**: Applies this filter to all other peaks in the compound.

   • **Set This Filter on All Compounds**: Applies this filter to all peaks in the method.

Figure 31. Signal page
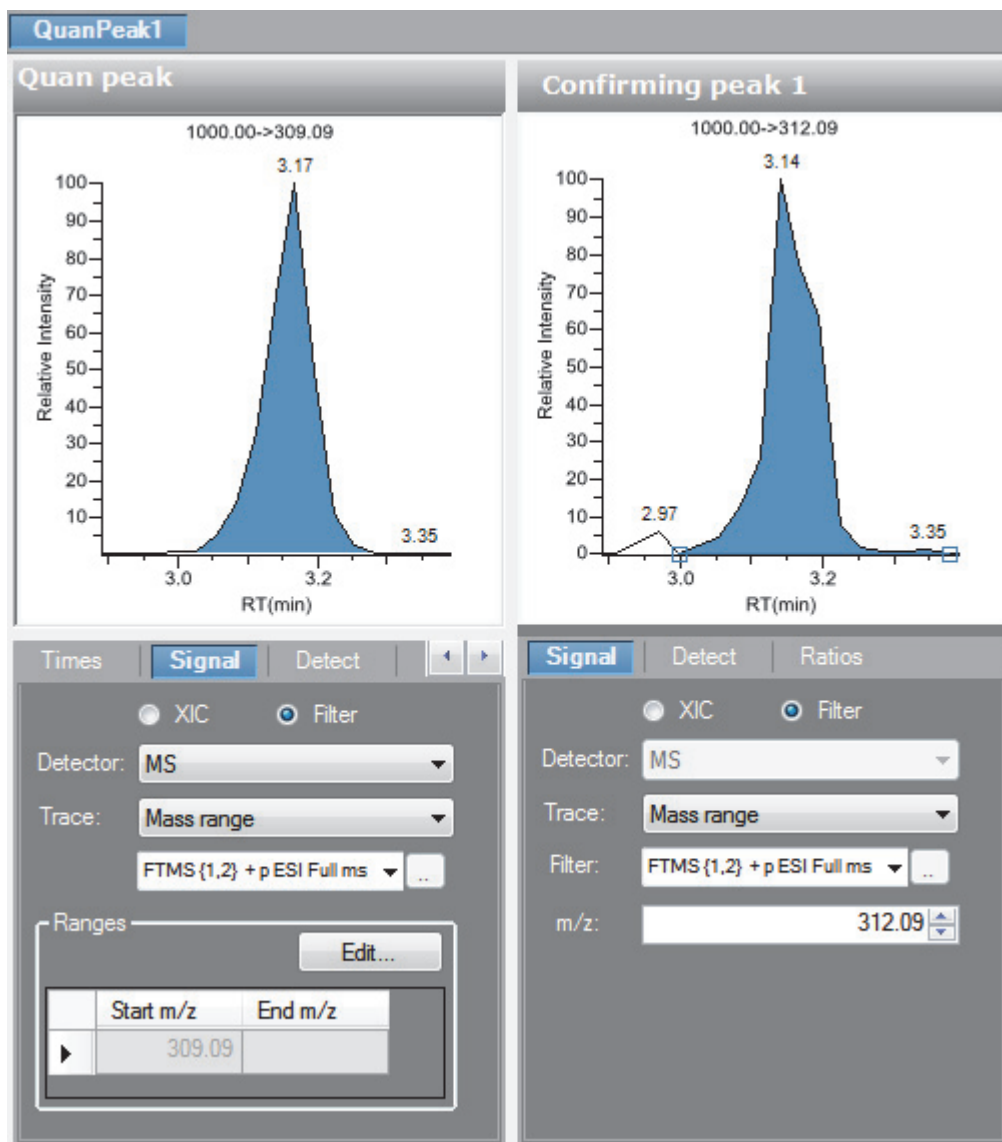
Table 27. Signal page parameters (Sheet 1 of 2)

Parameter	Description
XIC	Specifies an Extracted Ion Chromatogram experiment type that uses a single, full-scan mass filter that is post-processed to extract a peak for the ions of interest.
Filter	Select from the list of mass filters to use for processing the compound.

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

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.
	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.
Ranges	Available only when you select the Mass Range Trace.
Edit	Opens the Edit Mass Ranges dialog box where you can specify a range of ions for detection and integration. See "Edit Mass Ranges dialog box" on page 150.
Start *m/z* End *m/z*	Specifies ranges of ions for detection and integration. The application sums the multiple ions specified by these ranges.

Ranges specified by a center mass value are listed as a single value in the Start *m/z* column. The application uses a range of one amu centered on this value. |

Detect

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

See the following for detailed descriptions of all the features on the Detect page:

Figure 32. Detect page for Genesis
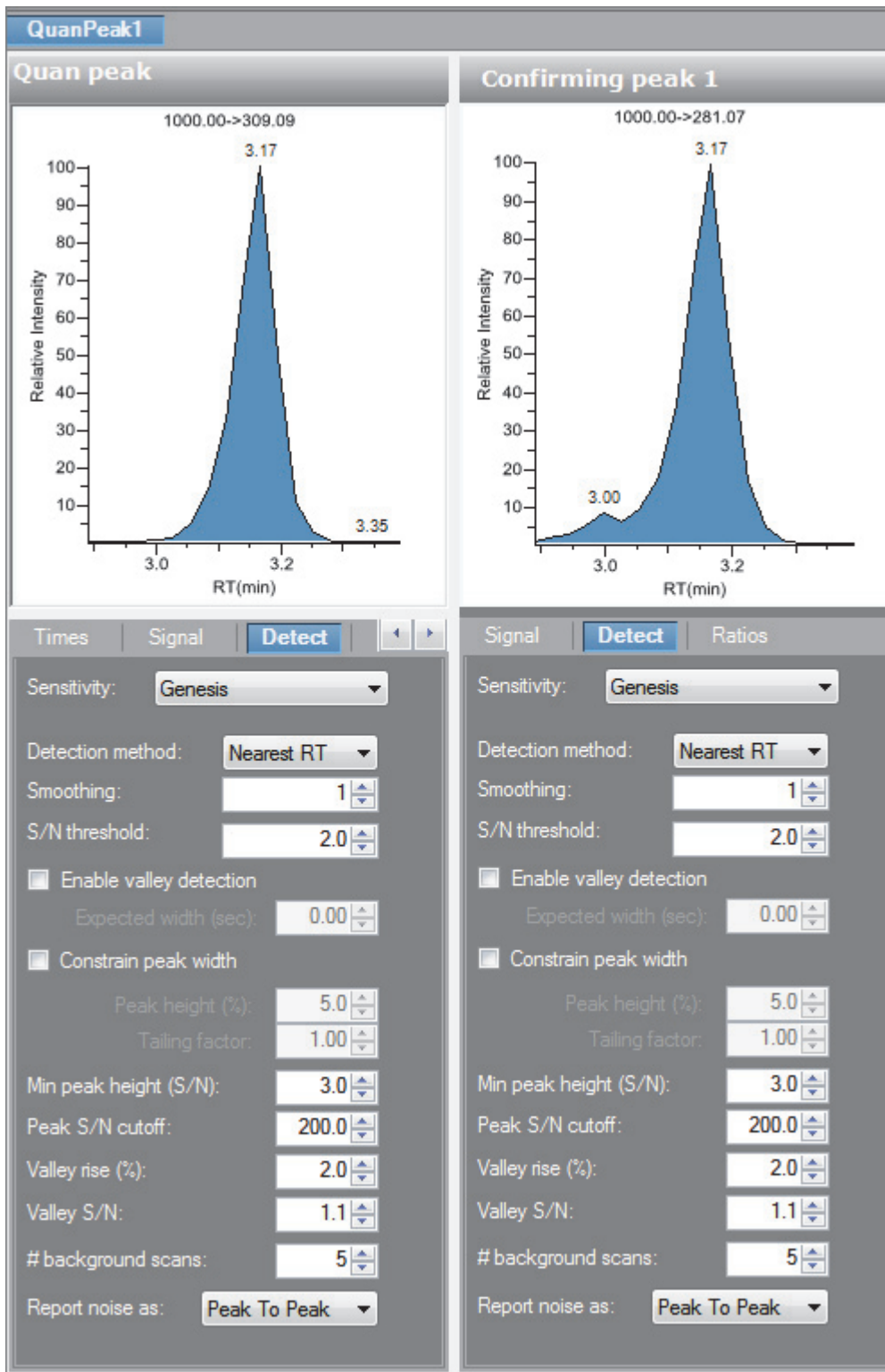
Table 28. Detect page parameters for Genesis (Sheet 1 of 3)

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 enables the Peak Height (%) and Tailing Factor options.
Peak Height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when you select the Constrain Peak Width check box. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0

Table 28. Detect page parameters for Genesis (Sheet 2 of 3)

Parameter	Description
Min Peak Height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0
Peak S/N Cutoff	The peak edge is set to values below this signal-to-noise ratio. This test identifies an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio. When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the TraceFinder application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 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 28. 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 33. Detect page for ICIS
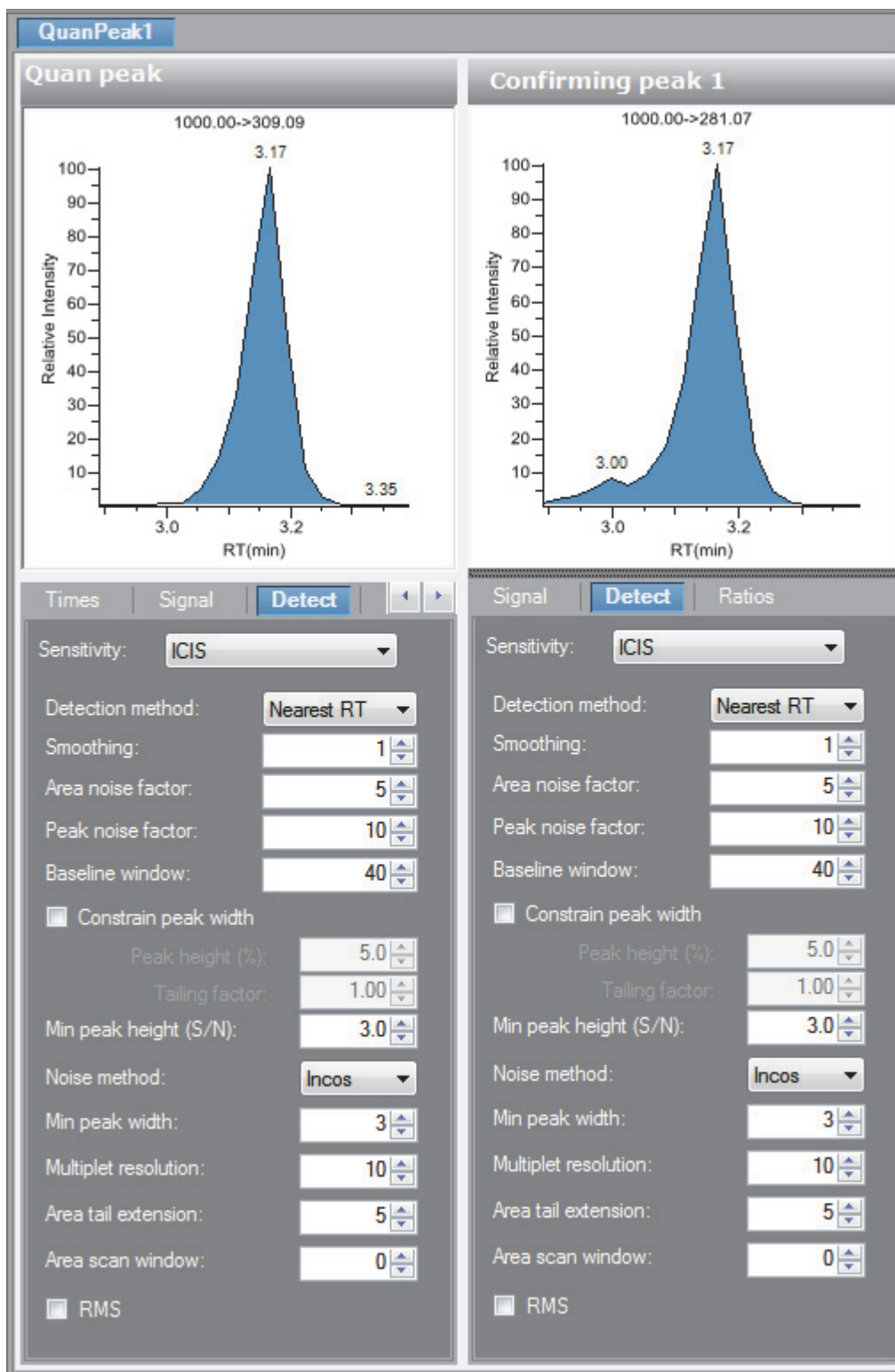
Table 29. Detect page parameters for ICIS (Sheet 1 of 2)

Parameter	Description
Sensitivity	Specifies the ICIS peak detection algorithm.
Detection Method	Highest peak: Uses the highest peak in the chromatogram for component identification. Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. 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 enables the Peak Height (%) and Tailing Factor options.
Peak Height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when you select the Constrain Peak Width check box. Range: 0.0 to 100.0%
Tailing Factor	A factor that controls how the TraceFinder application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when you select the Constrain the Peak Width check box. Range: 0.5 through 9.0
Min Peak Height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the TraceFinder application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0

Table 29. 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 criterion 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 34. Detect page for Avalon
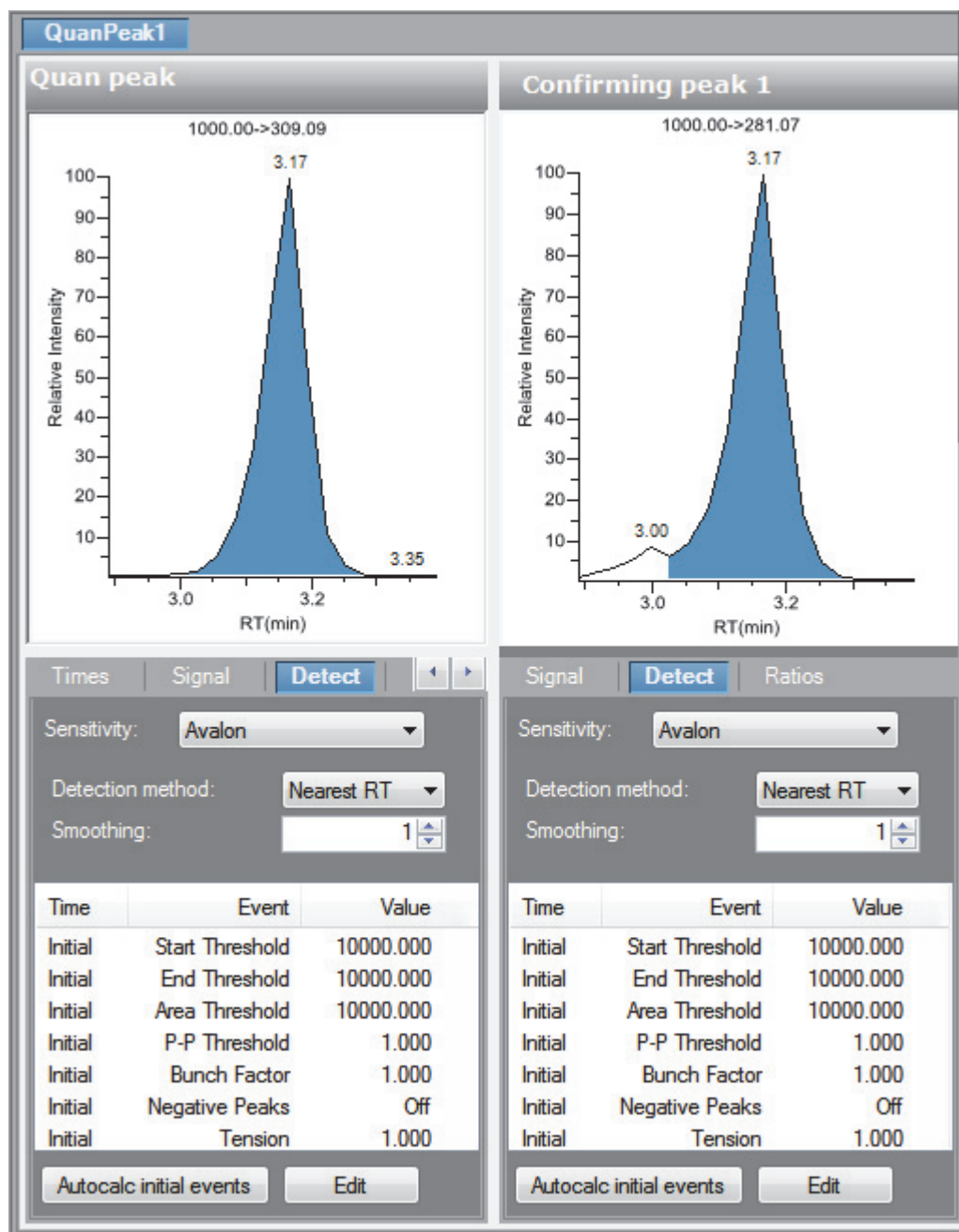
Table 30. Detect page parameters for Avalon (Sheet 1 of 2)

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

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

Parameter	Description
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. 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 85.
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.

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 shortcut menu commands" on page 170.

Follow these procedures:

- 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 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 35. Original quantitative peak mass example
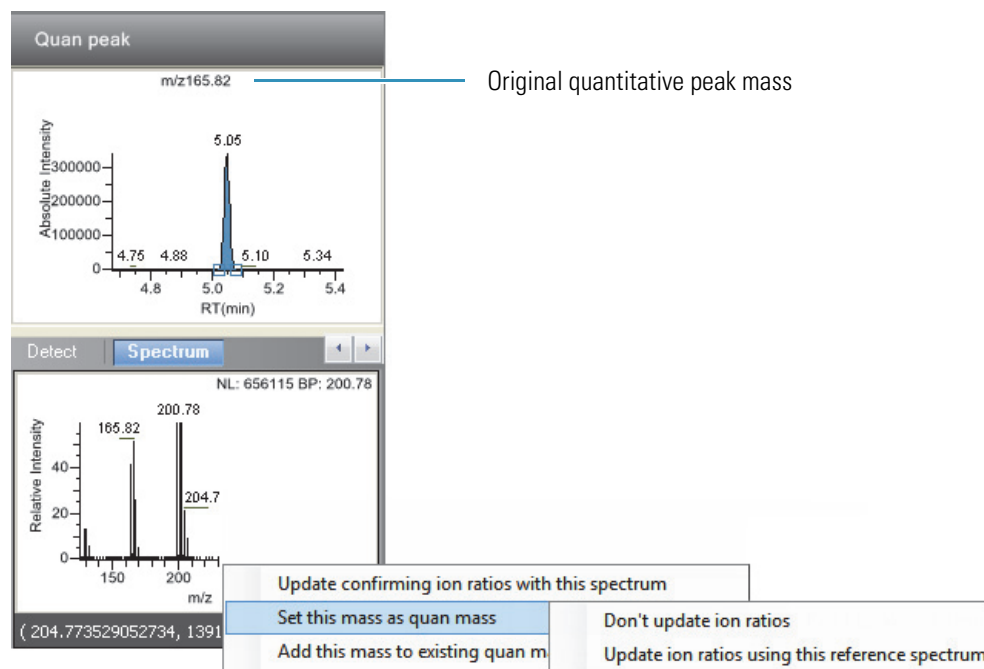
The TraceFinder application replaces the original quantitation mass with the selected mass.

Figure 36. Updated quantitative peak example
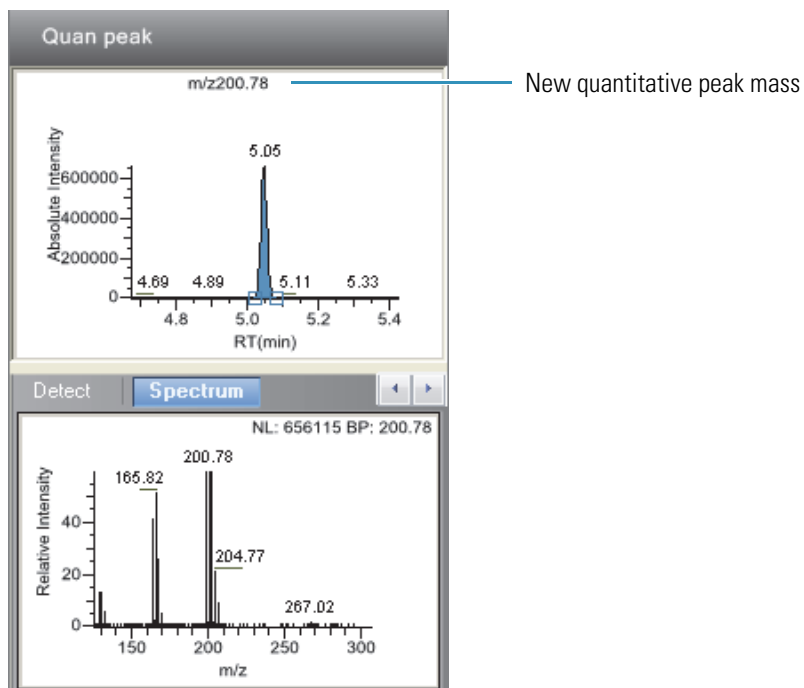
❖ **To add ions together to get an accumulated signal**

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

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

2. Right-click and choose **Add This Mass to Existing Quan Mass Range** from the shortcut menu.

   You can now update the ion ratios to adjust the confirming ion comparisons to the new summed quantitative peak signal.

❖ **To add a quantitative peak to an existing compound**

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

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

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

   A red box around the ion's *m/z* value indicates that the ion is selected.
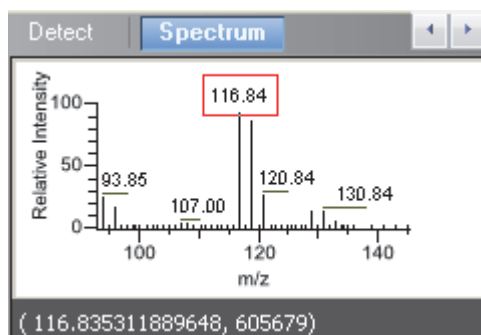
3. Right-click and choose **Set This Mass as New Quan Peak** from the shortcut menu.

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

New quantitative peak mass
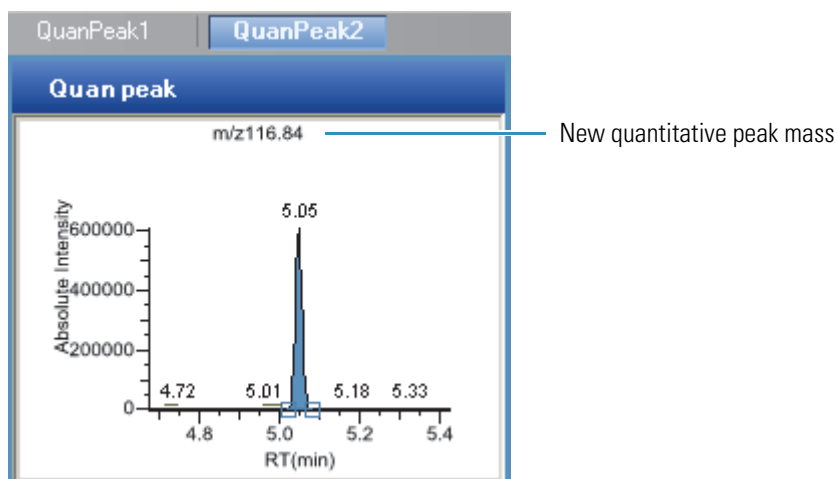
❖ **To add one or more confirming ions to an existing compound**

1. Click the 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.
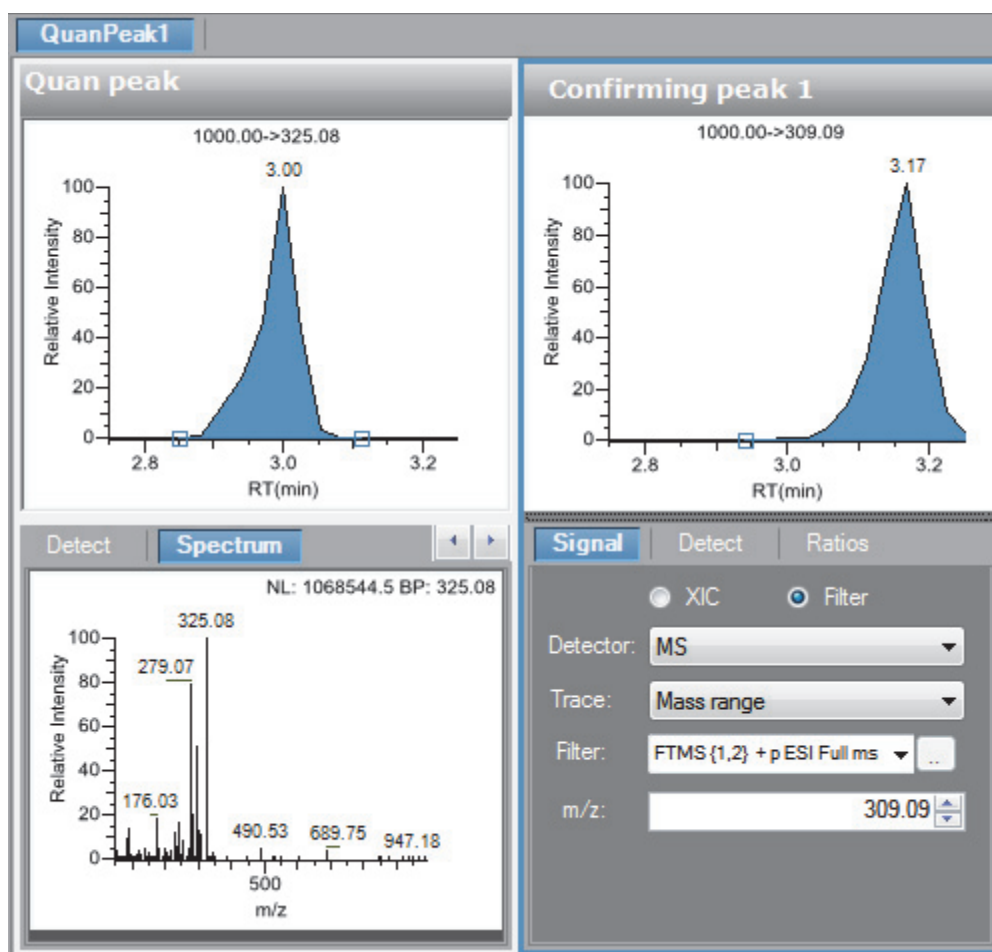
❖ **To zoom in on the chromatogram or spectrum displays**

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.

Figure 37. Spectrum page
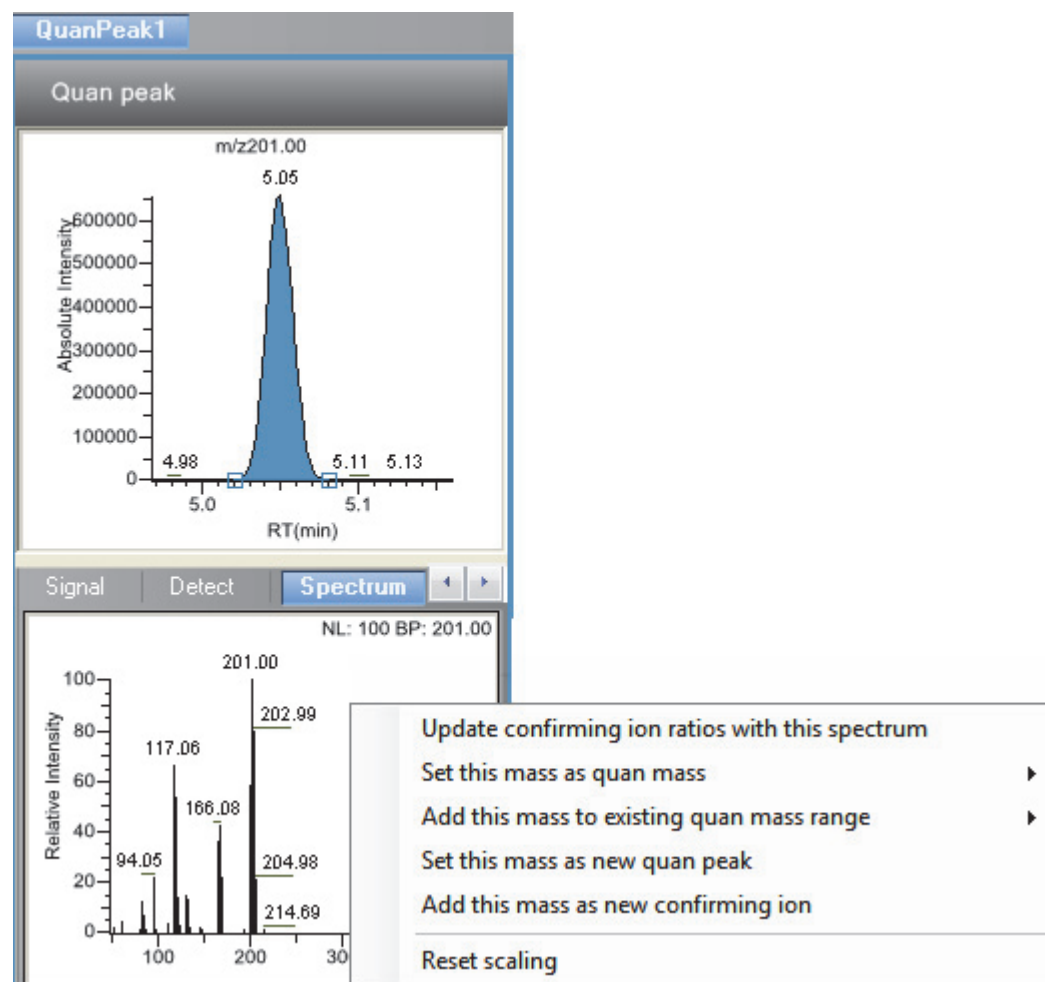
Table 31. Spectrum shortcut menu commands

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.

Ratios

Use the Ratios page (see "Ratios page" on page 172) 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 parameters" on page 172.

❖ **To specify ion ratio criteria**

1. Select the **Enable** check box to enable the confirming ion.

2. In the Target Ratio box, select the theoretical ratio of the confirming ion's response to the quantification ion's response.

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

4. In the Window (+/-%) box, select the acceptable ion ratio range.

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

   In the following example

   • The target ratio is expected to be 61.02% and the window is Absolute 20%, so the acceptable window for this confirming ion 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 38. Ratios page
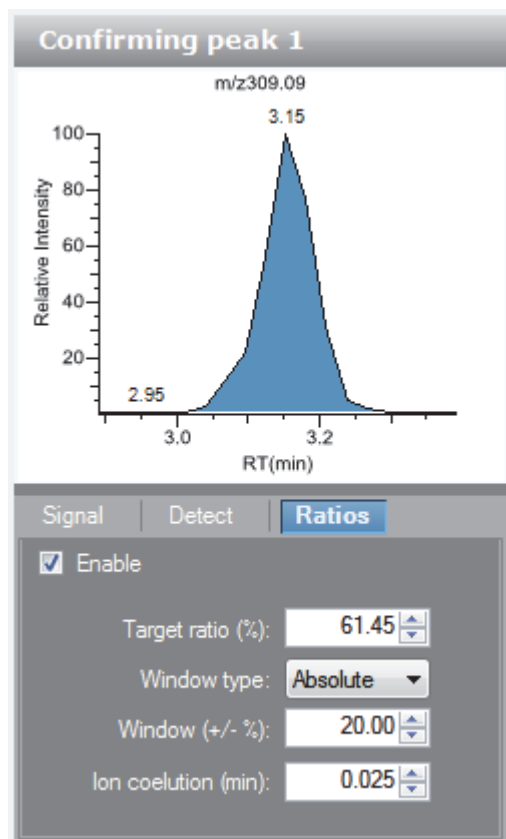
Table 32. Ratios page parameters

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

For detailed descriptions of all the features on the Calibration page, see Calibration page parameters.

❖ **To specify an internal standard 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 133.

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 "Peak Display Panes" on page 358.

Figure 39. Calibration page

Table 33. 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, Internal Standard, Surrogate, MSTune, Native, or Breakdown.

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

Parameter	Description
Standard Type	Specifies Internal or External standards.
Response Via	The use of area or height.
Curve Type	Specifies Linear, Quadratic, or AverageRF curve types.
Origin	The origin treatment as Ignore, Include, or Force. The Origin and Weighting columns are active only when you are using Linear or Quadratic curve types.
Weighting	Specifies the weighting as Equal, $1/X$, $1/X^2$, $1/Y$, or $1/Y^2$.
Units	The units to be displayed with the calculated values.
ISTD	The internal standard (ISTD) for a target compound or surrogate when the standard type is set to Internal. When you set the standard type to External, this field is inactive. The list displays all compounds with the compound type of Internal Standard.
Amount	The amount of the internal standard for ISTD compounds.
Shortcut menu	The Calibration page uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 181.

Calibration Levels

On the Calibration levels page (see "Calibration Levels page" on page 175) 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 parameters" on page 176.

❖ **To specify calibration levels and concentrations**

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

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.

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 to the table, do the following:

   a. Select the first calibration level table cell.

   b. Click the cell again to make it editable.

   c. Type a concentration value.

5. Repeat Step 4 for all calibration levels associated with the first compound.

6. To specify the same concentration values for all compounds, select the value that you want to copy, right-click, and choose **Copy Down** from the shortcut menu.

Figure 40. Calibration Levels page

Table 34. Calibration levels page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Cal1-Cal*n*	User-defined calibration levels for the compound.
Manage Calibration Levels	Defines values for each of the calibration level values for the selected compound.
Shortcut menu	The Calibration Levels page uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 181.

QC Levels

Use the QC levels page (see "QC Levels page") for a master method to define the standards for QC levels. You can edit QC levels for master methods only. The contents of this page are read-only when you are editing a local method. For detailed descriptions of all the features on the QC Levels page, see "QC levels page parameters."

❖ **To specify QC levels and concentrations**

1. Select the compound whose QC levels, percentage test values, and concentrations that 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 QC Levels area, type a name for the first QC level.

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

QC levels

	Level	% Test
1	QCLevel1	.00
✱ 2		NA

3. Type a value for the % Test.

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

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

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

5. To enter the concentration values to the table, do the following:

   a. Select the first QC level table cell.

   b. Click the cell again to make it editable.

   c. Type a concentration value.

6. Repeat Step 5 for all QC levels associated with the first compound.

	RT	Compound	QCLevel1	QCLevel2	QCLevel3
1	3.15	Pyrazinamide	5.000	10.000	15.000
2	3.67	1,3-Dioxolane, 2-heptyl-			

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 41. QC Levels page

Table 35. QC levels page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
QC1-QC*n*	User-defined quality control levels for the compound.
QC levels	
Level	User-defined quality control level names.
% Test	A value for the acceptable difference (as a percentage) between the known amount and calculated (measured) amount of each QC level.
Shortcut menu	The QC Levels page uses a right-click shortcut menu. See "Using the Shortcut Menu Commands" on page 181.

Real Time Viewer

Use the Real Time Viewer page to specify which traces display in the real-time status pane when you perform acquisition in the Acquisition mode or when you acquire a development batch in the Method Development mode. See "Real-Time Display" on page 279.

Figure 42. Real Time Viewer page
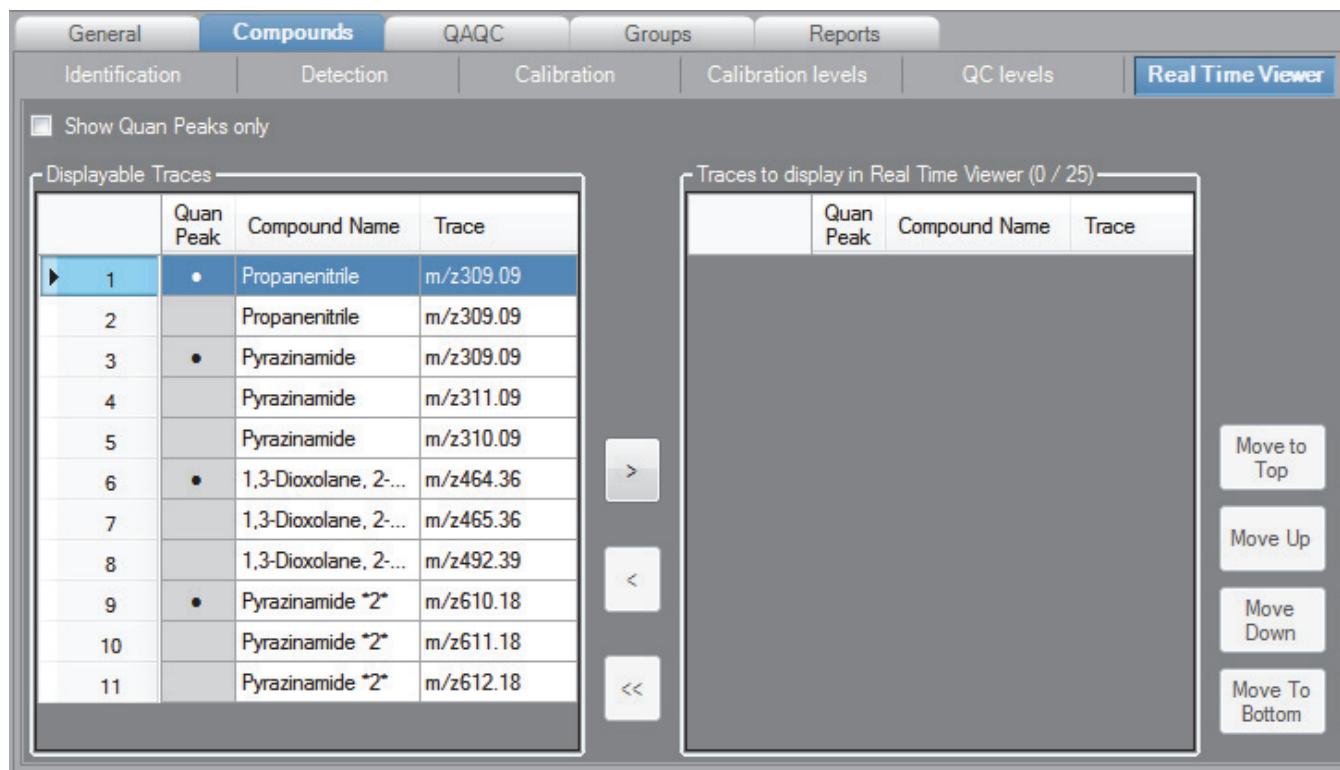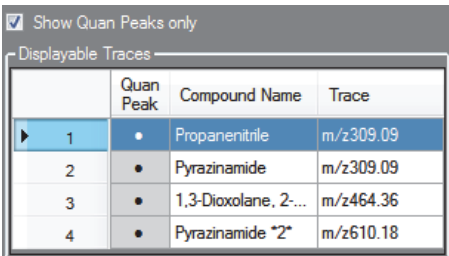
Table 36. Real Time Viewer page parameters (Sheet 1 of 2)

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	Checks indicate quantitative peak traces. Unchecked traces indicate confirming ion peaks.
Compound Name	Names of all compounds in the method.

Table 36. 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 (0/25)	List the traces to be displayed and the display order in the real-time viewer in the Acquisition mode. Maximum number of traces is 25.
Move to Top	Moves the selected trace to the top of the Traces to Display... list and the second position in the real-time display. The TIC is always the first position in the real-time display.
Move Up	Moves the selected trace up one position in the list.
Move Down	Moves the selected trace down one position in the list.
Move to Bottom	Moves the selected trace to the bottom of the list.

Using the Shortcut Menu Commands

Each page on the Compounds page (except the Acquisition List 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.
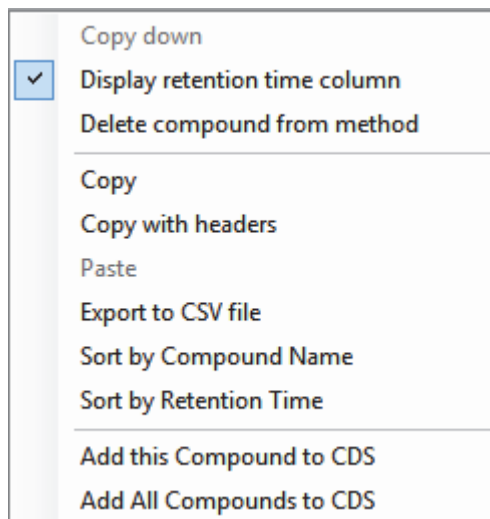
Table 37. Compounds page shortcut menu commands (Sheet 1 of 2)

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 B, "Using Copy Down and Fill Down."
Display Retention Time Column	Displays or hides the RT column in the compound list.
Delete Compound From Method	Removes the selected compound from the current master method.
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 37. 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 CDS	Adds the selected compound to the compound data store. When the compound already exists in the compound data store, the TraceFinder application updates the compound data store with the current compound information. This command is available only on the Detection page shortcut menu when the Compound Datastore is enabled. See "Enabling Optional Features" on page 88.
Add All Compounds to CDS	Adds all compounds in the current method to the compound data store. When any of these compounds already exist in the compound data store, the TraceFinder application updates the compound data store with the current compound information. This command is available only on the Detection page shortcut menu when the Compound Datastore is enabled. See "Enabling Optional Features" on page 88.

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.

From the QAQC page of the Master Method View, you can access these additional pages:

- Limits
- Calibration
- Chk Std
- Breakdown
- Matrix Blank
- ISTD
- Solvent Blank
- Surrogate
- Lab Control
- Meth Val
- Matrix Spike
- Tune

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 43. Limits page

Table 38. Limits page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
LOD (Detection Limit)	Limit of detection. The lowest amount that can be detected. Usually derived from a method detection limit (mdl) study.
LOQ (Quantitation Limit)	Limit of quantitation. The lowest amount that can be confidently and accurately quantitated. This is usually the lowest calibration amount.
LOR	Limit of reporting. Also called cutoff in some industries. This is the lowest amount that can be reported, as determined by each laboratory's standard operating practices.
ULOL (Linearity Limit)	Upper limit of linearity. This is usually the highest calibrator amount.
Carryover Limit	The highest amount of a substance that does not leave a residual amount in the instrument. If a substance has a carryover limit of 5, amounts higher than 5 usually dirty the instrument and leave residue behind, tainting the following sample. A carryover limit of less than 5 does not leave any residual amounts of the substance.

Calibration

Use the Calibration page to define acceptable criteria for initial calibration. The TraceFinder application makes the evaluation by comparing the initial calibration results for each compound found in the sample to the values defined on this page.

On the Calibration report, the application flags the calculated values for internal standard compounds that exceed these limits.

Figure 44. Calibration page

Table 39. Calibration page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
R^2 Threshold	The minimum correlation coefficient (r^2) for an acceptable calibration (when in linear or quadratic mode).
Max RSD (%)	The maximum relative standard deviation (RSD) for an acceptable calibration (when in average RF mode).
Min RF	The minimum average response factor (RF) for an acceptable calibration (when in average RF mode).
Max Amt Diff (%)	The maximum deviation between the calculated and theoretical concentrations of the calibration curve data points (when in linear or quadratic mode).

Chk Std

Use the Chk Std page to review the calibration on an ongoing basis. The TraceFinder application makes the evaluation by comparing the quality check standard results for each compound in the sample to the initial calibration using values defined on this page.

On the Check Standard report, the TraceFinder application flags the calculated values for internal standard compounds that exceed these limits.

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

Figure 45. Chk Std page

Table 40. Chk Std page parameters

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

Breakdown

Use the Breakdown page to view and edit values used for the evaluation of breakdown and degradation reporting. The TraceFinder application makes the evaluation by calculating the ratio of breakdown compounds to the native compounds.

❖ **To display the list of compounds in a group**

Click anywhere in the group row.

❖ **To select a group for breakdown calculation**

Select the **Active** check box in the group row.

You can select any group in the method for breakdown calculation, but the application calculates and reports only those that contain breakdown and native compounds.

Figure 46. Breakdown page

Table 41. Breakdown page parameters

Parameter	Description
Groups	Lists all groups created on the Groups page. See "Editing the Groups Page" on page 200.
Active	Specifies which groups are used for analysis.
Max % Breakdown	The maximum allowable percentage of breakdown to native compounds. This value is calculated by summing the responses of the breakdown compounds and dividing them by the sum of the native compounds. On the Breakdown Report, the application flags the calculated values for breakdown and native compounds that exceed these limits.
Compounds for Group	Lists all compounds in the selected group.

Matrix Blank

Use the Matrix Blank page to define acceptable levels of target compounds in blank samples. The TraceFinder application makes the evaluation by comparing the calculated concentration for each compound in the sample to the maximum concentration defined on this page. You can enter the maximum concentration as a percentage of a flag value or as a specified value.

For detailed descriptions of all the features on the Matrix Blank page, see Matrix Blank page parameters.

On the Matrix Blank report, the application flags the calculated values for target compounds that exceed these limits.

❖ **To specify the maximum concentration as a percentage**

1. From the Method column list, select one of the following methods:
   • % 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 47. Matrix Blank page

Table 42. Matrix Blank page parameters (Sheet 1 of 2)

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

Table 42. Matrix Blank page parameters (Sheet 2 of 2)

Parameter	Description
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 makes the evaluation by comparing the area and retention time results for each internal standard compound in the sample to a specified range.

If all of your target compounds are set to external calibration mode or if you have not identified any compounds as internal standards, this page does not show any values.

Figure 48. ISTD page

Table 43. ISTD page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Min Recovery (%) 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 makes the evaluation by comparing the calculated response for each compound in the sample to the maximum response defined on this page.

On the Solvent Blank report, the TraceFinder application flags the calculated values for target compounds that exceed these limits.

Figure 49. Solvent Blank page

Table 44. 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.

Surrogate

Use the Surrogate page to view or edit values for surrogate recovery reporting. The application makes the evaluation by comparing the calculated concentration for each compound in the sample to the theoretical concentration and range defined on this page.

You can use these parameters to evaluate the performance of your method. For this evaluation, prepare, analyze, and evaluate a number of samples (typically 4 to 10) to document method accuracy and precision as a comprehensive whole.

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

Figure 50. Surrogate page

Table 45. Surrogate page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Theo Conc	Values for the compounds that represent the expected theoretical concentration of that compound in the sample.
Min Recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that the application can determine by comparing the observed calculated concentration in the analysis to the expected concentration. Each method validation compound can have its own values for these fields, independent of other method validation compounds.
Max Recovery (%)	

Lab Control

Use the Lab Control page to view and edit QC values for lab control sample (LCS) and lab control sample duplicate (LCSD) analyses. The application makes the evaluation by comparing the calculated concentration for each compound in the sample to the theoretical concentration and range defined on this page.

You can prepare samples (typically known as clean matrices) as LCS or LCSD. These represent samples where you have added known concentrations of target analytes. To define an LCS and its duplicate in a batch, select the appropriate sample type and a common sample ID.

On the Lab Control report, the application flags the calculated values for spiked compounds that exceed these limits.

Figure 51. Lab Control page

	RT	Compound	Theo Conc	Min recovery (%)	Max recovery (%)	Max RPD
1	4.44	2-Chlorobenzimidazole	0.000	0.00	0.00	0.00

Table 46. Lab Control page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Theo Conc	Values for the lab control compounds that represent the expected theoretical concentration of that compound in the sample.
Min Recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that the application can determine by comparing the observed calculated concentration in the analysis to the expected concentration. Each LCS or LCSD compound can have its own values for these fields, independent of other LCS or LCSD compounds.
Max Recovery (%)	
Max RPD	Specifies a maximum value for relative percent difference (RPD) between two spiked samples.

Meth Val

Use the Meth Val page to view or edit QC values for method validation reporting. The application makes the evaluation by comparing the calculated concentration for each compound in the sample to the theoretical concentration and range defined on this page.

You can use these parameters to evaluate the performance of your method. For this evaluation, prepare, analyze, and evaluate a number of samples (typically four to 10) to document method accuracy and precision as a comprehensive whole. To define a method validation sample in the batch, select the appropriate sample type.

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

Figure 52. Meth Val page

Table 47. Meth Val page parameters

Parameter	Description
RT	Retention time for the compound.
Compound	The compound name.
Theo Conc	Values for the compounds that represent the expected theoretical concentration of that compound in the sample.
Min Recovery (%) Max Recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that the application can determine by comparing the observed calculated concentration in the analysis to the expected concentration. Each method validation compound can have its own values for these fields, independent of other method validation compounds.
Max RSD (%)	The maximum relative standard deviation of the set of observed concentrations for a component across the set of method validation samples.

Matrix Spike

Use the Matrix Spike page to view or edit QC values for matrix spike and matrix spike duplicate analyses. The application makes the evaluation by comparing the calculated concentration for each compound in the sample (after subtracting the original sample value) to the theoretical concentration and range defined on this page.

To evaluate matrix spike or matrix spike duplicate compounds, prepare samples as MS or MSD. These represent samples where you have added known concentrations of target analytes. To define a sample, its MS, and its MSD in the batch, select the appropriate Sample Type and a Sample ID.

Sample IDs must be unique. Duplicating Sample IDs can cause incorrect samples to be included in reports.

On the MS/MSD report, the application flags the calculated values for spiked compounds that exceed these limits.

Figure 53. Matrix Spike page

Table 48. Matrix Spike page parameters

Parameter	Description
RT	Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
Compound	The compound name.
Theo Conc	Values for the matrix spike compounds that represent the expected theoretical concentration of that compound in the sample. You can apply or not apply the dilution factor for a sample to the calculated matrix spike concentrations.
Min Recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that can be determined by comparing the observed calculated concentration in the analysis to the expected concentration. Each matrix spike sample can have its own values for these fields, independent of other matrix spike samples.
Max Recovery (%)	
Max RPD	Specify a maximum value for relative percent difference (RPD) between two spiked samples.

Tune

Use the Tune page (see "Tune page" on page 199) to specify mass spectral comparison criteria according to Environmental Protection Agency (EPA) tune methods. Your master method must include one (and only one) compound specified as an MSTune compound type. The QAQC evaluation compares the mass list of the compound to the values in the tune method.

An MSTune sample contains Decafluorotriphenylphosphine (DFTPP) or bromofluorobenzene (BFB) and is handled differently from other samples in the master method. The TraceFinder application handles it as a qualitative examination of the mass spectrum of a specific compound rather than evaluates it on a quantitative basis.

Follow these procedures:

- To select an EPA tune method

- To manually submit a mass spectrum for tune evaluation

❖ **To select an EPA tune method**

1. Choose a method from the Method list.

   - For some methods, the Use Only Selected Method option is available.

   - For some methods, the Perform Background Subtraction option is available.

   The application displays the mass spectral reference for the selected method.

Eval Mass	Base Peak?	Low Op	Lower Limit %	High Op	High Limit	Relative To
51		>=	10	<=	85	Base peak
68				<	2	69
70				<	2	69
127		>=	10	<=	80	Base peak
197				<	2	198
198	Yes	>	50	<=	100	Base peak
199		>=	5	<=	9	198
275		>=	10	<=	60	Base peak
365		>	0.5			198

2. (Optional) Select the **Use Only Selected Method** check box.

   The application uses only the specified EPA tune method for tune criteria testing.

   If this option is not selected and the tune spectrum fails against the specified tune criteria, the application performs the comparison against other EPA tune method criteria. The Tune report displays the pass/fail status of the tune spectra against all methods used for comparison.

3. (Optional) Select the **Perform Background Subtraction** check box.

   - The 8000 and CLP series methods require background subtraction.

   - The 500 and 600 series do not require background subtraction but you can choose to use it.

   The Tune report displays the retention time and scan range of the spectrum.

4. (Optional) Click **Max Stepoff** to select a number or type a number in the box.

   The Max Stepoff field defines the maximum number of scans as the range before and after the Tune compound peak that is to be used for background subtraction. For example, a maximum stepoff of 1 means that the background spectrum is taken one scan before the left edge of the tune peak or one scan after the right edge of the tune peak. If using the left edge background spectrum fails the tune test, the system automatically tries the right edge of the spectrum. A maximum stepoff of 2 means trying up to four tests using four different background spectrum: two scans before the left edge, one scan before the left edge, one scan after the right edge, and two scans after the right edge. EPA guidelines assign a maximum stepoff value of 20.

   > **Note** This Max Stepoff value is not related to the Stepoff Value parameter on the General page of the master method. The Stepoff Value on the General page applies only to the reference spectrum set for the master method and does not affect the Tune method.

❖ **To manually submit a mass spectrum for tune evaluation**
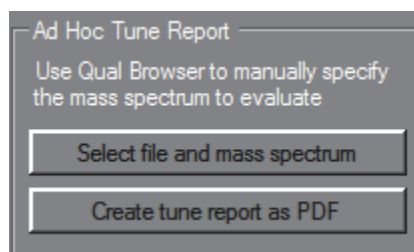
1. Click **Select File and Mass Spectrum**.

2. In the browser, select a raw data file and click **Open**.

   The Thermo Xcalibur Qual Browser opens.

Figure 54. Thermo Xcalibur Qual Browser
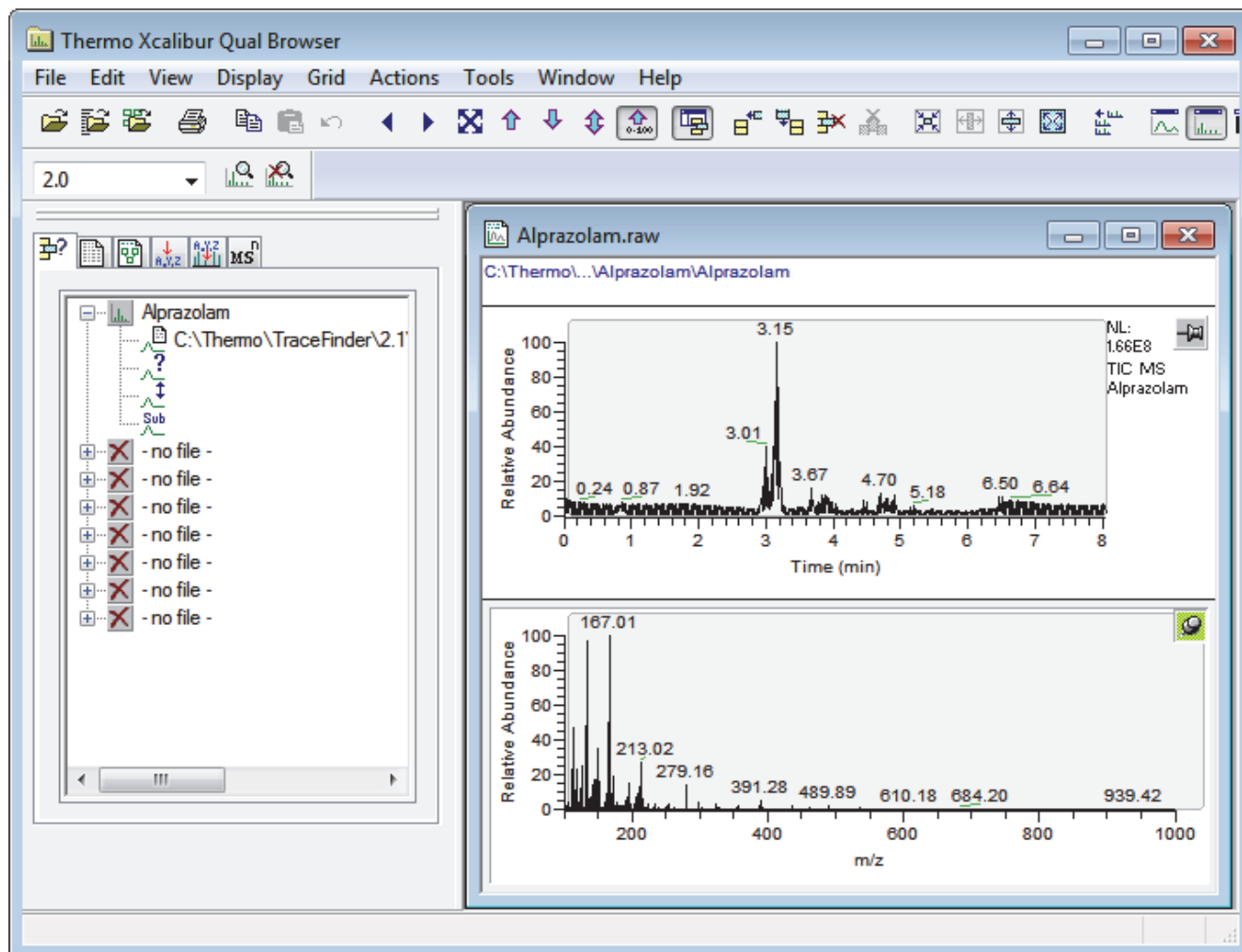
3. In the Qual Browser, do the following:

    a.   Select the tune compound peak that you want to use.

    b.   Select the background subtraction parameters to use, and generate the mass spectrum.

        For detailed instructions, refer to the Qual Browser documentation.

    c.   When the process is complete, choose **View > Spectrum List**.

    d.   Right-click the spectrum list and choose **Export > Clipboard**.

    e.   On the TraceFinder Tune page, click **Create Tune Report as PDF**.

Figure 55. Tune page

Table 49. Tune page parameters

Parameter	Description
Tune parameter	
Tune Compound	Compound specified as a tune compound on the Identification page. See "Identification" on page 133.
Method	Environmental Protection Agency (EPA) methods used for tuning.
Use Only Selected Method	Specifies that the application use only the specified EPA tune method for tune criteria testing.
Perform Background Subtraction	Specifies that the application average and subtract the mass spectra as specified in the background subtraction settings on the General page for the master method. See "To set automated background subtraction options" on page 123.
Max Stepoff	Specifies the maximum number of scans as the range before and after the Tune compound peak to be used for background subtraction.
Ad Hoc Tune Report	
Select File and Mass Spectrum	Opens a browser where you can select a raw data file to use for the tune report.
Create Tune Report as PDF	Creates an ad hoc tune report using the mass spectrum data saved to the Clipboard.

Editing the Groups Page

Use the Groups page of the Master Method View (see "Groups page") 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 parameters."

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

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

❖ **To create a group**

1. From the Show list, select the type of compounds that you want to view.
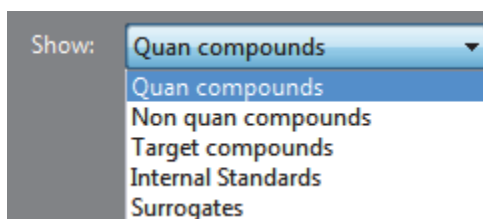
2. At the bottom of the Groups area, click **Add Group**.

   The Add a New Group dialog box opens.

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

   The new group appears in the Groups area.

4. Drag a compound from the Compounds area onto a group name (as if you were moving files into a folder).

5. To remove all the compounds from a group, rename the group, or delete it, right-click the group name and choose from the shortcut menu.
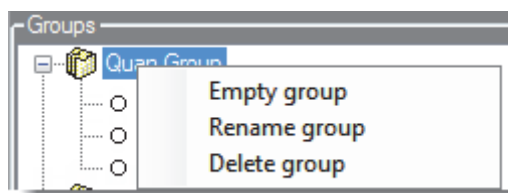
6. To remove a single compound, right-click the compound name in the group and choose **Remove from Group** from the shortcut menu.
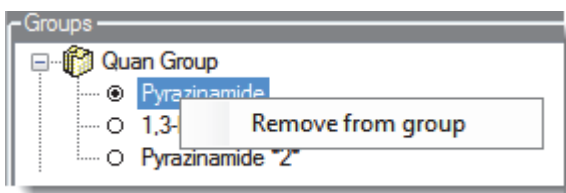
Figure 56. Groups page
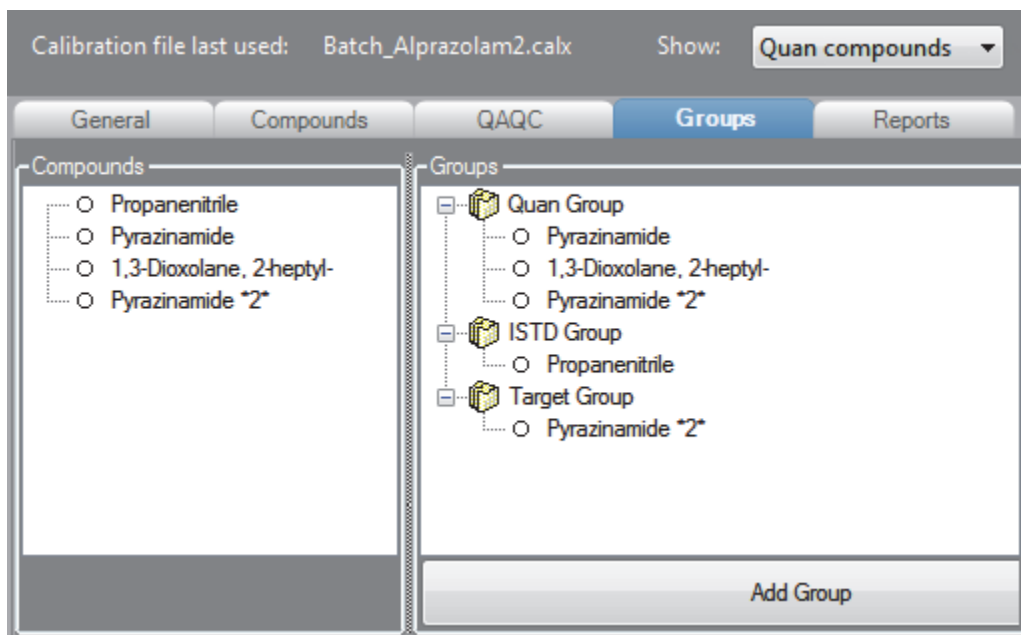
Table 50. Groups page parameters

Parameter	Description
Compounds	Lists all available compounds.
Groups	Lists all available groups.
Add Group	Opens the Add a New Group dialog box where you can create a new group.
Shortcut menu	
Empty Group	Removes all compounds from the selected group.
Rename Group	Changes the name of the selected group.
Delete Group	Removes the selected group and all the compounds in it.
Remove From Group	Removes the selected compound from its group.

Editing the Reports Page

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

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 target screening 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 Settings page.

This section includes instructions for the following tasks:

- Specifying Report Formats

- Specifying Quan Report Settings

- Specifying Target Screening Settings

Specifying Report Formats

- For each standard report, you can create a hardcopy printout, a PDF file, or an XML file.

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

- For each target screening report, you can create a hardcopy printout or a PDF file.

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

❖ **To specify report types and output formats**

1. Click the **Reports** tab.

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

   - Example: Click the magnifying glass icon to open an example PDF of the report type

   - Report Name, Report Description, and Report Type

   - For standard report types: Options to create a hardcopy, PDF file, or XML file

   - For custom report types: Options to create a hardcopy or Excel Macro-Enabled Workbook file

   - For target screening report types: Options to create a hardcopy or PDF file

   - Batch Level: Option that indicates which reports are batch-level reports

   For information about configuring which reports are available when you create a master method or which reports create a batch-level report, see "Specifying the Reports Configuration" on page 68.

2. To edit the Report Description, double-click the name and type your new description.

   The TraceFinder application uses this description for all reports that use this master method. You cannot edit the Report Description from other report views.

3. To specify the type of report output to create for each report type, select the check box in the appropriate column.

4. To duplicate the output type for all reports, click the cell to select it, and then right-click and choose **Copy Down** from the shortcut menu.
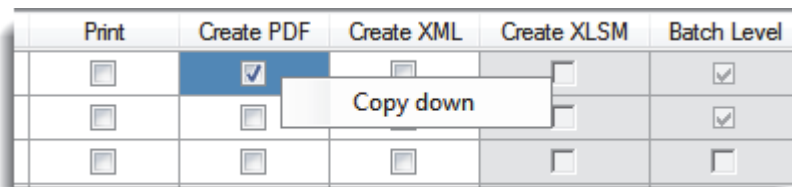
All check boxes in the column below the selected cell duplicate the selected or cleared state of the selected cell. This action applies only to reports where this output format is available.

By default, all report types are cleared.

Figure 57. Reports page

Table 51. Reports page parameters (Sheet 1 of 2)

Parameter	Description
Example	Opens a PDF that displays an example of the report type.
Report Name	The name of a report.
Report Description	The user-defined description to be used on a report.
Report Type	The type of report: 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	Exports reports in XML format. Available only for standard reports.

Table 51. Reports page parameters (Sheet 2 of 2)

Parameter	Description
Create XLSM	Exports reports 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 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 Configuration" on page 68.

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.

Follow these procedures:

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

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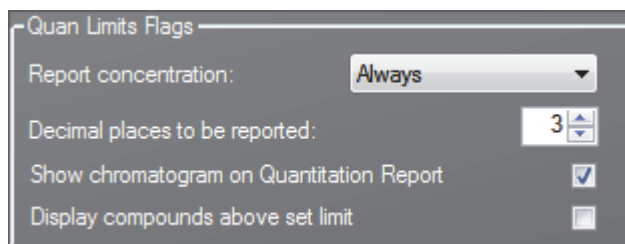
1. To report the calculated concentration at all times or only when the quantified value exceeds LOD, LOQ, or LOR, choose the appropriate value from the Report Concentration list.

   For a description of concentration limits, see "Editing the QAQC Page" on page 183.

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**
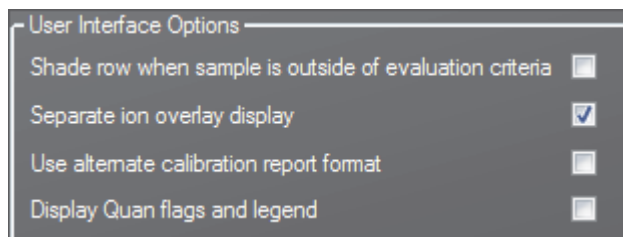
1. To shade a compound row on any of the reports if a value fails one of the criteria used for evaluation, select the **Shade Row when Sample is Outside of Evaluation Criteria** check box.

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."

❖ **To correct surrogates**

Surrogate Correction Option

Correct surrogates ☐
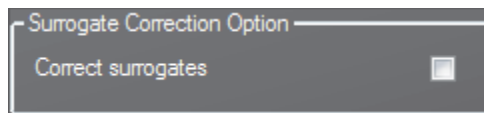
Select the **Correct Surrogates** check box.

The TraceFinder application applies the conversion factor (specified in the sample row in the batch) to the sample's calculated concentrations for surrogates as the conversion factor is applied to target compounds.

❖ **To track the use of the tune file**

Tune Time Tracking Options

Enable tune time tracking ☑

Tune file lifetime (hrs.) : 12
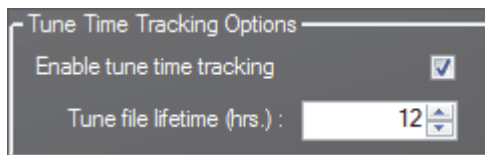
1. Select the **Enable Tune Time Tracking** check box.

   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 58. Quan Report Settings page

Table 52. Quan Report Settings page parameters (Sheet 1 of 2)

Parameter	Description
Quan Limits Flags	
Report Concentration	Reports the concentration at all times or only when the quantified value exceeds either the limit of detection (LOD), the limit of quantitation (LOQ), or the limit of reporting (LOR). Report concentration: Always, >LOD, >LOQ, or >LOR.
Decimal Places to be Reported	Number of decimal places to be included in the report. Maximum value is 6.
Show Chromatogram on Quantitation Report	Displays a chromatogram (TIC trace) of the sample on the quantitation report.
Display Compounds Above Set Limit	Prints only the positive compounds in a sample. If a compound is above the specified Quan Flag Options limits, the TraceFinder application reports the compound.
User Interface Options	
Shade Row When Sample is Outside of Evaluation Criteria	Shades a compound row on any of the reports if a value fails one of the criteria used for evaluation.
Separate Ion Overlay Display	Separates the ion overlay pane from the confirming ion plots in 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 52. Quan Report Settings page parameters (Sheet 2 of 2)

Parameter	Description
Quan Flag Options	Values that are above or below limits defined on the Limits page. These flags appear on a variety of reports.
Flag Values Below LOD	Flags values below the limit of detection (LOD).
Flag Values Below LOQ	Flags values below the limit of quantitation (LOQ).
Flag Values Above LOR	Flags values above the limit of reporting (LOR).
Flag Values Above ULOL	Flags values above the upper limit of linearity (ULOL).
Flag Values Above Carryover	Flags values above the carryover limit.
Flag Values Between LOD and LOQ	Flags values between the limit of detection and the limit of quantitation known as the J flag.
Surrogate Correction Option	
Correct Surrogates	Applies the conversion factor (specified in the sample row in the batch) to the sample's calculated concentrations for surrogates as the conversion factor is applied to target compounds. For example, if you added surrogates to the sample as part of sample preparation and you require a dilution for analysis, the TraceFinder application dilutes the surrogates and target compounds and applies a dilution correction to correct for this dilution. However, if you added surrogates after a dilution has occurred, then you can leave the option cleared so that, while the target compounds are corrected for the dilution, the surrogates are reported "as is."
Tune Time Tracking Options	
Enable Tune Time Tracking	Tracks the number of hours between the last instrument tune and each sample acquisition.
Tune File Lifetime	Specifies the maximum number of hours between the last instrument tune and a sample acquisition. Any sample acquired outside this maximum allowable time is flagged on the Batch report.

Specifying Target Screening Settings
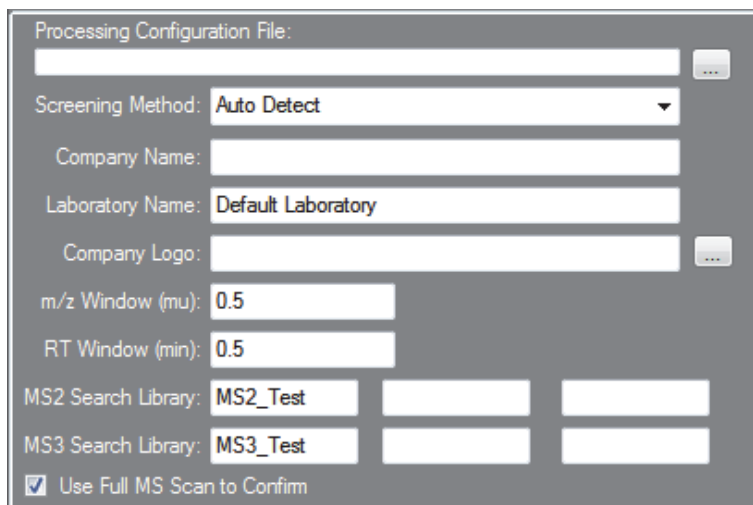
Use the options on the Target Screening Settings page to set the parameters required to produce Target Screening reports. For detailed descriptions of the features on the Target Screening Settings page, see "Target Screening Settings page parameters" on page 213.

The TraceFinder application uses these parameters to process a raw data file and create a report similar to a ToxID report. See "Example Target Screening Summary Report" on page 215.

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 **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 **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.

2. To search the entire raw data file for the specified peak, do the following:

   a. Select the **No Specified Retention Time** check box.

   b. Select either the **First Peak** or **Highest Peak** option.

      When the search finds more than one *m/z* match in the raw data file, the application uses the specified peak for processing.

3. Select the **Report All Compounds Listed in Configuration File** check box to report all compounds in the configuration file whether or not matches are found for them.

The default reports on only those compounds where matches are found in the raw data file. This option applies to the Exactive™ experiment only.

Figure 59. Target Screening Settings page

Table 53. Target Screening Settings page parameters (Sheet 1 of 2)

Parameter	Description
Processing Configuration File	Specifies a configuration file (.csv).
Screening Method	Specifies one of the following screening methods: • (Default) Auto Detect • Based on Full MS2 scans • Based on SRM and MS2 scans • Based on MS2 and MS3 scans • Based on MS3 scans • Based on accurate mass scans • Based on SRM scans • Based on Exactive screening method
	Note Using the Auto Detect method, the ToxID application can identify the screening experiment implemented in the acquired data file.
Company Name	Specifies the name of the company to print on the report.
Laboratory Name	Specifies the name of the laboratory to print on the report.
Company Logo	Specifies a graphic file (.jpg, .gif, or .bmp) to print on the report.
m/z Window (mu)	Specifies a value for the window above and below the *m/z* value for the compounds.

Table 53. Target Screening 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(%)	
Accurate Mass Experiment	
Exact Mass Window	Specifies a value in parts per million for the accurate mass experiment.
Exactive	
Adduct 1–*n*	Specifies the adducts listed in and applied throughout the configuration file. Adducts are polarity sensitive. For negative ionization, enter negative adduct values. Defaults: Adduct 1: H+, Adduct 2: NH4+, and Adduct 3: Na+
No Specified Retention Time	Specifies either First Peak or Highest Peak to use for processing when the search finds more than one *m/z* match in the raw data file.
Report All Compounds Listed in Configuration File	Specifies that in an Exactive experiment, the application reports all compounds in the configuration file whether or not matches are found for them. Default: Reports only those compounds where matches are found in the raw data file.

Figure 60. Example Target Screening Summary Report

Your Company Name
Summary Report

Raw File Name: C:\Xcalibur\examples\ToxID\Exact_Mass\Exact_Mass_Test.RAW

Config File Name: C:\Xcalibur\examples\ToxID\Exact_Mass\ConfigFile_Exact_mass.csv

Sample Name: Laboratory: Your Lab Name

Acquistion Start Time: 3/24/2008 4:46:43 PM

Screening Conditions: Based on accurate mass scans. Exact mass window (ppm): 30, RT window(min): 0.50.
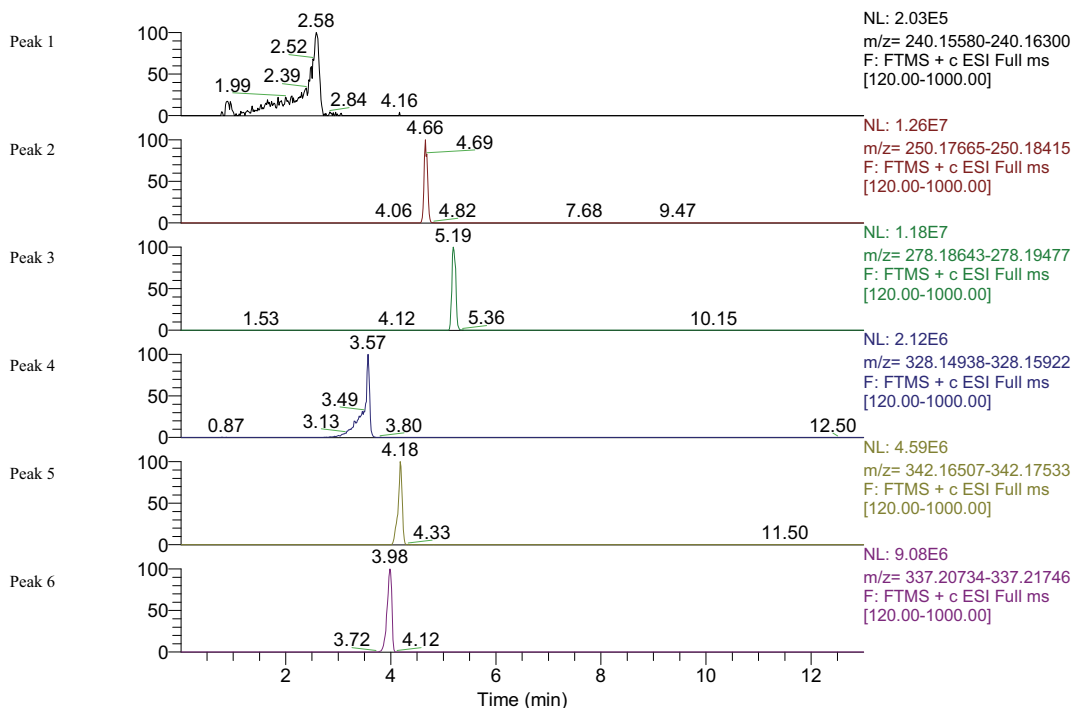
Peak Number	Compound Name	Expected m/z	Detected m/z	Delta (mDa)	Delta (ppm)	Expected RT	Actual RT	Intensity
1	Albuterol	240.15940	240.15939	-0.0	-0.0	2.58	2.58	199505
2	Alprenolol	250.18040	250.18039	-0.0	-0.0	4.50	4.66	12604499
3	Amitriptyline	278.19060	278.19061	0.0	0.0	5.00	5.19	11769755
4	6-Acetylmorphine	328.15430	328.15433	0.0	0.1	3.30	3.57	2112090
5	6-Acetylcodeine	342.17020	342.17035	0.1	0.4	4.10	4.18	4593306
6	Acebutolol	337.21240	337.21246	0.1	0.2	3.80	3.98	9077282

Creating a Method Template

In the TraceFinder application, you can create a processing method using a method template that contains common settings.

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** from the dashboard or the navigation pane.

The Method Development navigation pane opens.

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

3. From the main menu, choose **File > New > Method Template**.

The Method Template Editor opens. For a complete description of the Method Template Editor, see "Method Template Editor dialog box" on page 222.

❖ **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 largest peak.

4. To display a specific number of the largest peaks by height or area, select the **Only Select Top Peaks** check box and enter the number of peaks to display.

❖ **To identify the peaks**

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

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

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

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

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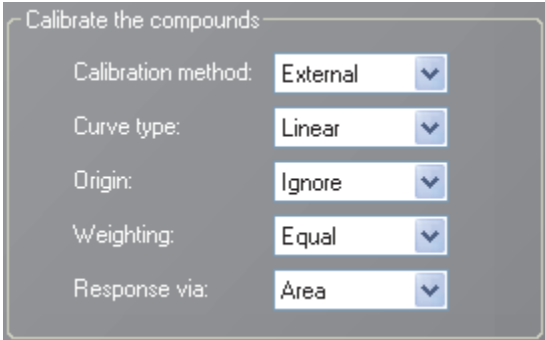
1. To set the number of confirming ions, select the **Include Confirming Ions** check box and enter a value in the Number of Confirming Ions box.

   This value is the number of other ions in the spectrum whose ratio is compared to the quantitation ion. Using this ratio, you can then determine if it is the target compound or something else. 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, all weighting values are unavailable except for Equal.

   • Quadratic: All other settings are available with this exception: When you select Include in the Origin list, all weighting values are unavailable except for Equal.

   • Average RF: No selections in the Weighting or Origin lists are available. The Weighting list is set to Equal, and the Origin list is set to Ignore.

3. From the Origin list, select one of the following:

   • Ignore: Specifies that the origin is not included as a valid point in the calibration curve when the curve is generated. When you select Ignore, the calibration curve might or might not pass through the origin.

   • Force: Specifies that the calibration curve passes through the origin of the data point plot when the calibration curve is generated.

   • Include: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select Include, the calibration curve might or might not pass through the origin.

4. From the Weighting list, select one of the following:

- Equal: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select Equal, the calibration curve might or might not pass through the origin.

- 1/X: Specifies a weighting of 1/X for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their quantity.

- 1/X^2: Specifies a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity.

- 1/Y: Specifies a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio).

- 1/Y^2: Specifies a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).

5. From the Response Via list, select **Area** or **Height**.

- Area: Specifies that the TraceFinder application use this area value in response calculations.

- Height: Specifies that the application use this height value in response calculations.

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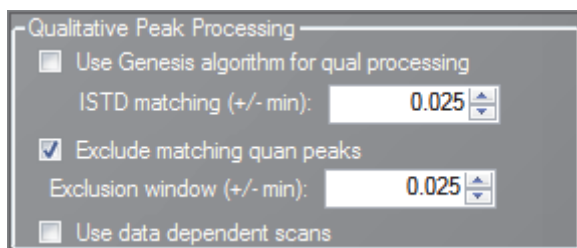
1. Select the **Use Genesis Algorithm for Qual Processing** check box and specify a value for internal standard matching.

The application uses the Genesis algorithm to match internal standards in a range plus/minus the value that you specify. For additional information about the Genesis algorithm, see "Genesis Detection Method" on page 78.

This parameter is available only when the Sensitivity parameter in the Find the Peaks area is set to ICIS.

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.

In addition to the peak information, the TIC Report and TIC Summary Report display information about the data-dependent filtered data. See Appendix A, "Reports."

❖ **To enter a note for the method**

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

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

❖ **To save the method template**

1. Choose **File > Save** from the Method Template Editor menu.

The Save Method Template dialog box opens.

2. Do one of the following:

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

–or–

Select a method name to overwrite and click **Overwrite**.

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

…\Thermo\TraceFinder\2.1\EFS\Templates\Methods

Figure 61. Method Template Editor dialog box

Table 54. Method Template Editor dialog box parameters (Sheet 1 of 3)

Parameter	Description
Find the peaks	
Sensitivity	Defines how extensively the peak detector algorithm searches for low-level peaks.
Limit the Retention Time Range	Min RT specifies the beginning of the range. Max RT specifies the end of the range.
Enable Peak Threshold	Specifies whether to select peaks by relative height or area and the percentage of the highest peak that results in compound selection.
Only Select Top Peaks	Displays a specific number of the largest peaks by height or area.
Identify the peaks	
Use These Libraries	Lists the libraries that you can search.
Limit Library Hits	Specifies the number of 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.
Specify Default Ion Ratio Ranges	Enables the ion ratio range features. Ion Coelution specifies the maximum difference in retention time between a confirming ion peak and the quantification ion peak. Window Type specifies an Absolute or Relative calculation approach for determining the acceptable ion ratio range. Window (+/-%) specifies the acceptable ion ratio range.
Include Compound Peak Spectrum as Reference Spectrum	Includes the peak spectrum in the processing method. Use this setting to perform a spectra comparison in Data Review.
Calibrate the compounds	
Calibration Method	Specifies an internal or external calibration method.
Curve Type	Specifies a linear, quadratic, or average RF curve type.

Table 54. Method Template Editor dialog box parameters (Sheet 2 of 3)

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

Table 54. Method Template Editor dialog box parameters (Sheet 3 of 3)

Parameter	Description
Exclude Matching Quan Peaks	Compares the retention time of the internal standard in the method to the found retention time of the internal standard in the library search and excludes peaks outside the Exclusion Window range.
Exclusion Window	Defines a range plus/minus the Exclusion Window value that you specify.
Use Data Dependent Scans	Constrains the Qual Mode view in the Data Review to only data-dependent scan spectra. See "Qual Mode" on page 375. In addition to the peak information, the TIC Report and TIC Summary report display information about the data-dependent filtered data.

Importing Published Master Methods

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

> …\Thermo\TraceFinder\2.1\EFS\Published Master Methods

❖ **To import a published master method**

1. From the Method View task pane, click **Import Published Method**.

   The Import Published Method dialog box opens.
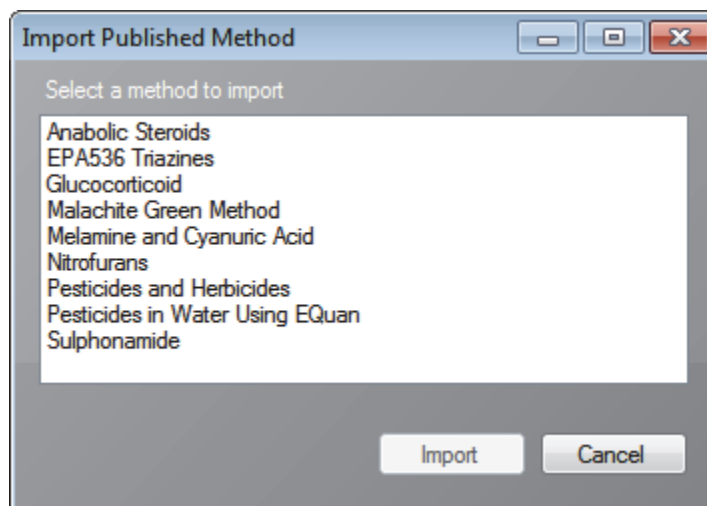
2. Select a method to import.

3. Click **Import**.

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

   > …\Thermo\TraceFinder\2.1\EFS\Methods

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

Exporting SRM Data

In the TraceFinder application, you can export your selected reaction monitoring (SRM) data to an XML file. The Export SRM Data command is displayed only when you enable the Compound Datastore option in the Configuration mode. See "Compound Datastore" on page 92.

❖ **To export SRM data to an XML file**

1. Open the master method whose SRM data that you want to export.

2. From the Method View task pane, click **Export SRM Data**.

   The TraceFinder application writes the data in the SRM table to the following file:

   …\Thermo\TraceFinder\2.1\EFS\Methods*methodname*.xml

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

Figure 62. SRM TSQ Quantum example
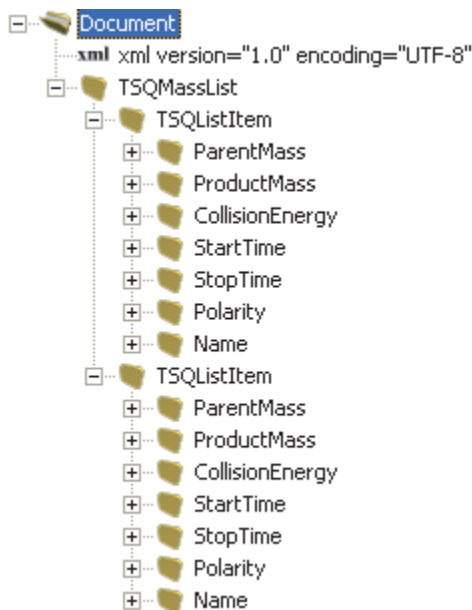
Working with Instrument Methods

An instrument method is a set of experiment parameters that define the operating settings for an autosampler, mass spectrometer, and so on. Instrument methods are saved as file type .meth.

> **IMPORTANT** Do not open the Thermo Foundation Instrument Configuration window while the TraceFinder application is running.

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 dashboard or the navigation pane.

The Method Development navigation pane opens.

2. Click the **Instrument View** task pane.

❖ **To create a new instrument method**

1. Click **New Instrument Method** in the Instrument View task pane.

The Thermo Xcalibur Instrument Setup window opens.

Figure 63. Example instrument setup showing multiple configured instruments
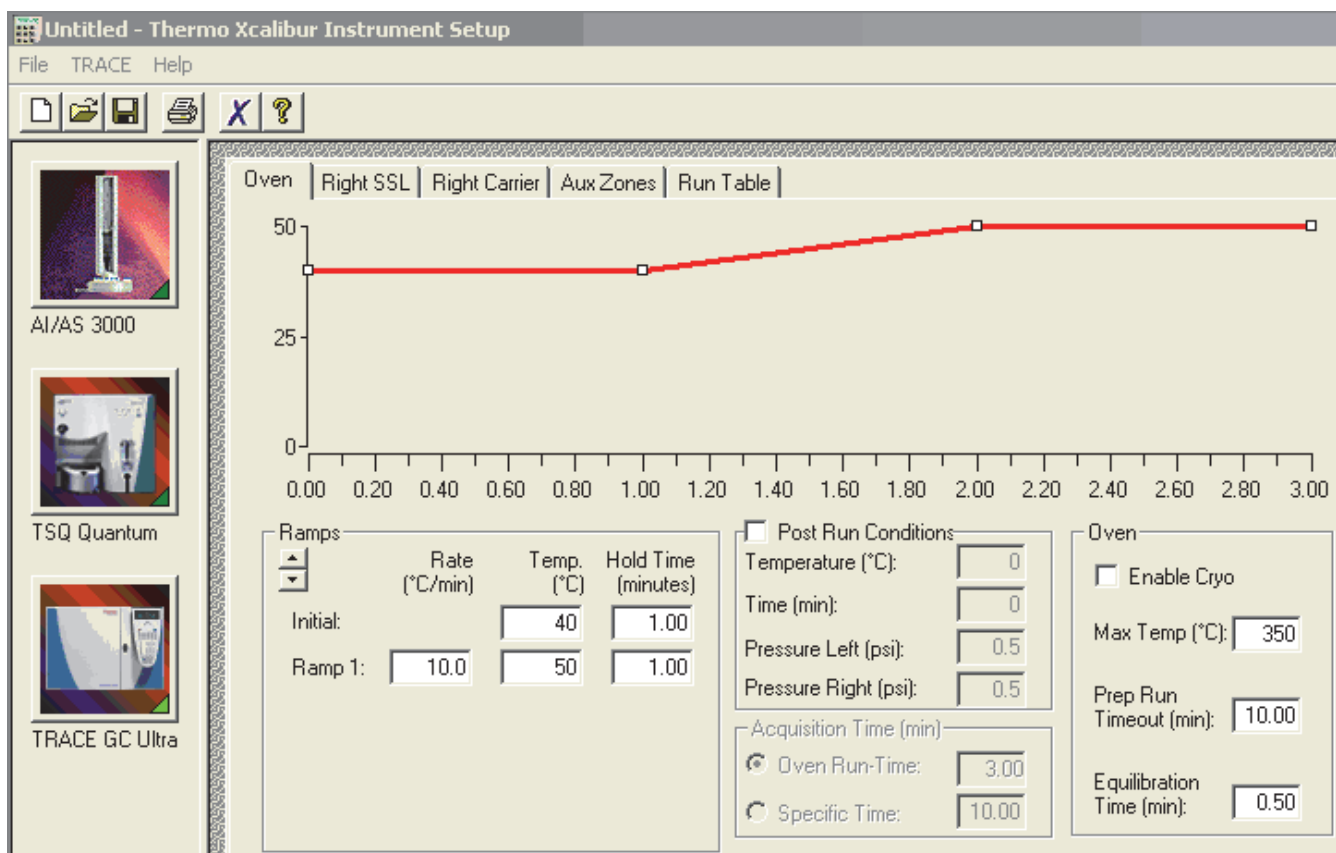
2. Click the icon for the instrument that you want to use for the method.

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.
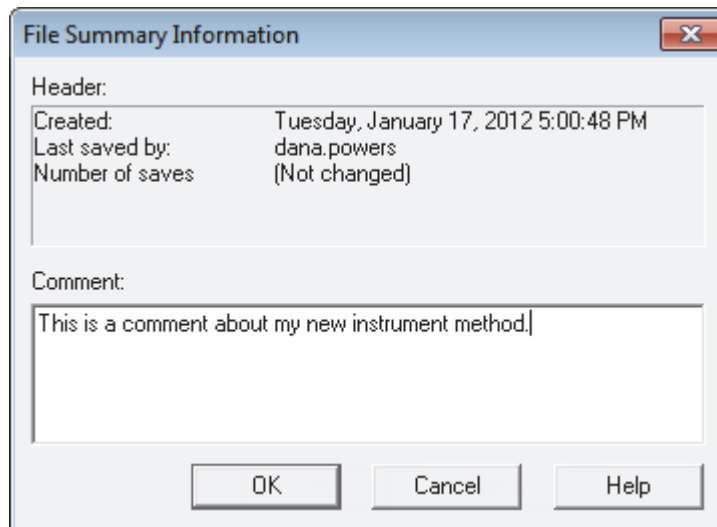
6. (Optional) Type a comment about the new instrument method.

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. Click **New Instrument Method** in the Instrument View task pane.

   The Thermo Xcalibur Instrument Setup window opens.

   Figure 64. Example instrument setup showing a configured multiplexed instrument
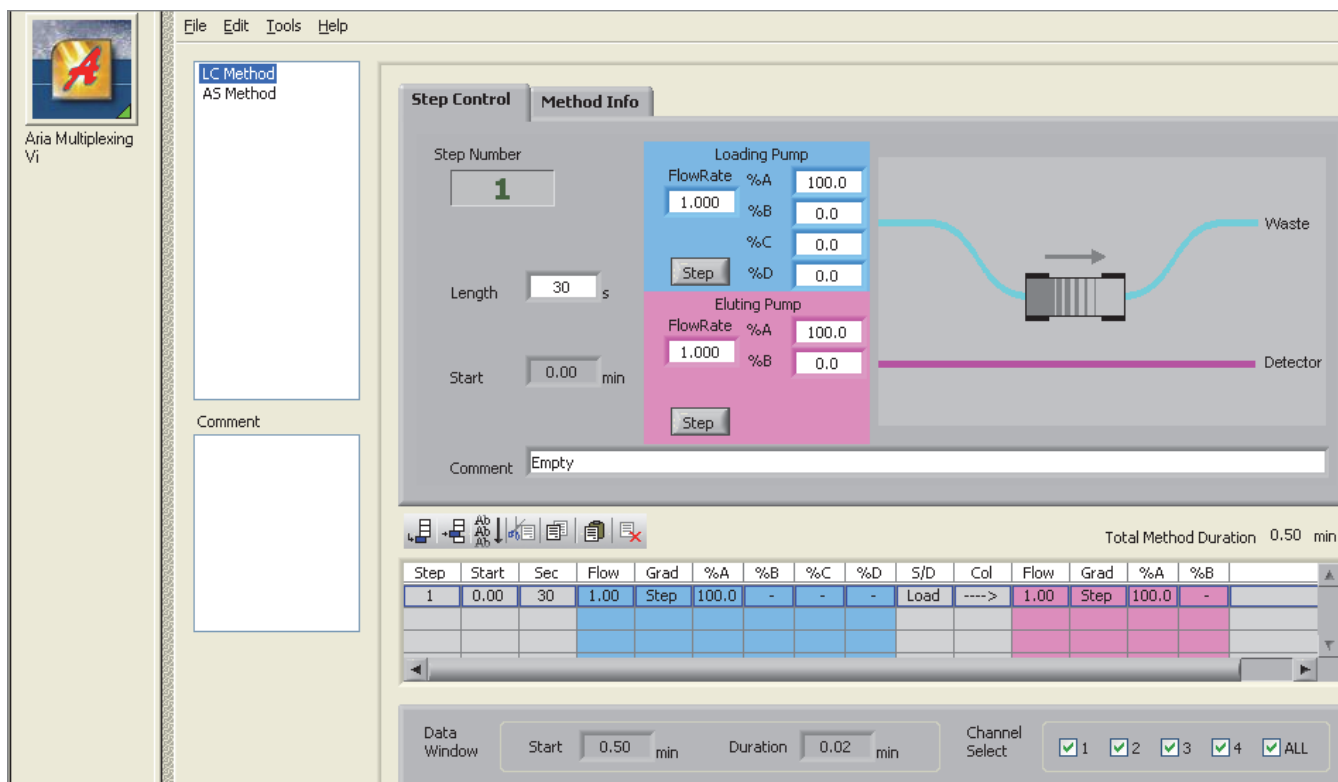
2. Click the icon for the instrument that you want to use for the method.

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.
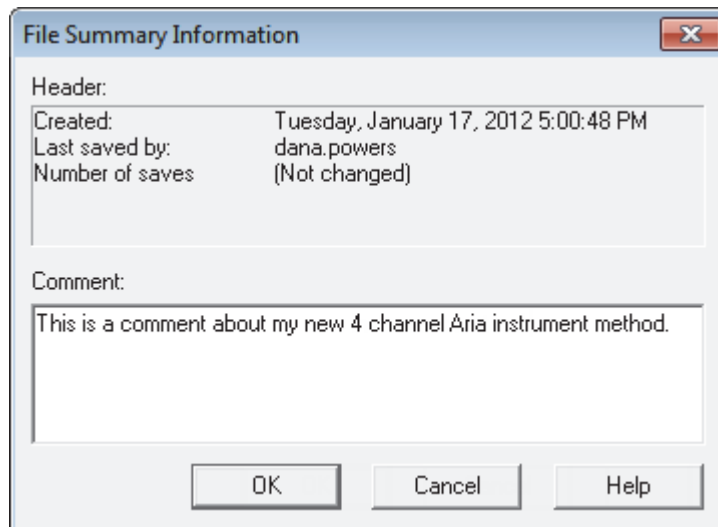
7. (Optional) Type a comment about the new instrument method.

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 task 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.

Figure 65. Example instrument setup showing multiple configured instruments
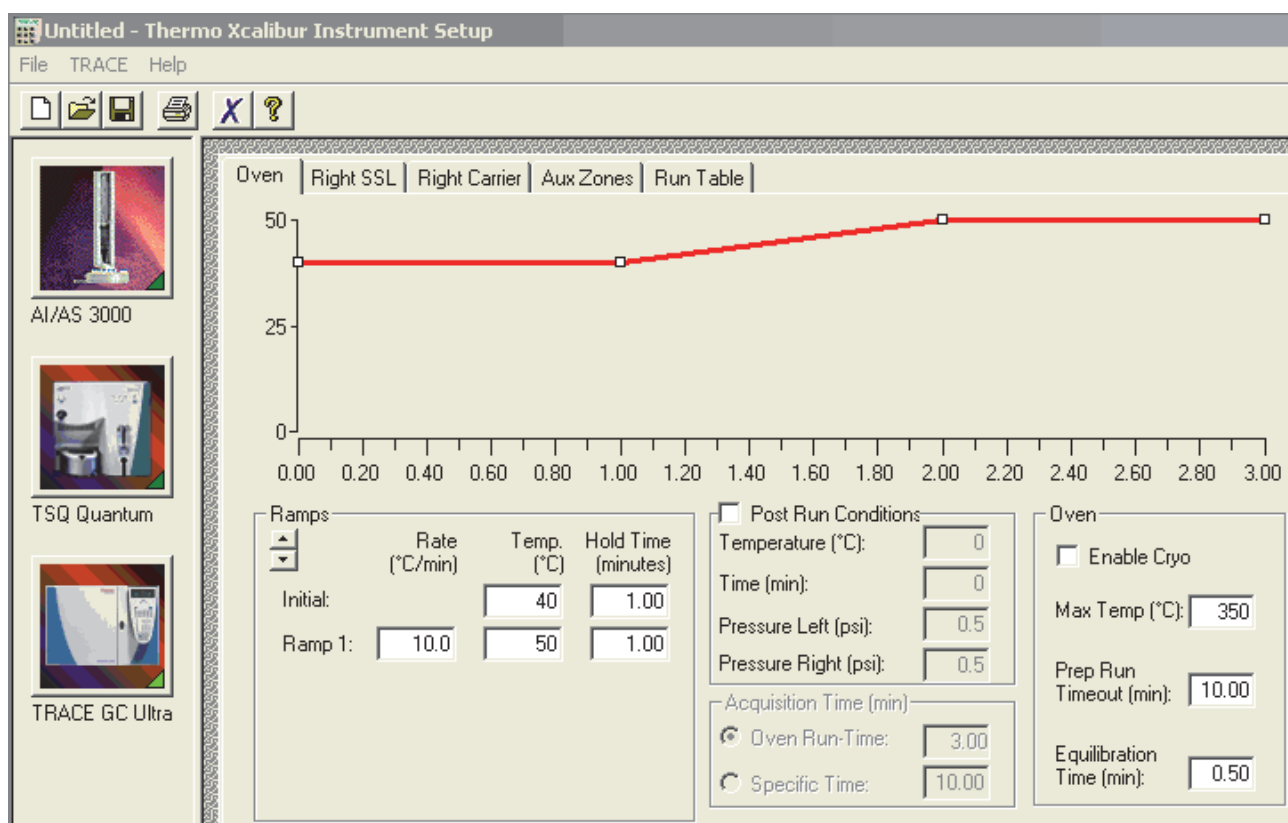
❖ **To import an instrument method**

1. From the Instrument View task pane, click **Import Published Method**.

   The Import Published Method dialog box opens. This dialog box lists the master methods in the Published Master Methods folder. You can import instrument methods that are associated with these published master methods.
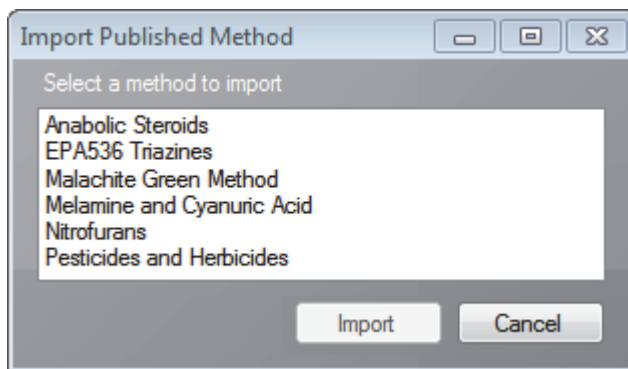
2. Select a method that includes the instrument method that you want to import.

   For instructions about importing the master methods, see "Importing Published Master Methods" on page 226.

3. Click **Import**.

   The Save Instrument Method dialog box opens.
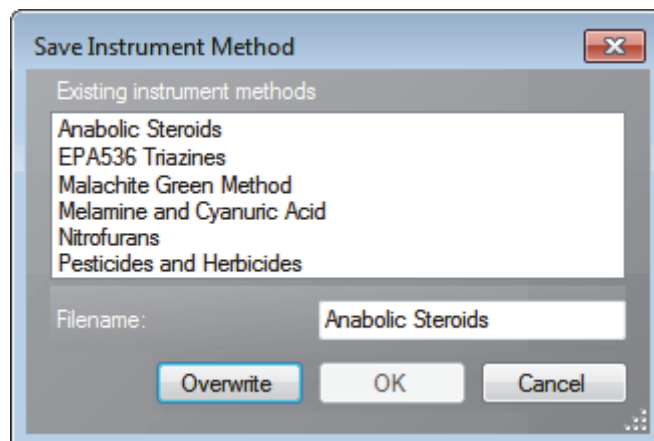
4. Do one of the following:

   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** from the dashboard or the navigation pane.

   Method Development

   The Method Development navigation pane opens.

2. In the Method Development navigation pane, click **Development Batch**.

   Development Batch ⌃

   The Development Batch view opens a new, empty batch.

Development Batch - [C:\Thermo\TraceFinder\2.1\...\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 enabled multiplexing in the Configuration mode. See "Multiplexing" on page 92.

❖ **To specify a location for development batch data**

1. To specify a location for the files, click **Select Batch Location** in the Development Batch task pane.

   By default, the TraceFinder application writes the temporary files, raw data files, and .sld method file to the following folder:

   …\Thermo\TraceFinder\2.1\EFS\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 file 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.
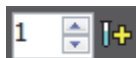
The application adds the specified number of new, empty samples to the end of the sample list.

❖ **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 B, "Using Copy Down and Fill Down."

A development batch uses the same shortcut menu features as a batch in the Batch View. For detailed descriptions of the right-click shortcut menu features, see "Batch View Shortcut Menu" on page 307.

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. To enter an instrument method for each sample, click the down arrow in the Instrument Method column and select a method from the list.

   This list contains all the available instrument methods.

6. To enter a channel for each sample, click the down arrow in the Channel column and select a channel from the list.

   You cannot specify the auto channel selection in a development batch.

   Note The Channel column is available only when you have enabled multiplexing in the Configuration mode. See "Multiplexing" on page 92.

Figure 66. Completed Development Batch

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.

2. Right-click and choose **Remove Selected Samples** from the shortcut menu.

To remove all samples from the list

1. Click **New Sample List** in the Development Batch task pane.

   One of the following happens:

   • If the samples in the current batch have all been acquired, the list is cleared.

   • If the samples in the current list have not been acquired, a message confirms that you want to clear them and start a new list.

2. To create a new empty list, click **Yes**.

   Note You cannot save a development batch when you create a new one; you can only create, acquire, and discard each batch after you use it. The TraceFinder application saves only the generated raw data files in the specified batch location.

Acquiring Samples in a Development Batch

In a development batch, you can submit the entire batch for acquisition or submit only selected samples.

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:

   …\Thermo\TraceFinder\2.1\EFS\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**

In the Development Batch task pane, click **Open Qual Browser**.

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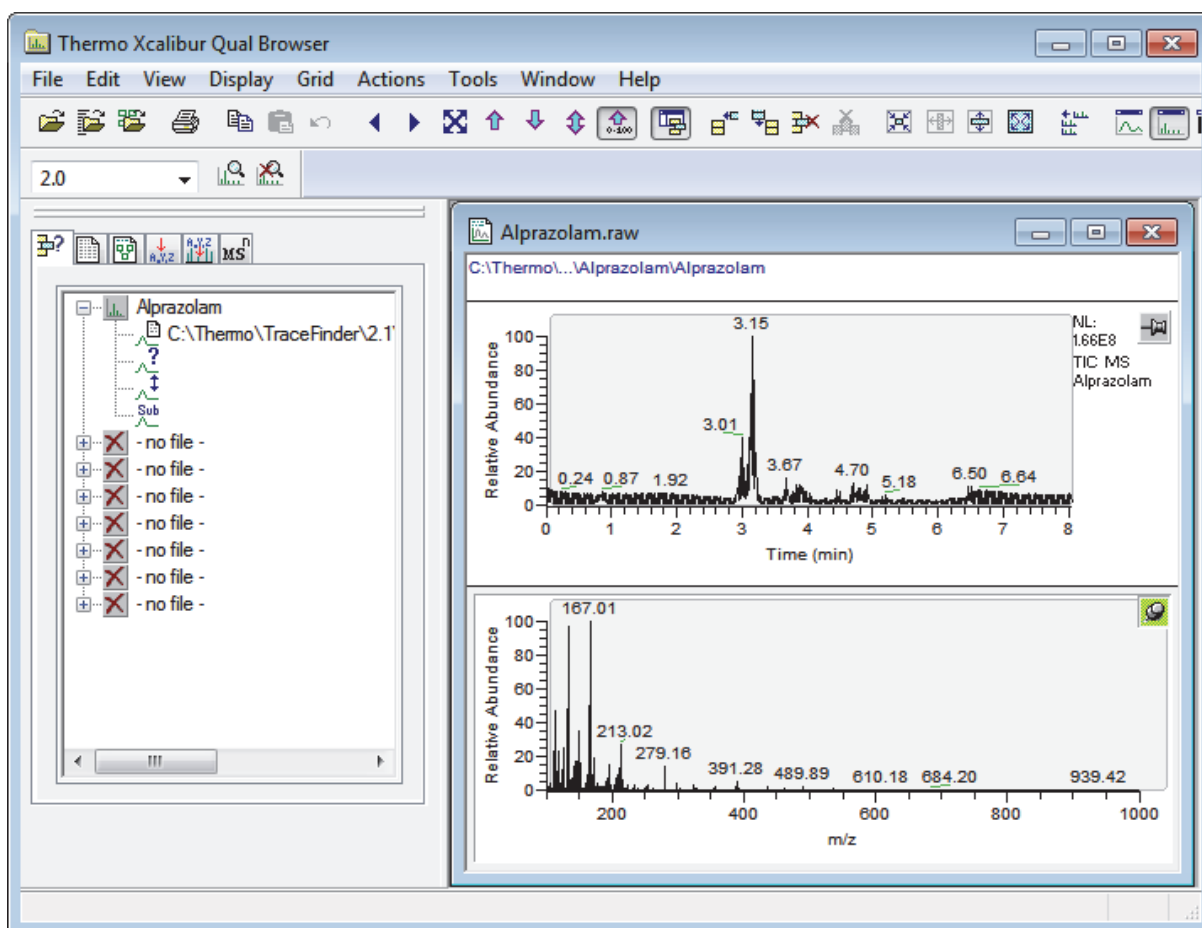
For detailed instructions about using the Qual Browser, refer to the Qual Browser Help.

❖ **To display the last completed raw data file in the Qual Browser**

On the Acquisition page of the real-time viewer, right-click and choose **View Last File in Qual Browser** from the shortcut menu.
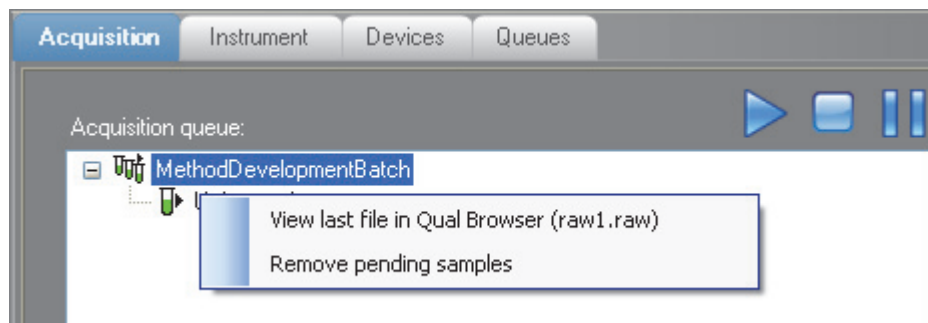
The last completed file opens in the Qual Browser.

When all samples are completed, you can view the last raw data file for the batch.
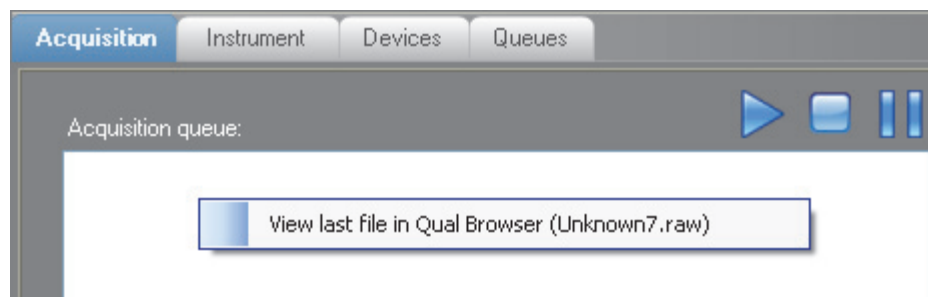
Using Quick Acquisition

You can use the quick acquisition feature to quickly submit a single sample from any view in the Method Development mode.

> **Note** The Quick Acquisition feature is available only when you enable it in the Configuration mode. See "Enabling Optional Features" on page 88.

❖ **To run a quick acquisition**

1. Choose **Go > Quick Acquire Sample** from the main menu.

   The Quick Acquisition dialog box opens.

2. Select an instrument method.

3. Type a name for the raw data file that you acquire.

4. Click the browse button and locate 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:

   a. Select the **Manual Injection** option.

   b. Click **OK**.

      The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 280.

   To perform autosampler injection, do the following:

a. Select the **Use Autosampler** option.

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

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

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

d. Click **OK**.

The Quick Acquisition dialog box opens.

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

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

This is usually the autosampler.

g. (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.

h. (Optional) Select the **Priority** check box to place the sample immediately after any currently acquiring sample.

i. (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.

j. Click **OK**.

The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 280.

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 mode. See "Batch Wizard Style" on page 94.

Contents

- Working with Batches
- Using Quick Acquisition
- Real-Time Display
- Sample Types

When you plan to work with multiple samples or use similarly designed batches, use the Acquisition mode to reduce the amount of data you must enter.

Because the nature and types of batches are often similar (in some cases specified by laboratory standard practices), you can define a batch template that supplies the basic structure of a batch.

Note When user security is enabled, only a user in the LabDirector or Supervisor role can create a batch template.

If you have a master method, you can create a batch and run the samples. Batches represent one or more samples that are to be acquired, processed, reviewed, and reported as a set. After you create a batch of samples, you can submit the batch and review the results in the 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 277.

Working with Batches

This section includes instructions for the following tasks:

- Opening and Navigating the Acquisition Mode

- Creating Batches

Opening and Navigating the Acquisition Mode

❖ **To access the Acquisition mode**

Click **Acquisition** from the dashboard or the navigation pane.

The Acquisition mode navigation pane opens.

The TraceFinder application does not use the navigation pane in the Acquisition mode in the same way it uses the navigation pane in other modes. In the Acquisition mode, this pane keeps track of your progress as you move through the views to create and submit a batch or a batch template.

Figure 67. Task pane when you enter the Acquisition mode
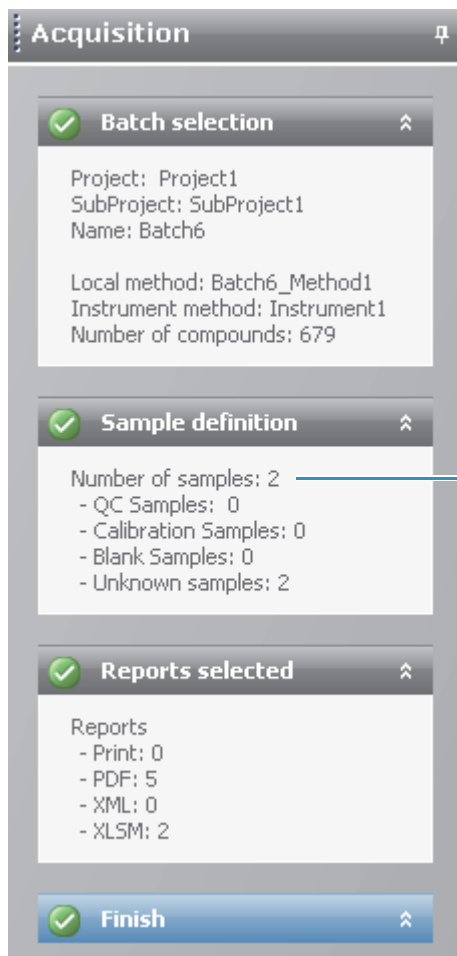
The status of each view in the Acquisition mode shows you which tasks are completed and which tasks are not.

 ———— Completed view

 ———— Incomplete required view

 ———— Current view

 ———— Unvisited view
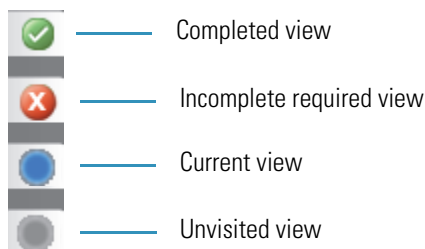
As you complete each view, the task panes display the parameters you specified for your batch.

Figure 68. Example task pane when you have completed the Acquisition mode

Categories in the Sample Definition list:

QC Samples: Chk Std

Calibration Samples: Cal Std

Blank Samples: Matrix Blank

Unknown Samples: All other samples

Creating Batches

To create a batch, follow these major steps in Acquisition mode:

1. Selecting a Batch

2. Defining the Sample List

3. Selecting and Reviewing Reports

4. Submitting the Batch

The following workflows show the different Acquisition views required for each batch creation approach. Depending on your approach to creating a batch, use one of these specific workflows.

❖ **To create an original batch**

Batch and Method

↓

Samples

↓

Reports

↓

Finish
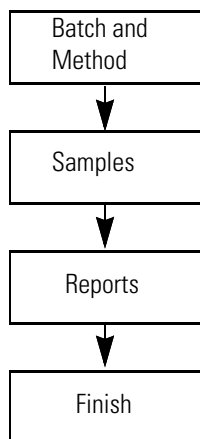
To create an original batch, start with the instructions "To start a new batch" on page 250.

❖ **To acquire a previously saved (.tbr) batch**

Batch

↓

Finish ⟷ Samples
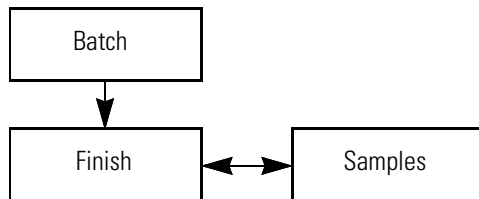
To acquire a previously saved batch, start with the instructions "To select a ready-to-acquire batch" on page 252.

❖ **To edit and process a previously acquired batch**

```
┌─────────────────┐
│      Batch      │
└─────────────────┘
         │
         ▼
┌─────────────────┐
│     Samples     │
└─────────────────┘
         │
         ▼
┌─────────────────┐
│     Finish      │
└─────────────────┘
```
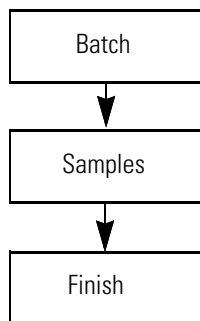
To process a previously acquired batch, start with the instructions "To select a previously acquired batch" on page 253.

❖ **To create a batch template**

```
┌─────────────────┐
│  Template and   │
│     Method      │
└─────────────────┘
         │
         ▼
┌─────────────────┐
│     Samples     │
└─────────────────┘
         │
         ▼
┌─────────────────┐
│     Finish      │
└─────────────────┘
```
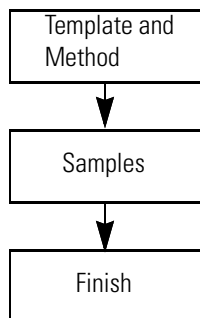
> **Note** When user security is enabled, this workflow is available only to users in the LabDirector or Supervisor role.

To create a batch template, start with the instructions "To create a batch template" on page 254 and then click **Save** on the Finish page.

Selecting a Batch

In a Template Selection view of the Acquisition mode, you can choose to create a new batch in any of your current projects/subprojects.

Follow these procedures:

- To start a new batch
- To start a new batch from a template
- To select a ready-to-acquire batch
- To select a previously acquired batch
- To create a batch template

❖ **To start a new batch**

1. Click the **New Batch** tab.

2. Select the project and subproject where you want to create the new batch.

3. Type a name for the new batch in the Batch Name box.

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

4. Select a method from the Method Selection list.

The Method Compound Data pane displays the compounds in the method. You cannot edit the compounds list from the Acquisition mode.

5. To continue to the next view, click **Next**.

The Sample Definition view opens. See "Defining the Sample List" on page 255.

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

1. Click the **New Batch** tab.

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

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

3. (Optional) Select a different project and subproject where you want to create the new batch.
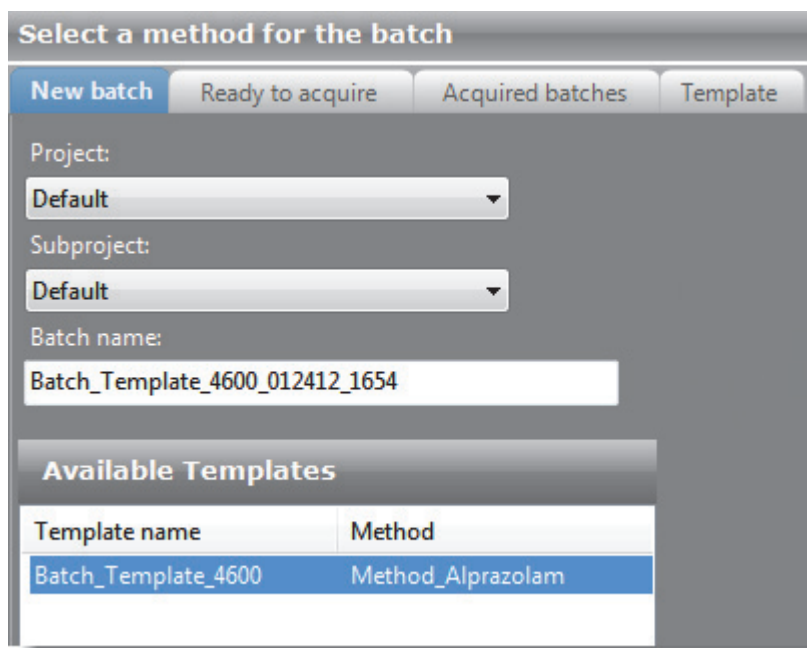
4. (Optional) Select a different method to use for the new batch.

5. To continue to the next view, click **Next**.

   The Sample Definition view of the Acquisition mode opens. See "Defining the Sample List" on page 255.
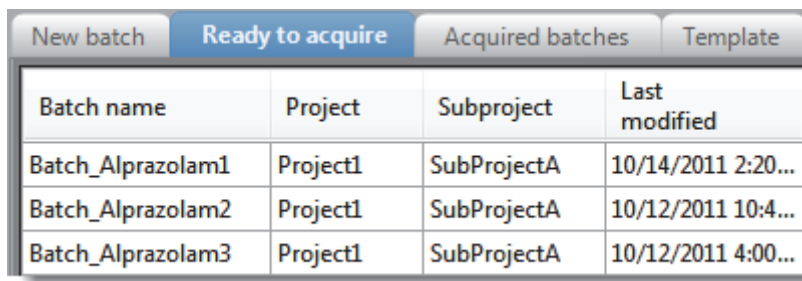
❖ **To select a ready-to-acquire batch**

1. Click the **Ready to Acquire** tab.

   All your unacquired, saved batches are displayed with the file extension .tbr (to be run). The TraceFinder application stores all .tbr batches in the following folder:

   …\Thermo\TraceFinder\2.1\EFS\Projects*projectname**subprojectname*

2. Select the batch you want to acquire.

3. To continue to the next view, click **Next**.

   The Finish view of the Acquisition mode opens. From the Finish view, you can save the batch, submit the batch for acquisition, or go to the Sample Definition view to edit the 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. Alternatively, you can browse in a new raw data file to replace the corrupt file.

4. Do one of the following:

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

     For detailed instructions, see "Submitting the Batch" on page 269.

   –or–

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

     For detailed instructions, see "Defining the Sample List" on page 255.

   –or–

   • To save the batch to the Ready to Acquire list, click **Save**.

     The TraceFinder application saves your batch as a to-be-run (.tbr) file, closes the Acquisition mode, and returns you to the application dashboard.

     The application saves the .tbr batches in the following folder:

     …\Thermo\TraceFinder\2.1\EFS\Projects*projectname**subprojectname*

❖ **To select a previously acquired batch**

1. Click the **Acquired Batches** tab.

   From this page, you can resubmit a previously acquired batch, edit the batch, or save it to be acquired later.

2. In the Project pane, select a project name.

   All subprojects included in the selected project are displayed in the Subproject pane.

3. In the Subproject pane, select a subproject name.

   The Batch pane displays all previously acquired batches included in the selected subproject.

4. In the Batch pane, select the batch you want to reacquire.
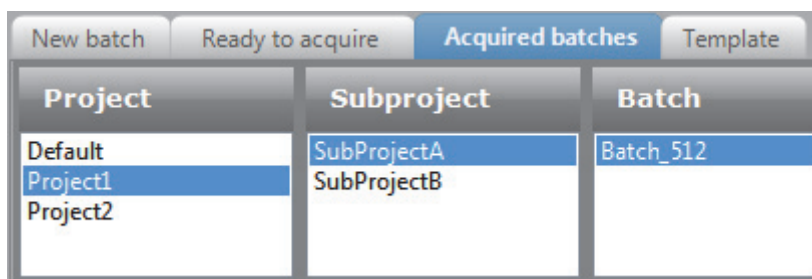
5. To continue to the next view, click **Next**.

   The Sample Definition view of the Acquisition mode opens. See "Defining the Sample List" on page 255.

   • 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. Alternatively, you can browse in a new raw data file to replace the corrupt file.

❖ **To create a batch template**

1. Click the **Template** tab.
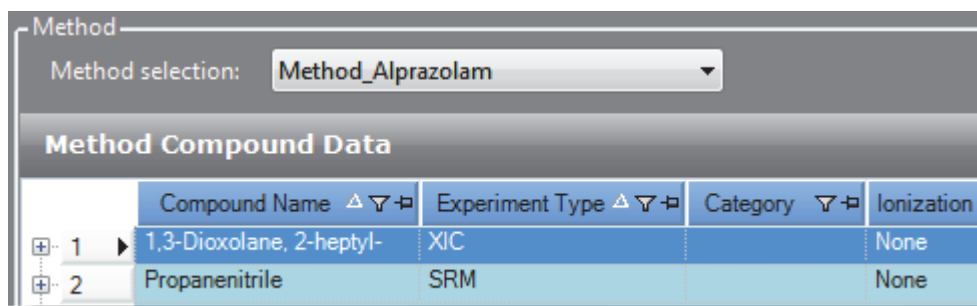
> **Note** When user security is enabled, this page is available only to users in the
> LabDirector or Supervisor role.

2. Select the project and subproject where you want to create the new batch template.

3. Type a name for the new batch template in the Template Name box.

4. Select a method from the Method Selection list.

5. 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 view, click **Next**.

7. The Sample Definition view of the Acquisition mode opens. See "Defining the Sample
List."

Defining the Sample List

In the Sample Definition view of the Acquisition mode, you can create a list of samples for the batch. You can add samples, insert samples, import a sample list, or remove samples from the list. 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 "Sample Definition view parameters" on page 263).

Icons in the toolbar

Add samples

Remove samples

Import samples

Insert samples
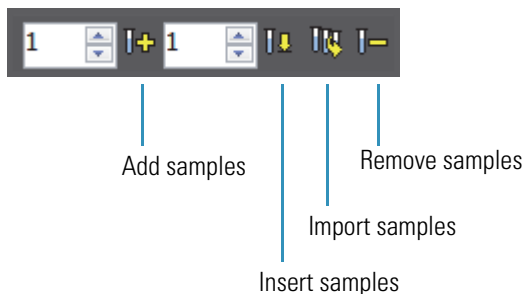
Buttons at the bottom of the template selection page

Add samples

Insert samples

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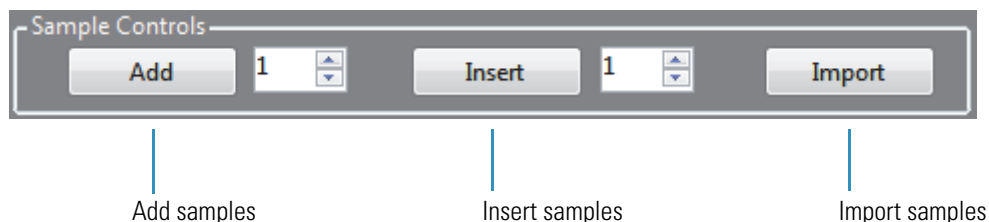
As you enter sample values, you can use the Copy Down and Fill Down commands to quickly enter column values. For detailed instructions on using Copy Down and Fill Down to enter column values, see Appendix B, "Using Copy Down and Fill Down."

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

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, the Report Selection view opens. See "Selecting and Reviewing Reports" on page 265.

- When you are editing a previously acquired batch or a .tbr batch, the Finish Selection view opens. See "Submitting the Batch" on page 269.

❖ **To add samples to the list**

1. Select the number of sample rows to add and click **Add**, [Add 1 ⬍].

2. Type a file name in the Filename column for each sample.

   Each file name must be unique.

3. Select a sample type from the Sample Type list for each sample.

Available sample types		
Matrix Blank	Solvent	Unknown/TIC
Cal Std	Chk Std	Unknown
LCS	MDL	MS
LCSD	Method Val	MSD
Tune	Tune/Breakdown	Breakdown

   For a detailed description of each sample type, see "Sample Types" on page 292.

4. For each Cal Std or Chk Std sample, select a level from the Level list.

   The sample levels are defined in the master method. If there is nothing 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 click **Update**.

   For detailed instructions, see Chapter 4, "Using the Method Development Mode."

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

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

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

   The minimum injection volume value allowed is 0.1 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, Sample Type, and Level columns stay fixed while the other columns scroll right and left.

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

❖ **To insert samples into the list**

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

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

2. Select the number of samples to insert and click **Insert**, [Insert] [1] [▲▼] .

   The application inserts the Unknown samples above the selected sample.

	Status	Filename	Sample type	Level	Sample ID
1	🟡	cal_std_5	Cal Std	5	cal std = 5 ng/uL
2	🔵	Unknown2	Unknown		
3	🔵	Unknown1	Unknown		
4	🟡	cal_std_10	Cal Std	10	cal std = 10 ng/uL

   Inserted samples → (rows 2 and 3)

3. Type a file name in the Filename column for each sample.

   Each file name must be unique.

4. Select a sample type from the Sample Type list for each sample.

   For a detailed description of each sample type, see "Sample Types" on page 292.

Available sample types		
Matrix Blank	Solvent	Unknown/TIC
Cal Std	Chk Std	Unknown
LCS	MDL	MS
LCSD	Method Val	MSD
Tune	Tune/Breakdown	Breakdown

5. For each Cal Std or Chk Std 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 Supervisor or LabDirector permissions to edit the method and specify the levels.

   For detailed instructions about defining sample levels, see Chapter 4, "Using the Method Development Mode."

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

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

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

   The minimum injection volume value allowed is 0.1 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, Sample Type, and Level 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.
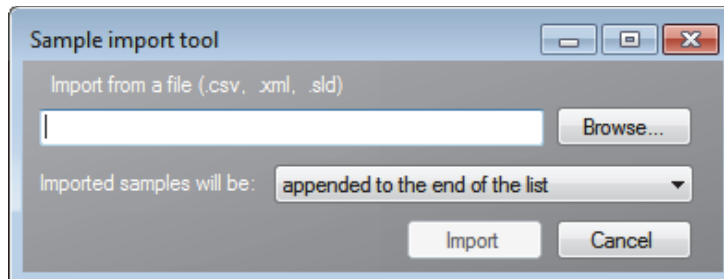
   Use this dialog box to import a sample list from a .csv, .xml, or .sld file.

2. Click **Browse** and select a .csv, .xml, or .sld file that contains the sample definitions you want to import.

   > **Note** The .csv, .xml, or .sld file format must match the TraceFinder file format.

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

4. Click **Import**.

   The Sample Import Tool dialog box closes, and the specified samples are added to the 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	Matrix Blank
QC	Chk Std
Std Bracket	Cal Std

5. For each Cal Std or Chk Std 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 Supervisor or LabDirector permissions to edit the method and specify the levels.

   For detailed instructions, see Chapter 4, "Using the Method Development Mode."

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

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

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

   The minimum injection volume value allowed is 0.1 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, Sample Type, and Level columns stay fixed while the other columns scroll right and left.

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

   Imported samples default to Auto.

❖ **To remove samples from the list**

1. Select the samples you want to remove.

> **Tip** Use the CTRL or SHIFT keys to select multiple samples.

2. Right-click and choose **Remove Selected Samples** from the shortcut menu.

❖ **To reinject a sample from a previously acquired batch**

1. In the sample list, select the sample you want to reinject.

2. Right-click and choose **Reinject This Sample** from the shortcut menu.

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

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

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

   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 enabled multiplexing in the Configuration mode. See "Multiplexing" on page 92.

To disable a configured channel, clear the check box for the channel in the Multiplexing Channels area at the bottom of the page.
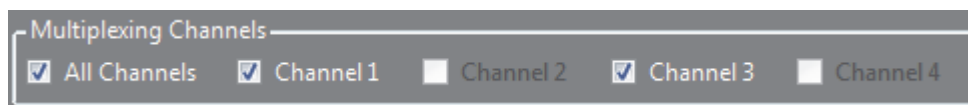
By default, all configured channels are selected. The configured channels are determined by the multiplexing settings in the Configuration mode. See "Enabling Optional Features" on page 88.

Disabling a channel in the Multiplexing Channels area does not remove this channel selection from the Channels list for each sample. When you assign a channel to a sample, be careful not to assign a channel that you disabled.

❖ **To assign a specific channel to a sample**

1. Scroll to the Channel column.

> **Note** The Channel column is available only when you have enabled multiplexing in the Configuration mode. See "Multiplexing" on page 92.

All samples default to Auto.

2. Select a channel from the Channel list.
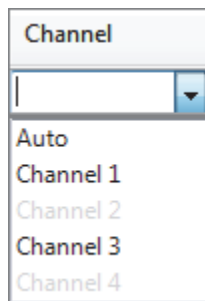
When you submit the batch, samples that are set to Auto run on any of the available channels and samples that are set to a specific channel run only on that channel.

If you select a channel that is not available for this batch, the application flags the sample sequence on the Finish page of the Acquisition mode. See the previous procedure, To select channels for the batch.
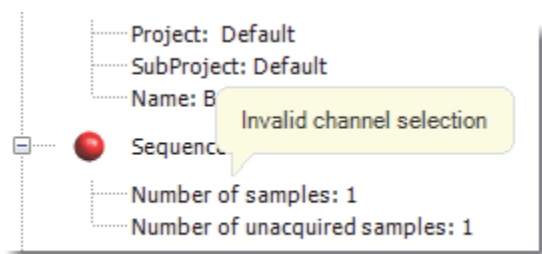
3. If you see this error, do the following:

   a. Click **Previous** to return to the Sample Definition view.

   The incorrect sample is marked with an error flag.

   b. Correct the channel selection.

Figure 69. Sample Definition view
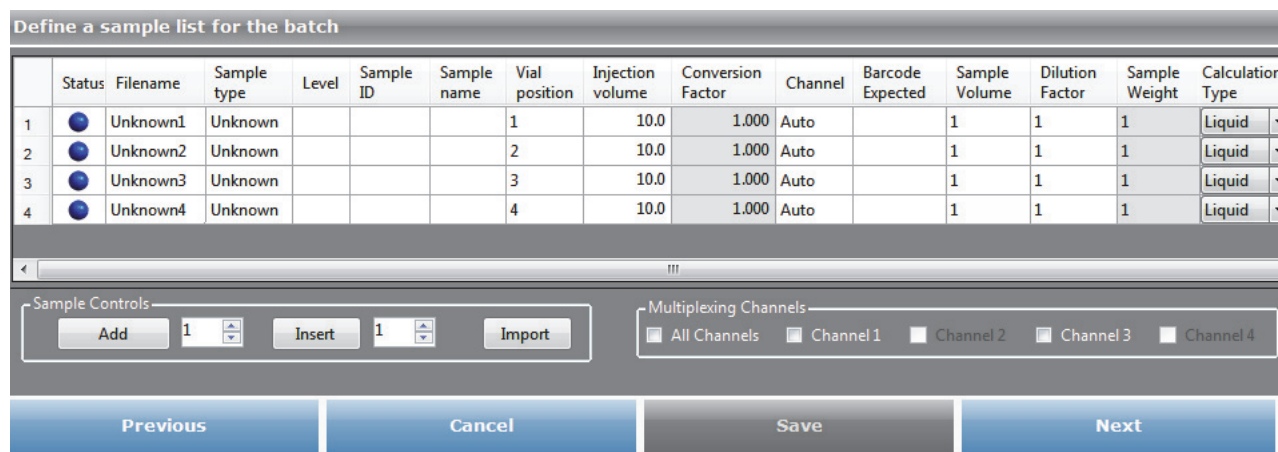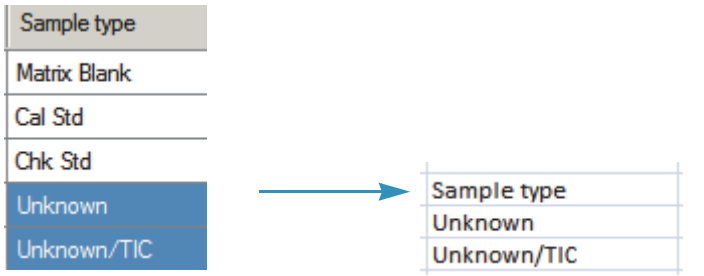
Table 55. Sample Definition view parameters (Sheet 1 of 2)

Parameter	Definition
Sample Controls	
Add	Adds the specified number of empty rows to the sample grid.
Insert	Inserts the specified number of empty rows above the selected row.
Import	Opens the Sample Import Tool where you can import samples defined in a .csv file or an .xml file.
Multiplexing Channels	These features are available only when you have enabled multiplexing in the Configuration mode. See "Multiplexing" on page 92.
All Channels	Uses all configured channels to acquire this batch.
Channel 1-n	Uses only the selected channels to acquire this batch.
Previous	Returns you to the previous Acquisition mode view.
Cancel	Confirms that you want to exit the Acquisition mode. When you cancel out of the Acquisition mode, your edits are not saved.
Save	Saves this batch as a to-be-run (.tbr) batch.
Next	Takes you to the next Acquisition mode view.
Shortcut menu	
Add Sample	Adds a single empty row to the sample grid.
Insert Sample	Inserts a single empty row to the sample grid above the selected row.
Insert Copy Sample	Copies the currently selected row and inserts a copy above the row.
Reinject Selected Samples	Creates a copy of the selected sample and appends INJ001 to the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth.
Remove Selected Samples	Removes selected samples from the sample grid.

Table 55. Sample Definition view parameters (Sheet 2 of 2)

Parameter	Definition
Copy Down	Copies the value in the selected row to all rows below it. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Fill Down	Enters sequential values in the column starting with the value in the selected row and ending with the last row in the column. For detailed instructions about using the Fill Down command, see Appendix B, "Using Copy Down and Fill Down."
Modify Columns	Opens the Modify Columns dialog box. See "Column Display" on page 350.
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. For example Copy With Headers from TraceFinder Paste into Excel spreadsheet
Paste	Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column.
Undo Last Paste	Removes the last pasted item in the Acquisition mode sample list.
Export to CSV File	Opens the Save As dialog box where you can save the current sample list to a .csv file.
Status Color Codes	● Sample is not acquired. ● Sample is acquired but not processed. ● Sample is acquired and processed. ● Sample is currently acquiring.

Selecting and Reviewing Reports

On the Report Selection view, you can specify the types of reports you want to create. See "Report Selection view" on page 267. For a complete list of report types and examples of output files, see Appendix A, "Reports." In addition to the report type, you can specify a report description for each of your reports.

For each standard report you generate, you can create a hardcopy printout, a PDF file, or an XML file.

For each custom report you generate, you can create a hardcopy printout or an XLSM file.

For each target screening report you generate, you can create a hardcopy printout or a PDF file.

When you finish specifying your report options, click **Next** to go to the Finish view and submit your batch. See "Submitting the Batch" on page 269.

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

…\TraceFinder\2.1\EFS\Projects*projectname**subprojectname**batchname*\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, XML, or XLSM file

- To export reports to a specific folder

❖ **To edit a report description**

Select the Report Description column and edit the default description.

The default report description is the same as the report name.

❖ **To preview a standard report**

1. Click the magnifying icon,   , to view an example of the report type as a PDF file.

   The right pane of the view displays an example PDF report with typical PDF viewer buttons.

2. To minimize the PDF viewer, click the minimize icon,   .

   Note Only Standard report types have preview documents.

❖ **To specify a standard report in print format or as a PDF, XML, or XLSM file**

1. For each type of report you want to create, select the check box in the Print, Create PDF, Create XML, or Create XLSM columns.

2. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell. 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 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 bottom of the view.
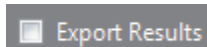
   The Browse For Folder dialog box opens.
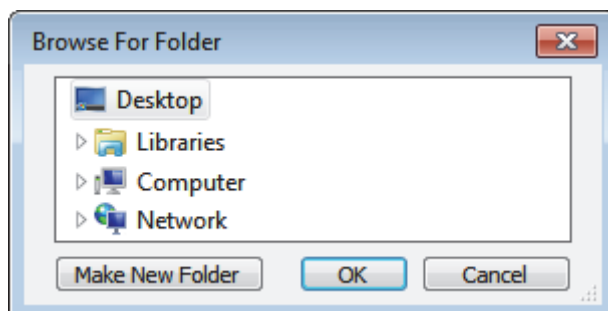
2. Locate and select the folder where you want to save the reports.

3. To create a new reports folder within the selected folder, click **Make New Folder** and type the new folder name.

4. Click **OK**.

The application writes all reports to the specified folder in addition to the batch Reports folder.

Figure 70. Report Selection view

Table 56. Report Selection parameters (Sheet 1 of 2)

Parameter	Description
🔎	Displays an example PDF for the report type. This example provides a model of the report type only; it does not reflect your specific data. This is available for standard reports only.
Report Name	The name of a report.
Report Title	User-editable description to be used on a report.
Report Type	The type of report: Standard, Custom, or Target Screening.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files. Available only for standard 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.

Table 56. Report Selection parameters (Sheet 2 of 2)

Parameter	Description
Batch Level	Rather than creating separate reports for each sample, the application uses a composite of the data from all the samples to create a single report for the entire batch. Batch-level reports are prepended with a **B** to differentiate them. You cannot select this option from the Report Selection page. You must select the Batch Level option for the report in the report configuration. See "Specifying the Reports Configuration" on page 68.
Shortcut menu: Copy Down	Copies the selected or cleared state to all subsequent reports in the column.

Submitting the Batch

In the Finish view of the Acquisition mode, you can specify a startup method, a shutdown method, or a calibration batch. You can save the batch to be acquired later, or you can acquire and process data and optionally create reports. See "Finish view" on page 275.

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

Follow these procedures:

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

❖ **To specify startup or shutdown methods**

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

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

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

   The TraceFinder application runs this method after running the batch. This feature is not available for all instruments.
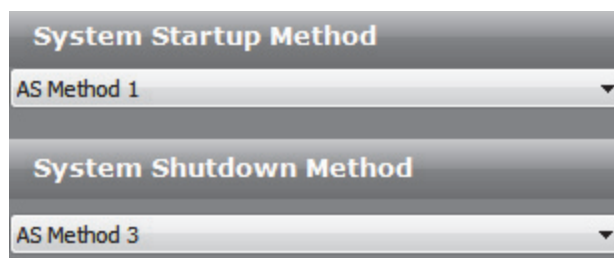
❖ **To automatically update the timed SRM information**

Select the **Auto TSRM Update** check box.
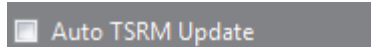
When you submit the batch, the application updates the TSQ method with mass transitions, collision energy, and other appropriate data for TSRM functionality.

❖ **To specify a calibration batch**

1. In the Calibration area, select a calibration (.calx) file from the list.
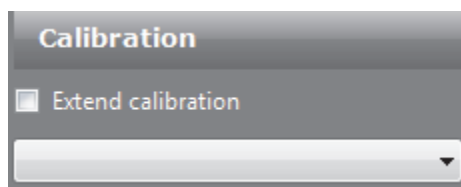
> **Note** You must acquire at least one batch with the current method to create a .calx calibration file.

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.
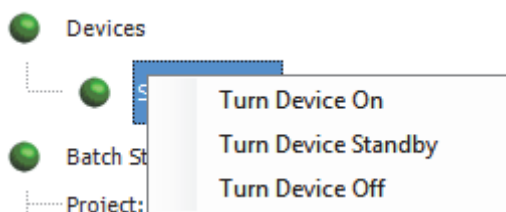
Table 57. Instrument states (Sheet 1 of 2)

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 57. Instrument states (Sheet 2 of 2)

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

❖ **To save a batch for later acquisition**

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

The TraceFinder application saves your batch as a to-be-run (.tbr) file, closes the Acquisition mode, and returns you to the application dashboard.

❖ **To start an acquisition**

1. Click **Submit**.

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

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

   > **Note** By default, the application acquires and processes data when you submit the batch.

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

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

   This is usually the autosampler.

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

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

6. (Optional with multiplexing enabled) Select the **Priority Sequence** check box.

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

7. (Optional without multiplexing enabled) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

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

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

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

8. Do one of the following:

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

The selected processes begin, and the TraceFinder application returns you to the dashboard and shows the real-time display at the bottom of the dashboard. The real-time display is visible from the dashboard and all modes. You can begin another batch in the Acquisition mode while you watch the real-time display of the currently acquiring batch.

–or–

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

Figure 71. Submit Options dialog box
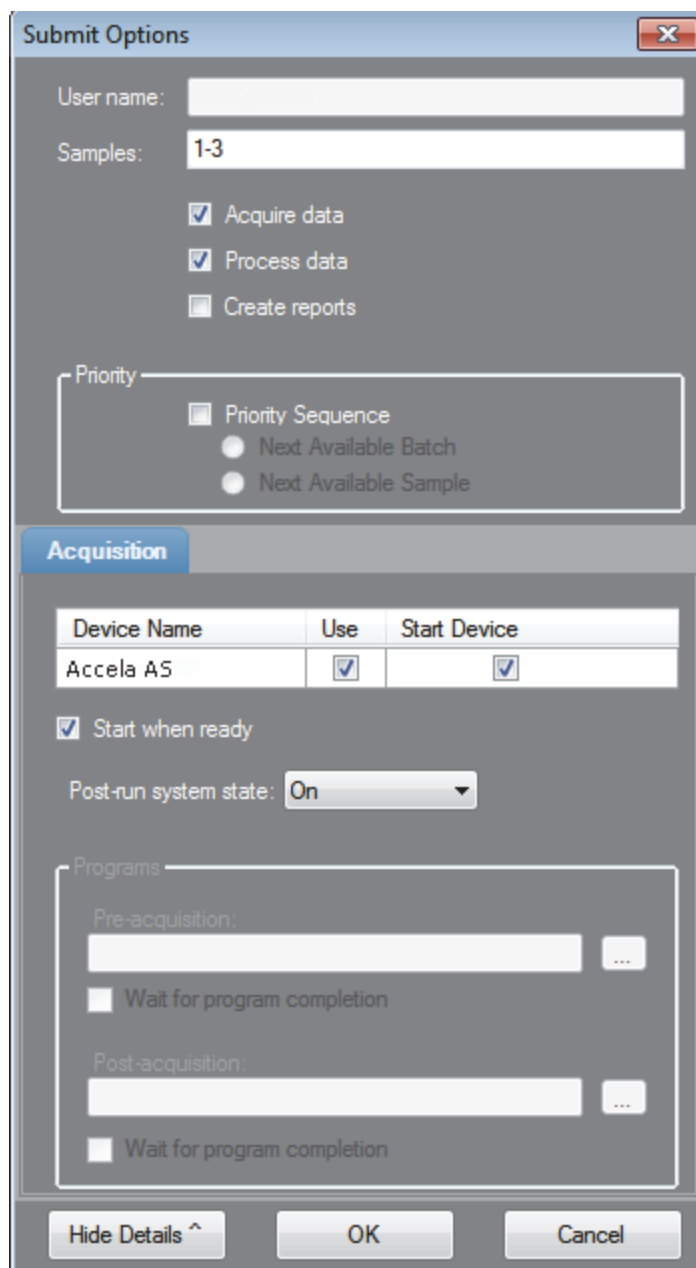
Parameter	Description
User Name	Name of the current user.
Samples	Range of samples to be submitted for acquisition, processing, or reporting.
Acquire Data	(Default) Submits the current batch to acquisition.
Process Data	(Default) Processes the data for the current batch.
Create Reports	Creates reports for the current batch.

Parameter	Description
Priority Sequence	With multiplexing enabled, places the batch immediately after the currently acquiring batch.
	Without multiplexing enabled, specifies one of the following priority options to place the batch in the queue:
	Next Available Batch: Places the batch immediately after the currently acquiring batch.
	Next Available Sample: Places the batch immediately after the currently acquiring sample.
	Note When you select Full Sequence Submission in the Configuration mode, 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 you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the TraceFinder application. You cannot configure an instrument while the TraceFinder application is running.
Use	Specifies the instruments used for this acquisition.
Start Device	Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler.
Start When Ready	Starts the specified device when all the instruments are ready to acquire data. When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
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**

- The TraceFinder application writes saved batches to the subproject folder with the file extension .tbr (to be run):

  …\TraceFinder\2.1\EFS\Projects*projectname**subprojectname*

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

  …*projectname**subprojectname**batchname*\Data

- The application saves method information to the batch Methods folder:

  …*projectname**subprojectname**batchname*\Methods*methodname*

- The application writes the reports to the batch Reports folder:

  …*projectname**subprojectname**batchname*\Reports

Figure 72. Finish view
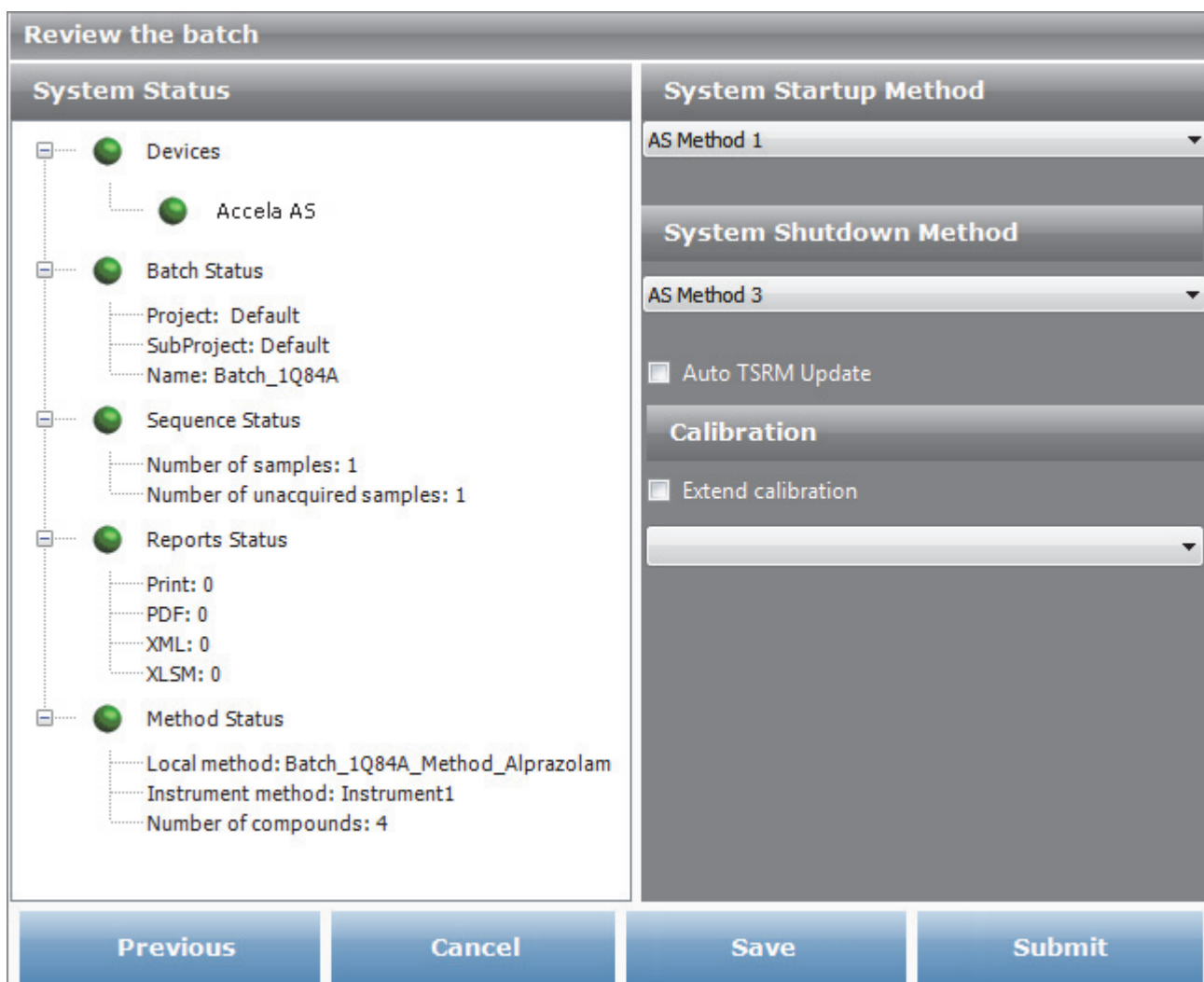
Table 58. Finish view parameters

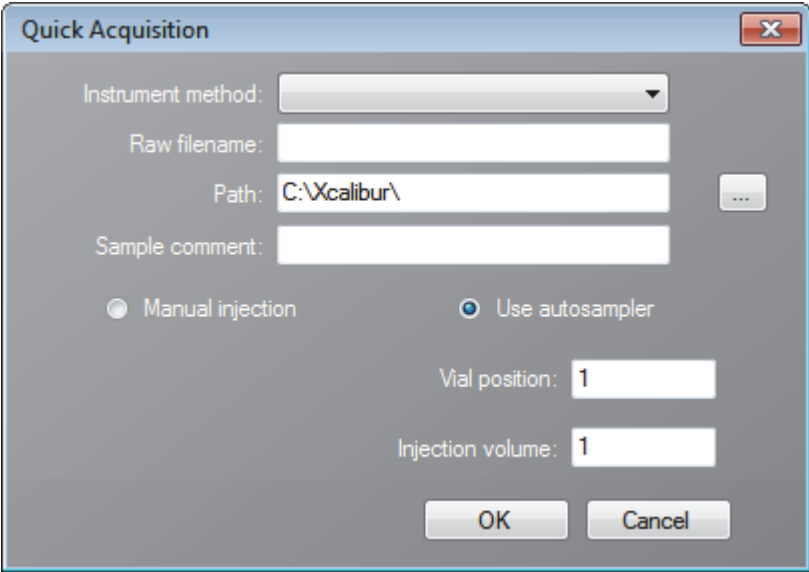| Parameter	Description
System Status	The System Status pane displays the following: • Devices used for the acquisition • Project, subproject, and name of the batch • Number of samples in the batch • Number of standard and custom reports to be printed and saved as PDF, XML, or XLSM files • Local method and instrument method used for the batch • Number of compounds in the method
System Startup Method	The instrument method that runs before the batch. No autosampler injection takes place. This feature is not available for all instruments.
System Shutdown Method	The instrument method that runs after the batch. No autosampler injection takes place. This feature is not available for all instruments.
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 to-be-run (.tbr) file.
Submit	Opens the Submit Options dialog box where you can optionally choose to generate reports.

Using Quick Acquisition
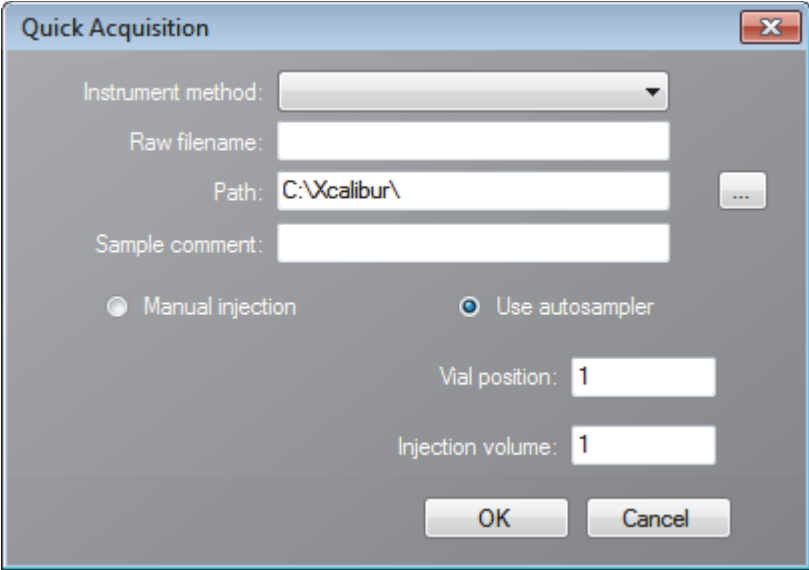
The quick acquisition feature lets you quickly submit a single sample from any view of the Acquisition mode.

> **Note** The quick acquisition feature is available only when you enable it in the Configuration mode. See "Enabling Optional Features" on page 88.

❖ **To run a quick acquisition**

1. Choose **Go > Quick Acquire Sample** from the main menu.

   The Quick Acquisition dialog box opens.

2. Select an instrument method.

3. Type a name for the raw data file that you acquire.

4. Click the browse button and locate 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:

   a. Select the **Manual Injection** option.

   b. Click **OK**.

   The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 280.
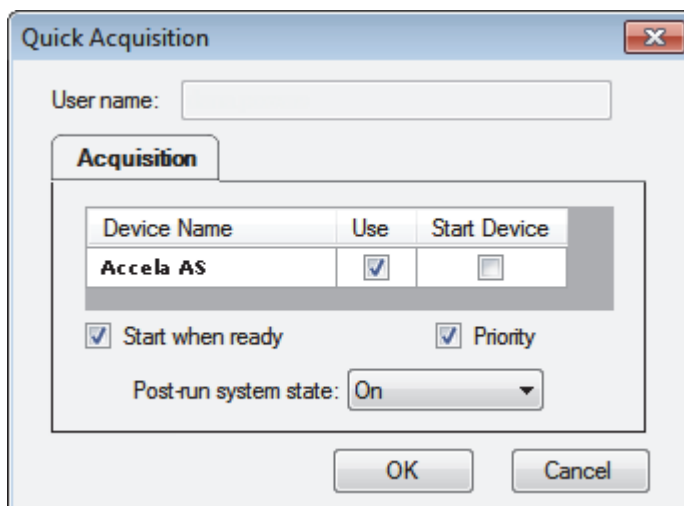
To perform autosampler injection, do the following:

a. Select the **Use Autosampler** option.

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

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

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

d. Click **OK**.

The Quick Acquisition dialog box opens.

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

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

This is usually the autosampler.

g. (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.

h. (Optional) Select the **Priority** check box to place the sample immediately after any currently acquiring sample.

i. (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.

j. Click **OK**.

The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 280.

Real-Time Display

You can access the real-time display from the dashboard and from any mode in the TraceFinder application.

❖ **To access the real-time display from the dashboard**

Click **Real Time Status**.
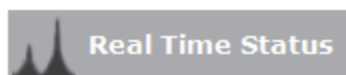
The real-time status displays at the bottom of the dashboard.

❖ **To access the real-time display from all modes**

Click **Real Time Status**.

The real-time status displays at the bottom of the current view.

Figure 73. Real Time Status display
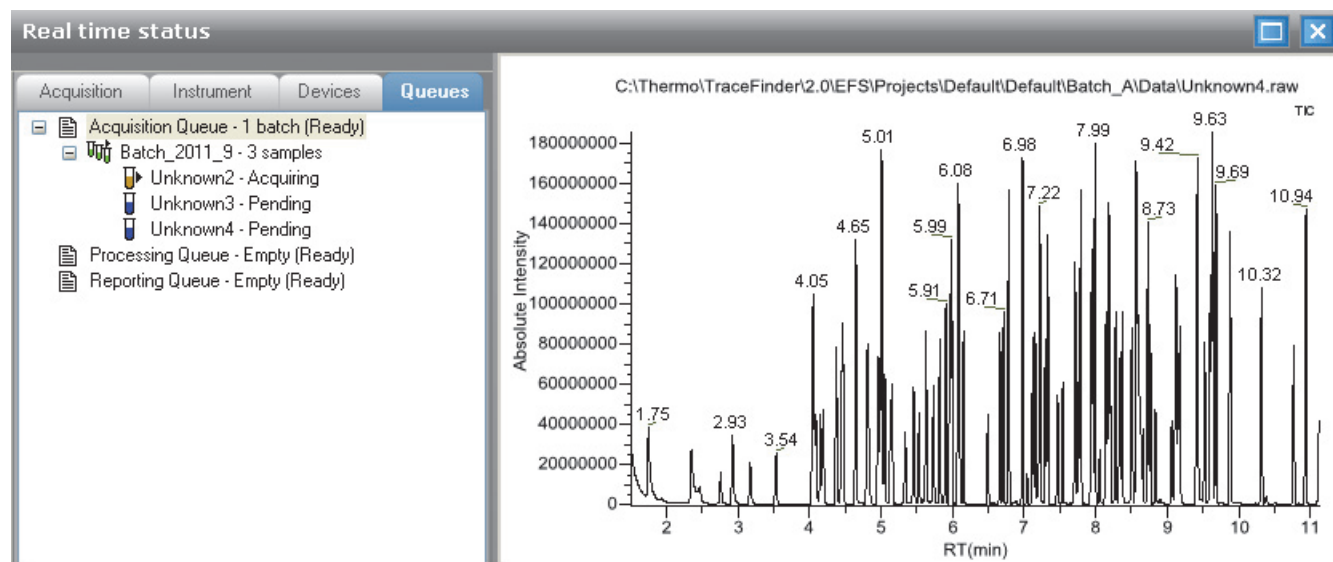
The real-time status display has four pages of information and a real-time trace pane:

- Acquisition Page

- Instrument Page

- Devices Page

- Queues Page

- Real-Time Trace Display

Acquisition Page

Use the Acquisition page to monitor the progress as the application acquires the samples.
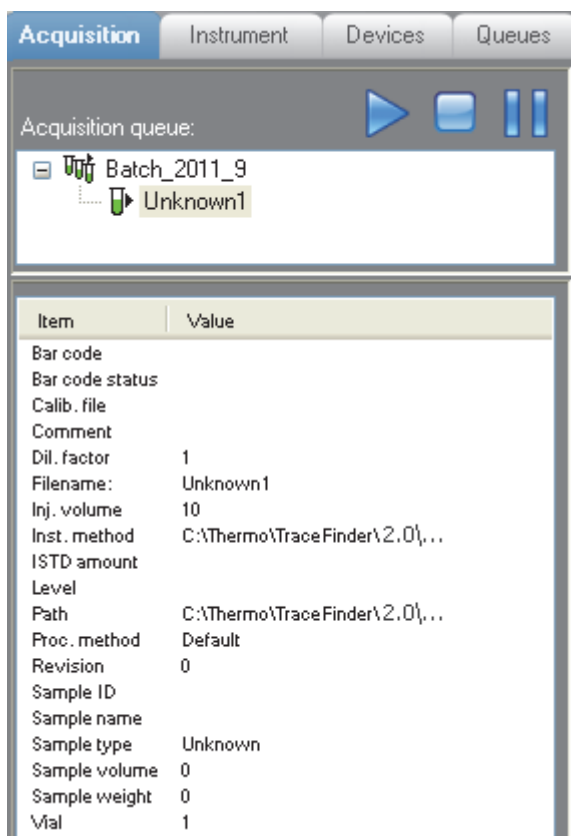
❖ **To pause or stop the batches in the queue**

Use the **Start**, ▷, **Stop**, ▢, or **Pause**, ‖, icons to control batches in the Acquisition queue.

Instrument Page

Use the Instrument page to monitor the currently acquiring sample.

Devices Page

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

Accela Autosampler Feedback

Aria Multiplexing Feedback

Follow these procedures:

- To pause the autosampler

- To control the channels

- To view the pressure trace

- To control the channels

❖ **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.
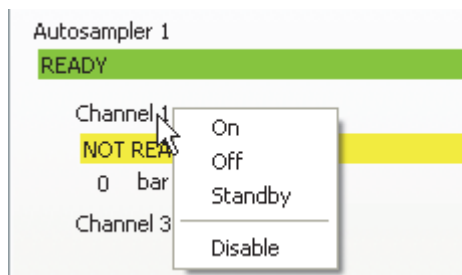
Table 59. Autosampler shortcut menu commands

Command	Description
On	Turns on a stopped pump and continues acquiring the sample list assigned to that channel.
Off	After the current sample completes, the application stops acquiring and the pump shuts down.
Standby	After the current sample completes, the application stops acquiring. The pump continues to run.
Disable / Enable	**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.
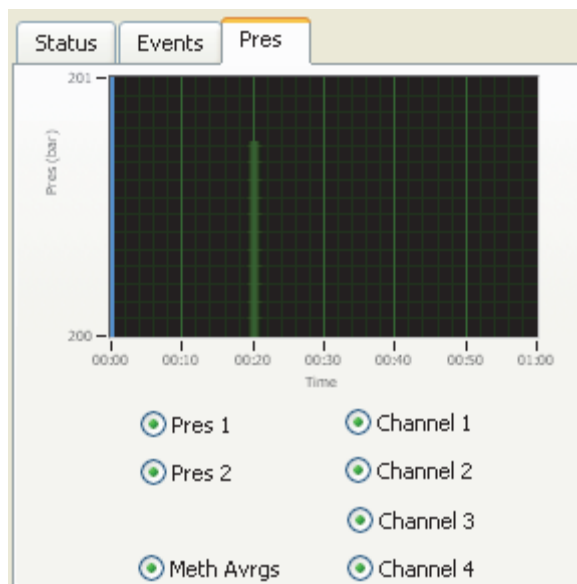
2. To view the pressure for a specific pump, select the **Pres 1** or **Pres 2** option.

   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.*

Queues Page

Use the Queues page to monitor and control the Acquisition, Processing, and Reporting queues:

- Use the Queue-Level Commands to pause or remove batches in any of the queues.

- Use the Batch-Level Commands to pause or remove entire batches or samples within batches from any of the queues.
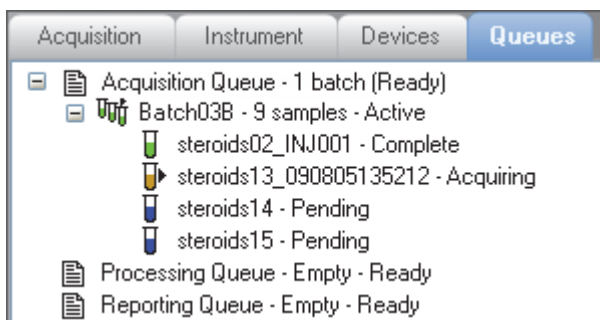
Queue-Level Commands

Use the queue-level commands to pause or remove batches in any of the queues on the Queues page. See "Queue-level shortcut menu" on page 287.

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 enabled, 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.
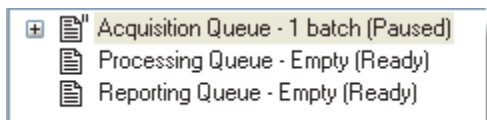
3. To restart a paused queue, select the queue, right-click, and choose **Resume Queue** from the shortcut menu.

❖ **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.

Figure 74. Queue-level shortcut menu
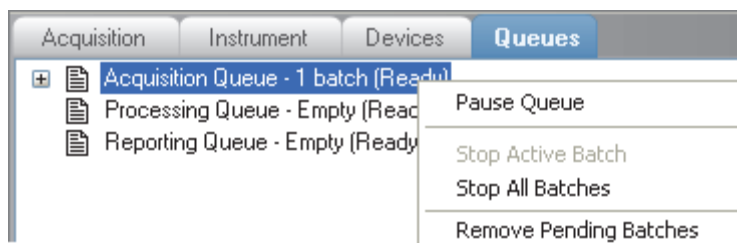
Table 60. Queue-level shortcut menu commands (Sheet 1 of 2)

Command	Description
Pause Queue	After the current sample completes, the application pauses the specified queue. Only the selected queue is affected.
Stop Active Batch	Removes all pending samples from the specified queue. The active sample is not affected.

Table 60. Queue-level shortcut menu commands (Sheet 2 of 2)

Command	Description
Stop All Batches	Removes all pending samples and batches from the specified queue. The active sample is not affected.
Remove Pending Batches	Removes all pending batches from the specified queue. The active batch is not affected.

Batch-Level Commands

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

Follow these procedures:

- To stop a batch
- To remove a pending batch
- To remove pending samples from a batch
- To remove a single pending sample from a batch

❖ **To stop a batch**

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

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

2. Right-click and choose **Stop Batch** from the shortcut menu.

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

❖ **To remove a pending batch**

1. Select a pending batch in any of the queues (Acquisition, Processing, or Reporting).

   Note A pending batch is a batch in which all samples are pending. If any sample in the batch is active, this command is not available.

2. Right-click and choose **Remove Pending Batch** from the shortcut menu.

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

❖ **To remove pending samples from a batch**

1. Select a batch in any of the queues (Acquisition, Processing, or Reporting).

   The batch must have at least one pending sample.

2. Right-click and choose **Remove Pending Samples** from the shortcut menu.

   The application confirms that you want to remove all pending samples from the batch and then removes the samples. If the batch includes only pending samples, the application removes the batch from the queue.

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

1. Select a pending sample.

2. Right-click and choose **Remove Sample** from the shortcut menu.
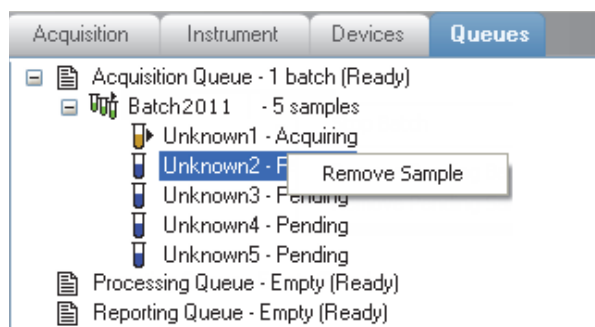
   The application confirms that you want to remove the selected sample from the batch and then removes the sample.

Figure 75. Batch-level shortcut menu
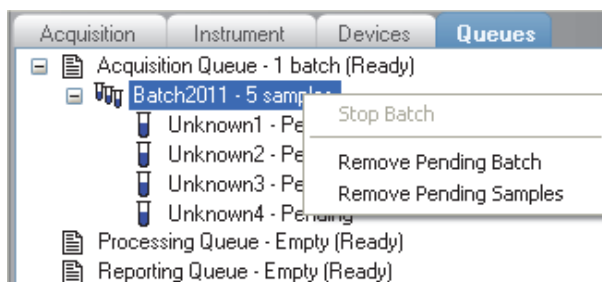
Table 61. Batch-level shortcut menu commands

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.

Real-Time Trace Display

As each sample acquires, the real-time chromatogram pane shows the retention time and intensity of the TIC trace.
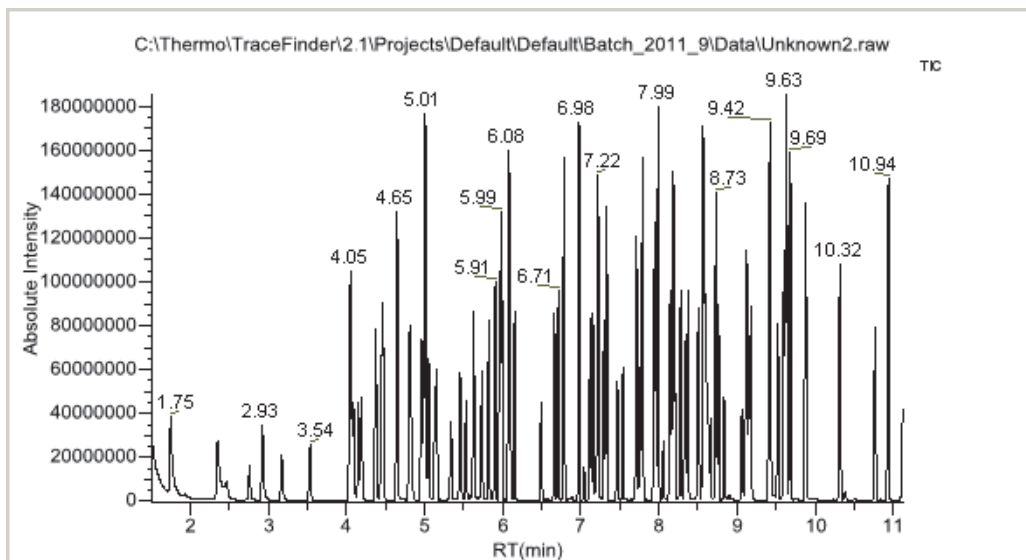
By default, the real-time display shows only the TIC trace as each sample acquires. To observe specific traces, such as the internal standard, use the RTV Display Traces function to display multiple traces.

When you create your method, you can specify additional traces to display in the real-time viewer and in which order the traces are displayed. The application always displays the TIC trace in the top pane. See "Real Time Viewer" on page 179.

❖ **To display multiple traces**

Right-click the chromatogram pane and choose the number of traces you want to display.
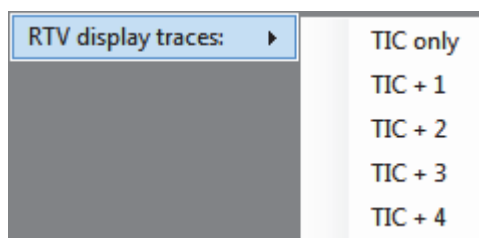
The chromatogram pane displays real-time chromatograms for the selected number of traces.

The TIC is always displayed at the top. When there are more traces than can fit in the pane, you can scroll through the traces.

For each trace, the application displays the mass or precursor mass.

Figure 76. Real-time display with multiple traces
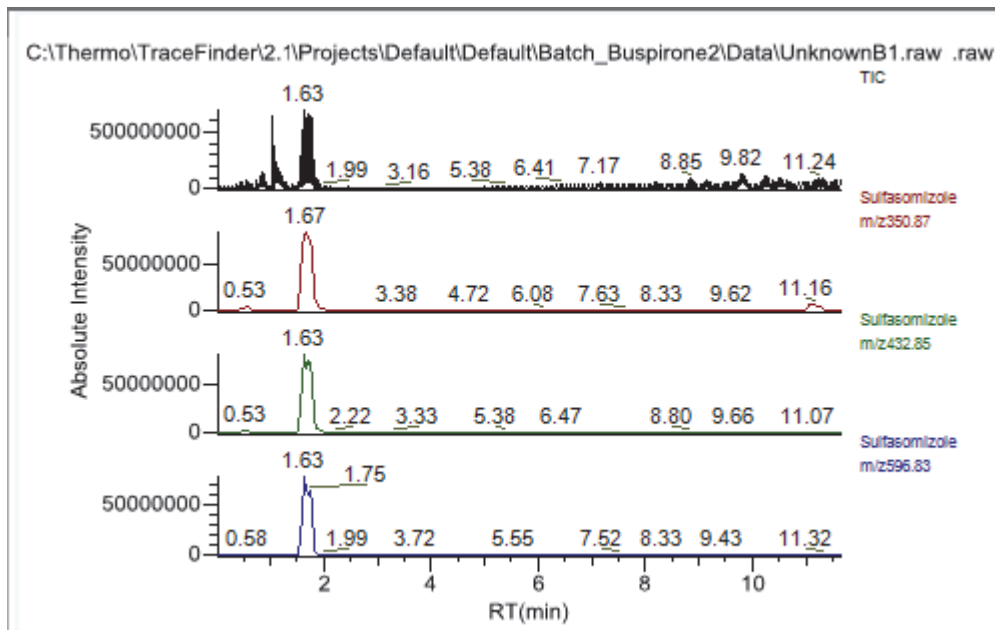
Sample Types

The TraceFinder application uses the following sample types in all sample definitions and reports. To view example standard reports specific to a sample type, see Appendix A, "Reports."

Table 62. Sample type definitions

Sample type	Definition
Matrix Blank	Contains no target compounds but might contain an ISTD when you use the internal standard quantitative analysis technique. By analyzing a blank sample, you can confirm that there are no residual compounds in the solvent system that can cause erroneous results.
Cal Std	(Calibration standard) Contains known amounts of all target compounds. The purpose of a standard is to measure the response of the instrument to the target compounds so that the processing software can generate a calibration curve for each compound.
Chk Std	(Check standard) Contains a known amount of one or more specific target compounds. The application places check standard samples in the sequence so that it can test quantitative analysis results for quality assurance purposes. After the application analyzes the Chk Std sample, it compares the measured quantity with the expected value and an acceptability range. The quantitative analysis of a Chk Std sample is classified as *passed* if the difference between the observed and expected quantities is within the user-defined tolerance. A Chk Std sample is classified as *failed* if the difference between the observed and expected quantities is outside the user-defined tolerance.
Solvent	Contains only solvent.
Unknown	Used for quantitative analysis of samples.
Unknown/TIC	Used for quantitative and qualitative analysis of samples.
LCS	Lab control sample.
LCSD	Lab control sample duplicate.
MDL	Method detection limits sample.
Method Val	Method validation sample.
MS	Matrix spike sample.
MSD	Matrix spike duplicate sample.
Tune	Verifies the tune of the system according to EPA guidelines.
Tune/Breakdown	Verifies the tune of the system according to EPA guidelines, allowing for the degradation of compounds.
Breakdown	Checks the degradation of compounds.

Using the Analysis Mode

This chapter includes instructions for 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 View
- 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** from the dashboard or the navigation pane.

The Analysis navigation pane opens.
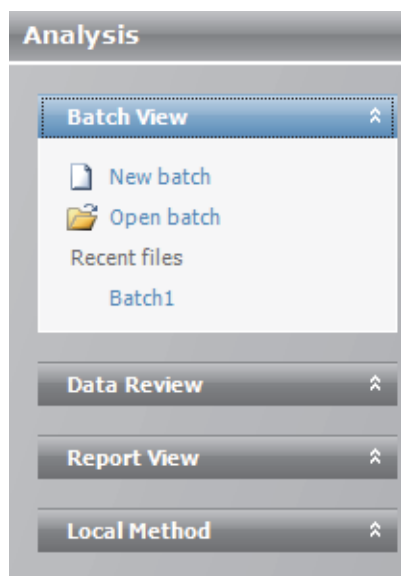
Using Quick Acquisition

With the quick acquisition feature, you can quickly submit a single sample from any view of the Analysis mode.

> **Note** The quick acquisition feature is available only when you enable it in the Configuration mode. See "Enabling Optional Features" on page 88.

❖ **To run a quick acquisition**

1. Choose **Go > Quick Acquire Sample** from the main menu.

   The Quick Acquisition dialog box opens.

2. Select an instrument method.

3. Type a name for the raw data file that you acquire.

4. Click the browse button and locate a folder where you want to save the acquired raw data file.

5. Select either the manual injection or the autosampler option:

   To perform manual injection, do the following:

   a. Select the **Manual Injection** option.

   b. Click **OK**.

      The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 280.

To perform autosampler injection, do the following:

a. Select the **Use Autosampler** option.

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

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

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

d. Click **OK**.

The Quick Acquisition dialog box opens.

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

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

This is usually the autosampler.

g. (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.

h. (Optional) Select the **Priority** check box to place the sample immediately after any currently acquiring sample.

i. (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.

j. Click **OK**.

The application submits the sample to the Acquisition queue. See "Acquisition Page" on page 280.

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.

❖ **To open the Batch View**

1. Do one of the following:

   From the dashboard, click **Analysis**.

   –or–

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

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

The Batch View opens for the currently selected batch.

This section contains information about the following topics:

- Batch View Panes

- Creating a New Batch

- Editing a Batch

- Editing Report Output Formats

- Submitting a Batch

Batch View Panes

The Batch View is divided into three panes:

- Sample List

  Use the sample list pane to create a batch. See "Creating a New Batch" on page 309.

- Automated Batch Reports

  Use the Automated Batch Reports pane to select the type of output formats that you want to generate for the reports. See "Editing Report Output Formats" on page 320.

- Compound Active Status

  Use the Compound Active Status pane to make specific compounds active or inactive. See "Setting Compound Active Status" on page 322.

Use the Batch View toolbar or shortcut menu to create the sample list and submit samples for acquisition. See "Batch View Toolbar" on page 304 or "Batch View Shortcut Menu" on page 307.

Sample list

Automated Batch Reports pane

Compound Active Status pane

> **Tip** To resize the panes, drag the separators that divide the panes.

Sample List

The sample list includes the following features:

- Column Display

- Status Indicators

- Sample Weight Calculation

Column Display

The sample list can contain many columns of information. You can scroll to see all the columns of information, and you can customize which columns to display and their display order.

Follow these procedures:

- To scroll the sample list

- To customize the column display

❖ **To scroll the sample list**

Use the horizontal scroll bar at the bottom of the sample list to view all the information.

When you use the scroll bar at the bottom of the sample list, the Status, Filename, Sample Type, and Level 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.

   All the columns you select are displayed after the Status, Filename, Sample Type, and 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, 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 77. Modify Columns dialog box
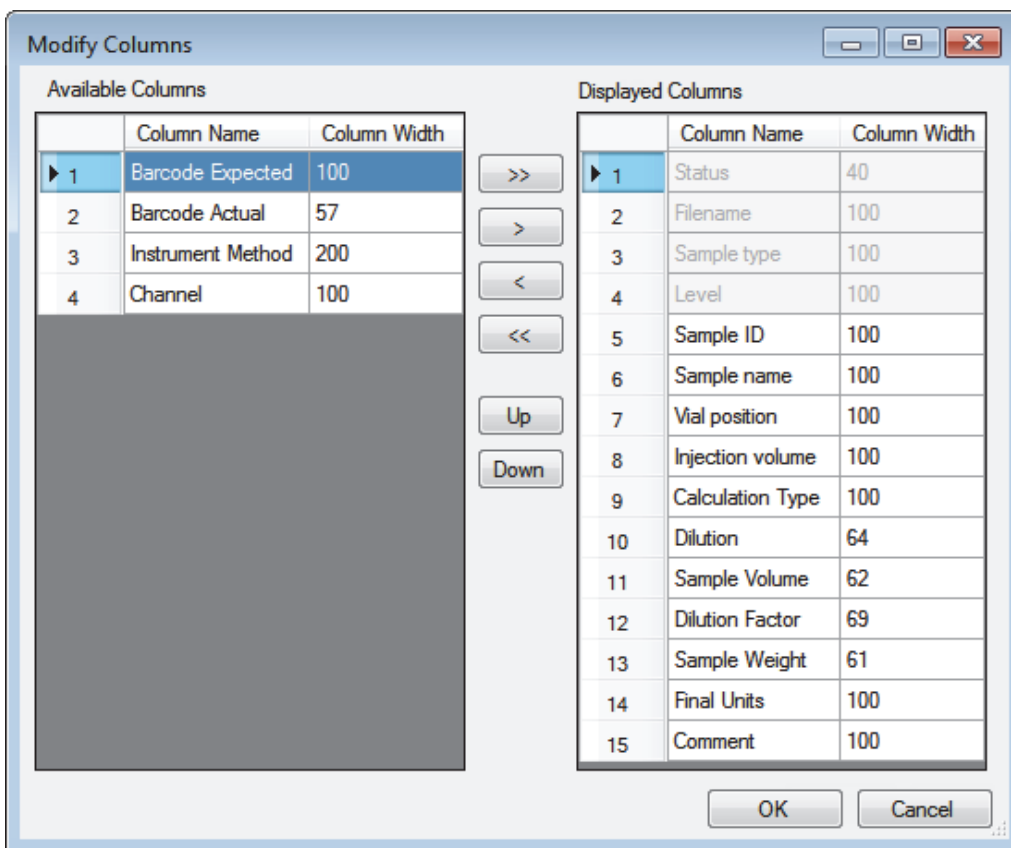
Table 63. Modify Columns function buttons (Sheet 1 of 2)

Function	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.

Table 63. Modify Columns function buttons (Sheet 2 of 2)

Function	Description
∨	Moves the selected column to the Available Columns pane. You cannot move the Status, Filename, Sample Type, or Level column.
∨∨	Moves all columns except Status, Filename, Sample Type, and 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 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, Sample Type, or Level column.

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

Sample Weight Calculation

Use the features for calculating sample weight 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 Weight, Sample Volume, Calculation Type, Dilution Factor, and Final Units columns are not visible, right-click and choose **Enable Sample Weight Calculation** from the shortcut menu.

Sample Weight	Sample Volume	Calculation Type	Dilution Factor	Final Units
1	1	Liquid ▼	1	
1	1	Solid ▼	1	
1	1	Manual ▼	1	

❖ **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.

Batch View Toolbar

The Batch View includes this toolbar for creating and submitting a batch.

Icon	Description
1 I+	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 310.
1 I↓	Inserts a new, empty sample or samples above the selected sample. See the instructions "To insert samples into the list" on page 311.
I−	Removes the selected samples from the sample list. See the instructions "To remove samples from the list" on page 312.
I↳	Adds imported samples from a .csv, .xml, or .sld file to the sample list. See the instructions "To import samples into the list" on page 311.
⊣I▸	Submits only the selected samples for acquisition, processing, or report generation. See the instructions "To submit selected samples" on page 326.
⊞▸	Submits the batch for acquisition, processing, or report generation. See the instructions "To submit all samples in the batch" on page 325.
◀	Closes/Opens the Analysis navigation pane.
⊣I1	Opens the Quick Acquisition dialog box where you can quickly submit a single sample. See "Using Quick Acquisition" on page 295.

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 78. Batch View sample list

Cells in the sample list that are not editable, such as Barcode Actual, are shaded and empty.

Table 64. 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.
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:
	Matrix Blank, Solvent, Cal Std, Chk Std, Unknown, Unknown/TIC, LCS, LCSD, MDL, MS, MSD, Method Val, Tune, Tune/Breakdown, or Breakdown
	Default: Unknown
Level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined, alphanumeric string that identifies a sample.

Table 64. Batch View sample list columns (Sheet 2 of 2)

Column	Description
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
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.
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 enabled multiplexing in the Configuration mode. See "Multiplexing" on page 92.
Barcode Expected	
Barcode Actual	
Comment	A user-defined comment for the sample.

Batch View Shortcut Menu

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

Table 65. 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 311.
Browse In Raw File	Opens a dialog box where you can select a raw data file to use for the selected sample row.
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 350.
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.
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
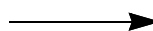
Paste into Excel spreadsheet |

Table 65. Batch View shortcut menu commands (Sheet 2 of 2)

Command	Description
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.

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. Click **New Batch** in the Batch View task pane or choose **File > New > Batch**.

   The Create a New Batch dialog box opens.
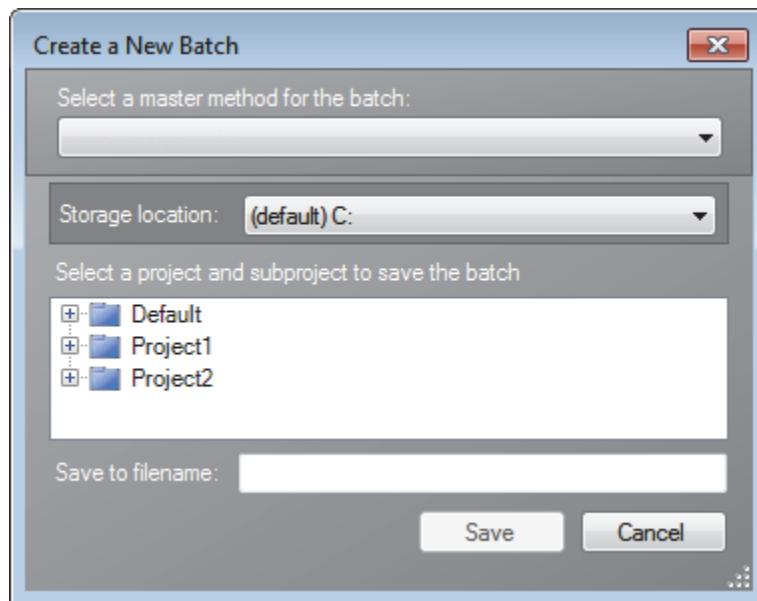
2. Select a master method from the Method list.
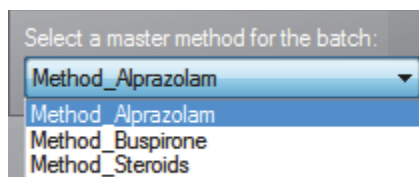
3. Select a drive from the Storage Location list.
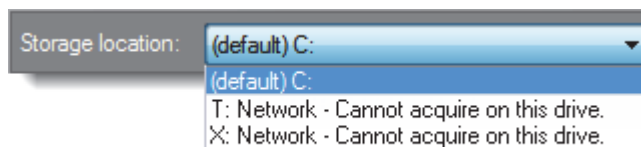
The project list displays all projects, subprojects, and batches on the selected drive.

> **Tip** The application does not display drives that do not have a project and subproject.

You cannot use network drives to acquire data. For more information about network drives, see "Working with Drives" on page 50.

4. Select a project and a subproject and type a name for your new batch.

> **Tip** To enable the Save button, you must select a subproject and enter a unique batch name. If the Save button is not enabled, either you have entered a name that is already used or you have not selected a subproject.

5. Click **Save**.

A new, unnamed batch opens with one Unknown sample.
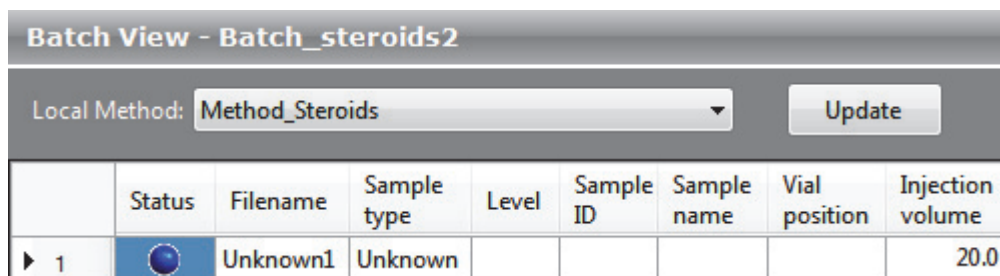
❖ **To add samples to the list**

1. To add a single sample row, right-click the sample list and choose **Add Sample** from the shortcut menu.

2. To add multiple sample rows, select the number of rows and then click the **Add Sample** icon, ☐ .

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

❖ **To insert samples into the list**

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

- To insert a single sample row, right-click and choose **Insert Sample** from the shortcut menu.

- To insert multiple sample rows, select the number of rows and then click the **Insert Sample** icon 1 [⬆⬇] [🔽] .

The application inserts the Unknown samples above the selected sample.

	Status	Filename	Sample type	Level	Sample ID
1	🟡	cal_std_5	Cal Std	5	cal std = 5 ng/uL
2	🔵	Unknown2	Unknown		
3	🔵	Unknown1	Unknown		
4	🟡	cal_std_10	Cal Std	10	cal std = 10 ng/uL

Inserted samples → (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.
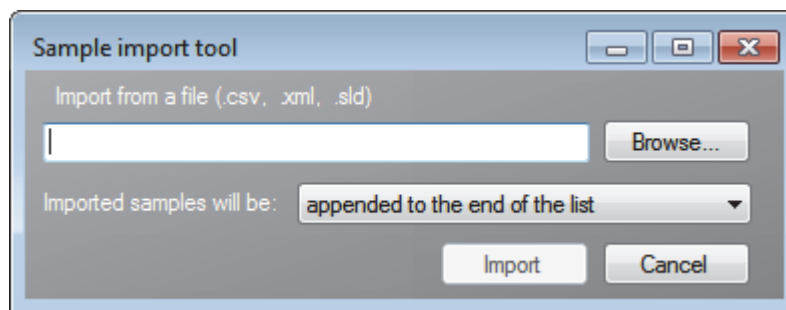
   From this dialog box, you can import samples from a .csv, .xml, or .sld file.

2. Click **Browse** and select a .csv, .xml, or .sld file that contains the samples 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	Matrix Blank
QC	Chk Std
Std Bracket	Cal Std

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

Imported samples default to Auto.

> **Note** The Channel column is available only when you have enabled multiplexing in the Configuration mode. See "Multiplexing" on page 92.

❖ **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		
Matrix Blank	Solvent	Unknown/TIC
Cal Std	Chk Std	Unknown
LCS	MDL	MS
LCSD	Method Val	MSD
Tune	Tune/Breakdown	Breakdown

3. For each Cal Std or Chk Std sample, select a level from the Level list.

   The sample levels are defined in the master method. If there is nothing 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_Steroids ▼	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, Sample Type, and Level columns stay fixed while the other columns scroll right and left.

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

❖ **To 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 inserts any additional browsed in files above the selected sample.

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

   > **Note** You cannot overwrite an acquired sample. When you select a sample that is acquired, the application inserts all browsed in files above 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.
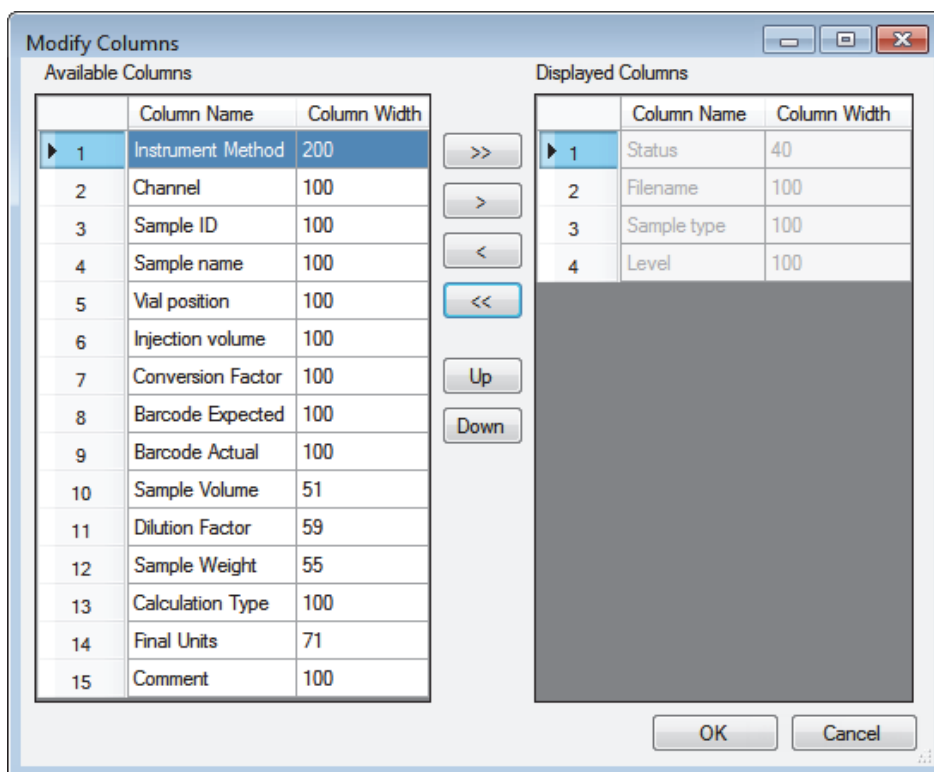
Table 66. Modify Columns dialog box function buttons

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, Sample Type, or Level 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.

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 to-be-run (.tbr) 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 submit all samples in the batch
- To submit selected samples

❖ **To open a saved batch**

1. From the Batch View task pane, click **Open Batch.**

   The Open Batch dialog box opens.
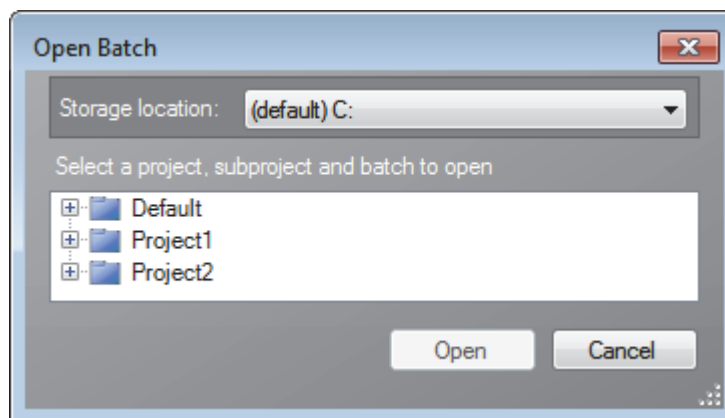
2. Select a drive from the Storage Location list.
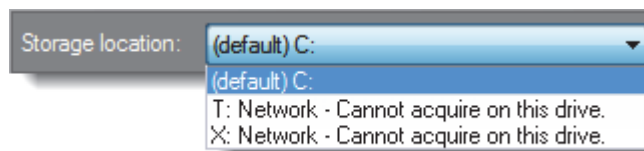
   The project list displays all projects, subprojects, and batches on the selected drive.

3. Select a project, subproject, and batch.

4. Click **Open**.

   The selected batch opens in the Batch View.

❖ **To open a recent batch**

Click a batch name in the Recent Files list.

The selected batch opens in the Batch View.

> **Tip** To view the drive, project, and subproject for a recent batch, hold your cursor over the batch name.
>
>
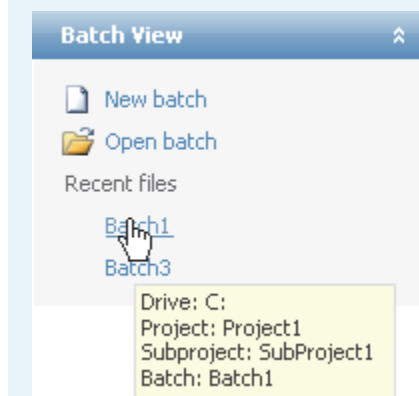
❖ **To edit samples in a batch**

Use the commands described in "Working in the Batch View" on page 297.

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

❖ **To reinject a sample from a previously acquired batch**

1. In the sample list, select the sample 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).

   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 .tbr batch. You can open this batch from the Ready to Acquire page in the Acquisition mode and submit the batch. The application acquires all submitted samples—both the reinjection samples and the previously acquired samples. The application appends a timestamp to the acquired raw data files to differentiate each acquisition.
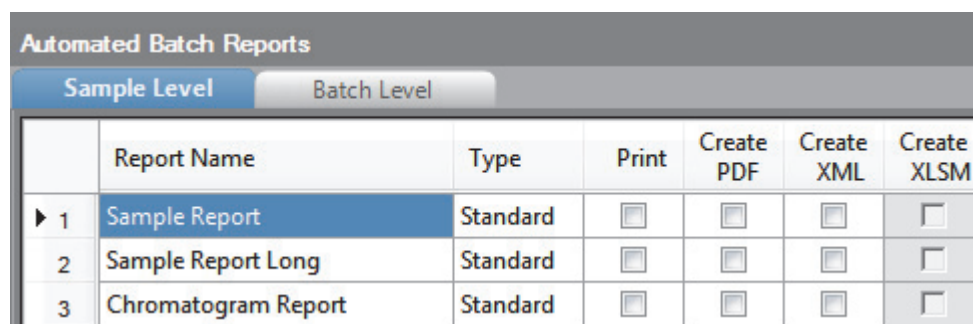
Editing Report Output Formats

In the Automated Batch Reports pane, you can view the reports that are selected for this batch and modify which output formats are generated for each report.

❖ **To edit the sample-level output formats**

1. Click the **Sample Level** tab.

   The application displays reports and the output formats as they were specified in the method.

	Report Name	Type	Print	Create PDF	Create XML	Create XLSM
▶ 1	Sample Report	Standard	☐	☐	☐	☐
2	Sample Report Long	Standard	☐	☐	☐	☐
3	Chromatogram Report	Standard	☐	☐	☐	☐

   For detailed instructions for specifying which reports and output formats are generated, see "Specifying the Reports Configuration" on page 68.

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						
Sample Level			**Batch Level**			
	Report Name	Type	Print	Create PDF	Create XML	Create XLSM
▶ 1	Batch Summary Report	Standard	☐	☐	☐	☐
2	Calibration Curve Report	Standard	☐	☐	☐	☐

   For detailed instructions for specifying which reports and output formats are generated and which reports are batch-level, see "Specifying the Reports Configuration" on page 68.

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.

Setting Compound Active Status

In the Compound Active Status pane, you can choose specific compounds to be active or inactive.

❖ **To set a compound as active or inactive**

1. In the sample list, select a sample.

   All compounds in the selected sample are listed in the Compound Active Status pane. The default active/inactive status is determined by the identification settings in the local method. For information about setting the identification parameters, see "Identification" on page 133.

   • 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.

Compound Active Status			
	RT	Compound	Active
1	3.67	1,3-Dioxolane, 2-heptyl-	☐
2	3.14	Propanenitrile	☑
3	3.15	Pyrazinamide	☑
▶ 4	4.70	Pyrazinamide *2*	☑

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

   When you specify a compound as inactive in this pane, it becomes inactive in the Compounds pane in the Data Review view. Inactive compounds are grayed out:

Compounds
Propanenitrile
Pyrazinamide
Pyrazinamide *2*
1,3-Dioxolane, 2-heptyl-

For instructions for changing the active/inactive status in the Data Review view, see "Inactive and Excluded Compounds" on page 354.

Compound Active/Inactive Status

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

Figure 79. Active and inactive compounds in the Local Method View

For details about setting the status on the Identification page, see "Identification" on page 133.

Figure 80. Active and inactive compounds in the Batch View

For details about setting the status in the Batch View, see "Setting Compound Active Status" on page 322.

Figure 81. Active and inactive compounds in the Data Review view

Inactive

For details about setting the status in the Data Review view, see "Inactive and Excluded Compounds" on page 354.

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 327.

Follow these procedures:

- To submit all samples in the batch
- To submit selected samples

For a description of commands on the shortcut menu, see "Batch View shortcut menu commands" on page 307.

❖ **To submit all samples in the batch**

1. Click the **Submit Batch** icon, ▫.

   The Submit Options dialog box opens. See "Submit Options dialog box" on page 327.

2. Select the tasks that you want to perform: acquire data, process data, or create reports.

3. (Optional) Click **Show Details** to display additional Acquisition parameters.

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

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

   This is usually the autosampler.

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

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

7. (Optional with multiplexing enabled) Select the **Priority Sequence** check box.

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

8. (Optional without multiplexing enabled) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

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

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

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

❖ **To submit selected samples**

1. Select the samples to submit.

2. Click the **Submit Selected Samples** icon, .

   The Submit Options dialog box opens. See "Submit Options dialog box."

3. Select the tasks that you want to perform: acquire data, process data, or create reports.

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

5. (Optional) Click **Show Details** to display additional Acquisition parameters.

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

   This is usually the autosampler.

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

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

8. (Optional with multiplexing enabled) Select the **Priority Sequence** check box.

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

9. (Optional without multiplexing enabled) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   • **Next Available Batch** places the batch immediately after the currently acquiring batch.

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

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

Figure 82. Submit Options dialog box
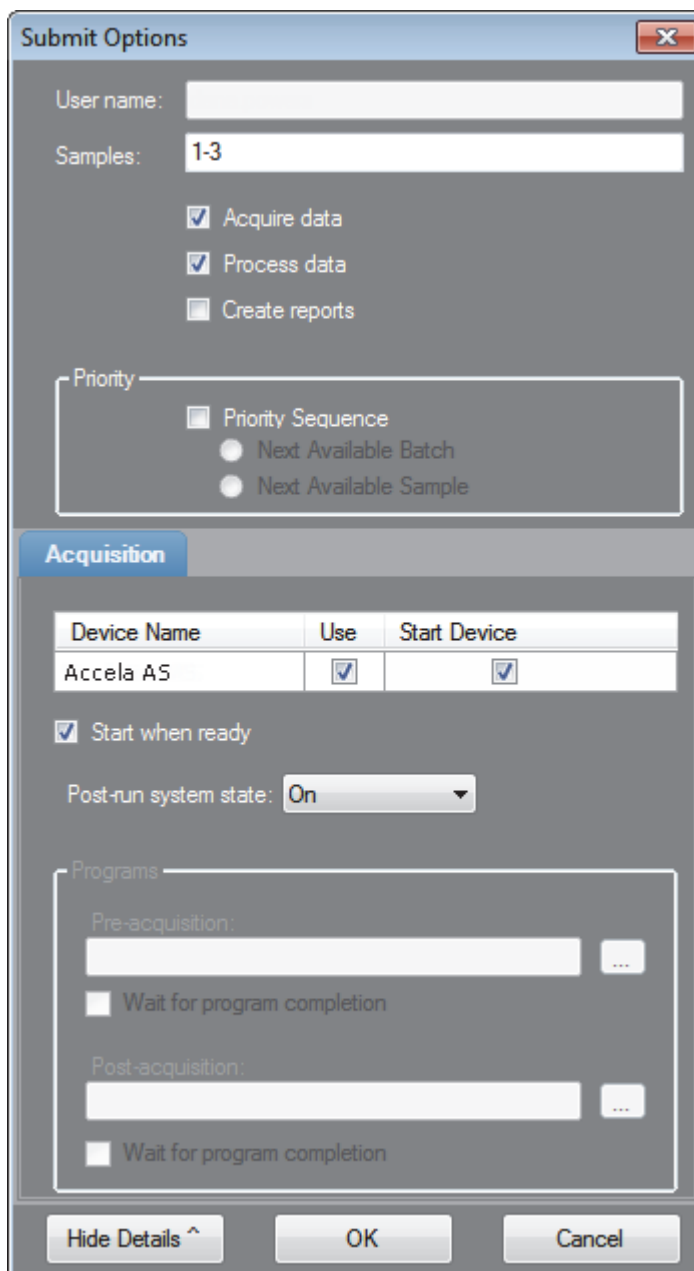
Table 67. Submit Options dialog box parameters (Sheet 1 of 2)

Parameter	Description
User Name	Name of the current user.
Samples	Range of samples to be submitted for acquisition, processing, or reporting.
Acquire Data	(Default) Submits the current batch to acquisition.
Process Data	(Default) Processes the data for the current batch.

Table 67. Submit Options dialog box parameters (Sheet 2 of 2)

Parameter	Description
Create Reports	Creates reports for the current batch.
Priority Sequence	With multiplexing enabled, places the batch immediately after the currently acquiring batch. Without multiplexing enabled, specifies one of the following priority options to place the batch in the queue: • **Next Available Batch** places the batch immediately after the currently acquiring batch. • **Next Available Sample** places the batch immediately after the currently acquiring sample.
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.
Use	Specifies the instruments used for this acquisition.
Start Device	Specifies the instrument that initiates the communication with the other instruments. This is usually the autosampler.
Start When Ready	Starts the specified device when all the instruments are ready to acquire data. When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
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 and subproject, or you can make a copy of the current batch and save the copy to a different project and subproject.

Follow these procedures:

- To save a batch to another project or subproject

- To move a batch to another project or subproject

❖ **To save a batch to another project or subproject**

1. Choose **File > Save > Save Batch As** from the main menu in the Analysis mode.
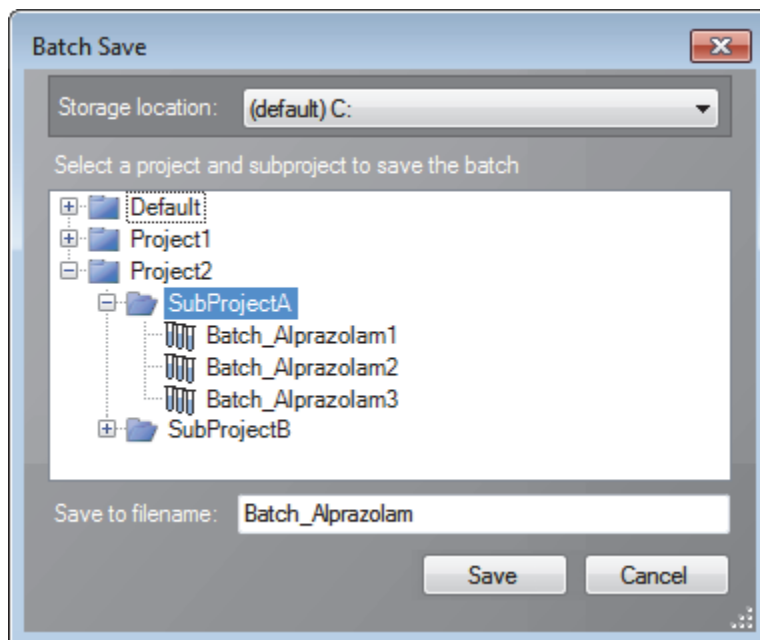
   The Batch Save dialog box opens.

2. Select a storage location.

3. Select a project.

4. Select a subproject.

5. Type a name for the new batch.

   If you are saving the batch to a different subproject, you must give it a unique name. You cannot overwrite an existing batch in the new subproject.

6. Click **Save**.

   When you save the batch to a different subproject, the reports reflect the original project/subproject and the application does not save the calibration history.

❖   **To move a batch to another project or subproject**

1. Choose **File > Save > Move Batch** from the main menu in the Analysis mode.
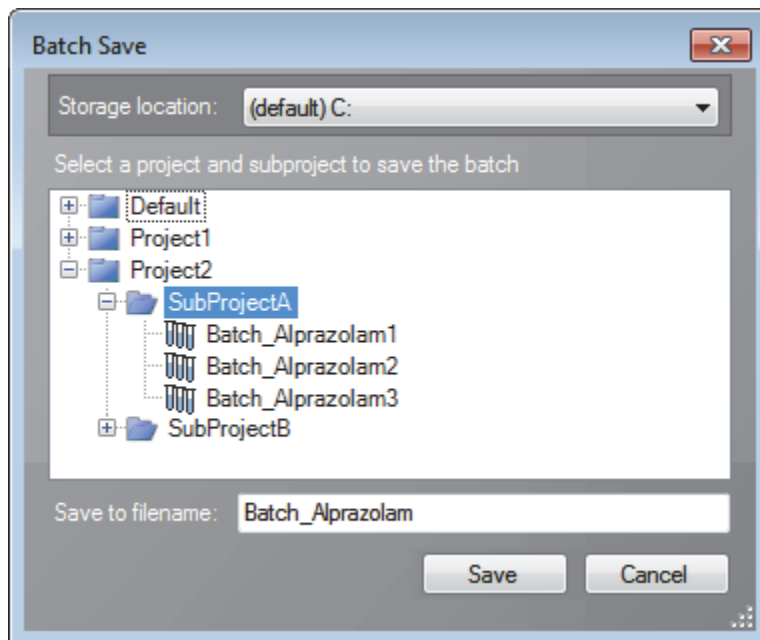
   The Batch Save dialog box opens.

2. Select a storage location.

3. Select a project.

4. Select a subproject.

5. Type a name for the new batch.

   You must give the batch a unique name in the new subproject. You cannot overwrite an existing batch.

6. Click **Save**.

   When you move the batch, the reports reflect the original project/subproject and the application does not save the calibration history.

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 101 and "Working in the Batch Template Editor" on page 415.

> **Note** This batch wizard is available only when you select the Batch Template Wizard (EnviroLab/ToxLab/QuanLab forms) style in the Configuration mode. See "Application Configuration" on page 67.

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:

```
┌─────────────────────────┐
│ Batch Template Selection │
└─────────────────────────┘
            │
            ▼
┌─────────────────────────┐
│   Batch Specification   │
└─────────────────────────┘
            │
            ▼
┌─────────────────┐       ┌──────────────────────────┐
│     Finish      │ ◄────► │ Calibration and Compound │
└─────────────────┘       │        Selection         │
                          └──────────────────────────┘
```
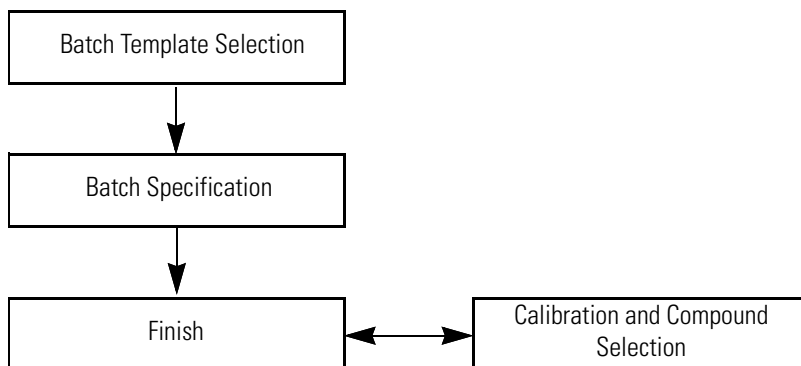
❖ **To open the Batch Wizard**

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 415.

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 333.

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.
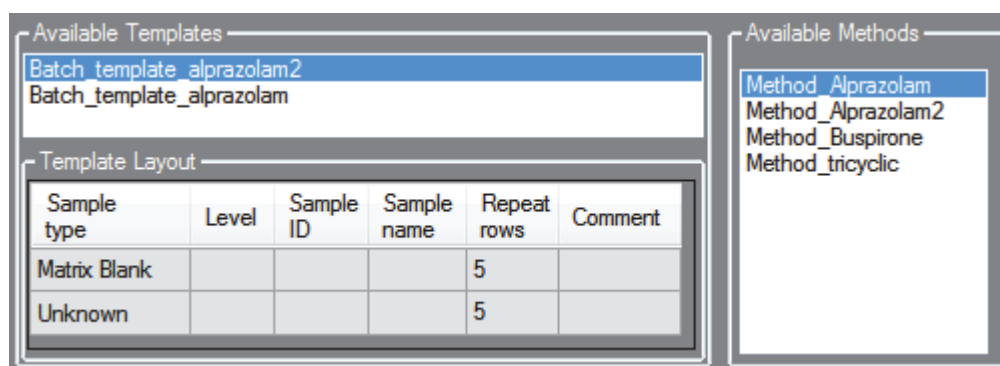
6. Select an available method.

   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 83. Batch Template Selection page
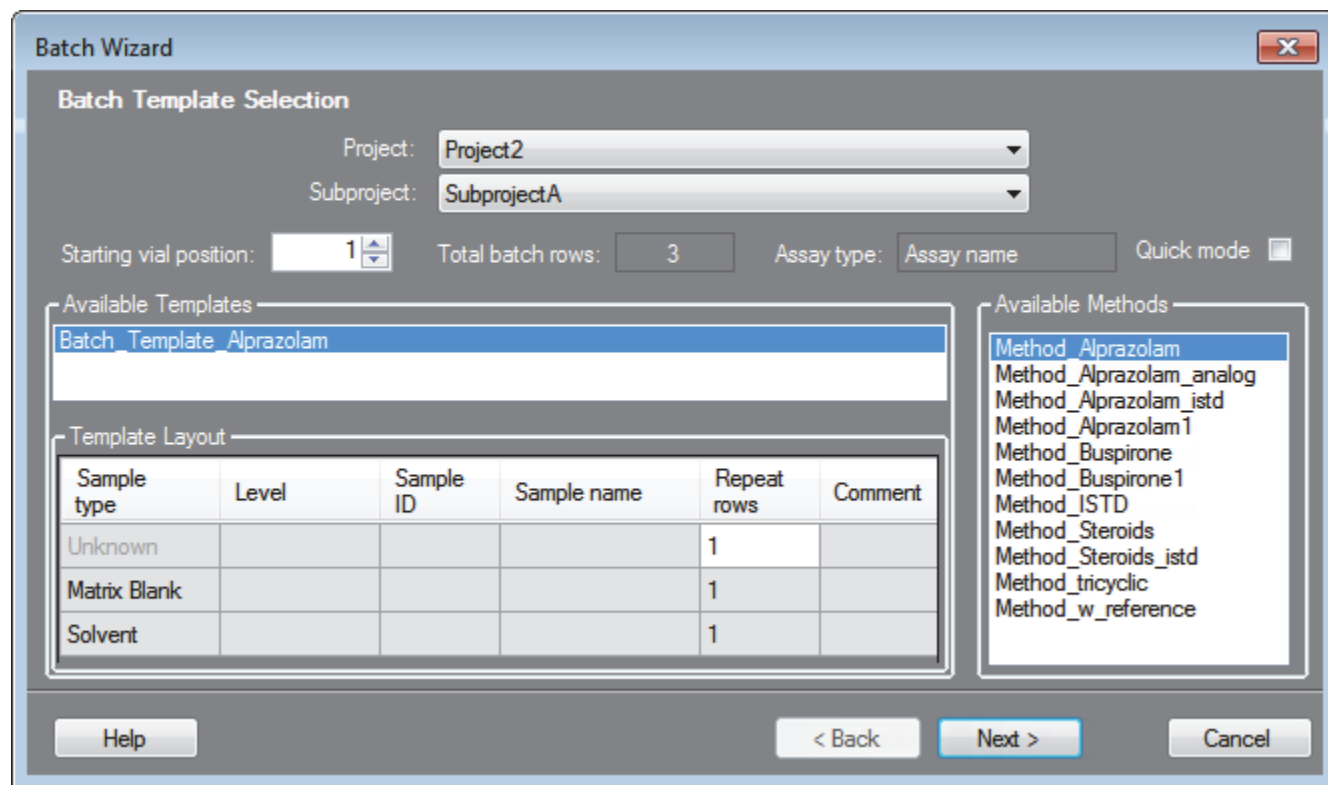
Table 68. Batch Template Selection parameters (Sheet 1 of 2)

Parameter	Description
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: …\Thermo\TraceFinder\2.1\EFS\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.
Help	Opens the "Creating a Batch Using the Batch Wizard" topic (this topic) in the application Help tool.

Table 68. Batch Template Selection parameters (Sheet 2 of 2)

Parameter	Description
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 335.
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 338.

❖ **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 add samples to the batch
- 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 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, Unknown sample to the end of the sample list.

2. In the Filename column for each sample, type a 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."

3. Select a sample type from the Sample Type list for each sample.

Available sample types		
Matrix Blank	Solvent	Unknown/TIC
Cal Std	Chk Std	Unknown
LCS	MDL	MS
LCSD	Method Val	MSD
Tune	Tune/Breakdown	Breakdown

4. For detailed descriptions of sample types, see "Sample Types" on page 292.

5. For each Cal Std or Chk Std sample, select a level from the Level list.

   The sample levels are defined in the master method. If there are no levels to select from the Level list, do the following:

   a. Cancel 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, [⊟] .

   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, Unknown 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.

Figure 84. Batch Specification page

Table 69. Batch Specification 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.
	Adds a new, Unknown sample to the end of the sample list. This function is not available in Quick Mode.
	Removes the selected sample. This function is not available in Quick Mode.
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.

Table 69. Batch Specification 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.
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, Unknown 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 B, "Using Copy Down and Fill Down."

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 325.

❖ **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 342.

❖ **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 342.

Figure 85. Finish page
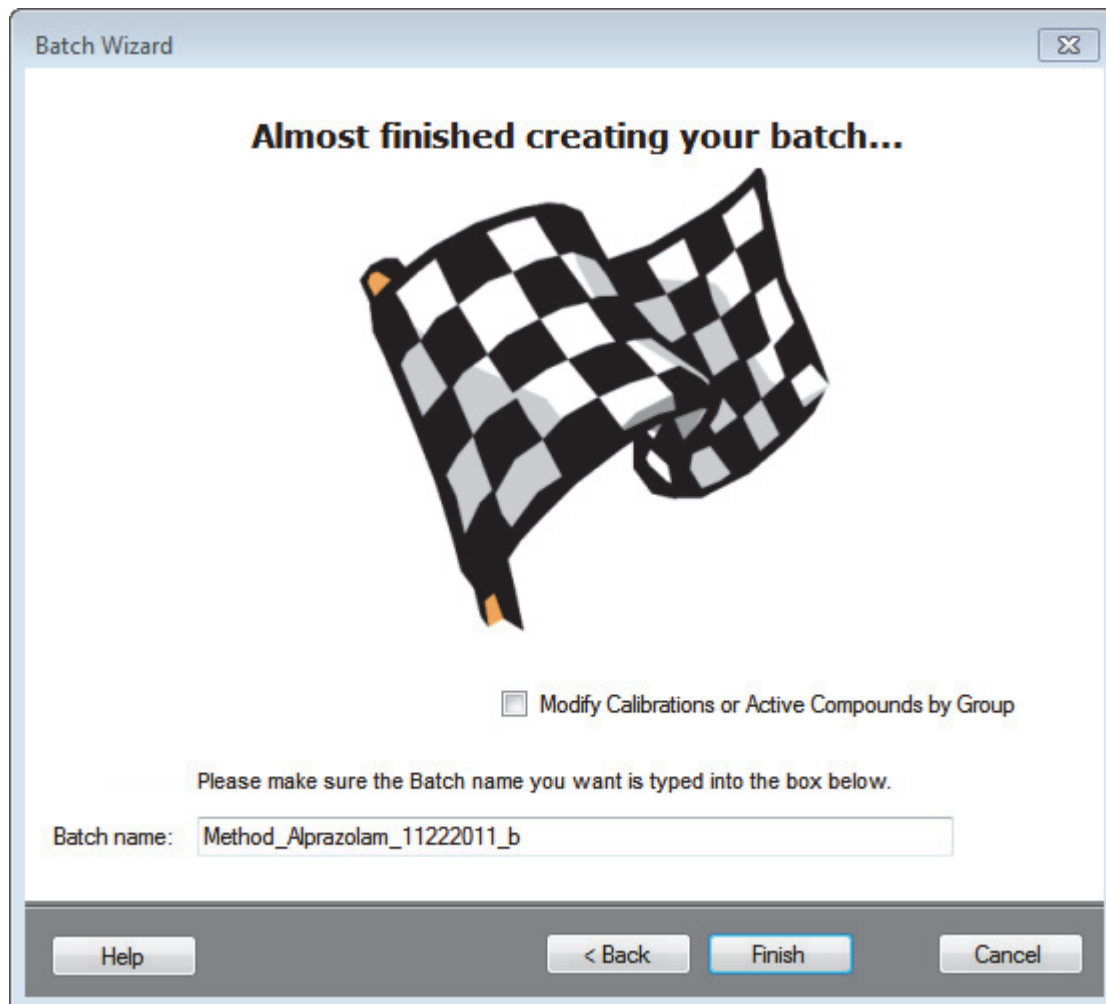
Table 70. Finish parameters (Sheet 1 of 2)

Parameter	Description
Modify Calibrations or Active Compounds by Group	Enables the Next button that lets you access the Calibration and Compound Selection page. If 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: *MasterMethodName_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 335.

Table 70. Finish parameters (Sheet 2 of 2)

Parameter	Description
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 325.
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.
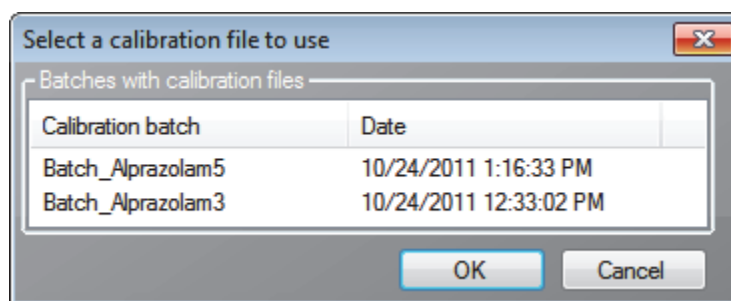
2. Select a calibration file to append to the current calibration file and click **OK**.

   The application appends the selected calibration file to the current file.
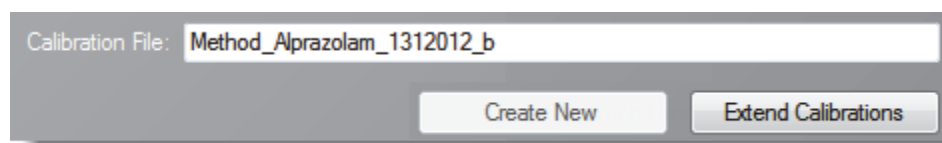
3. To save calibration data from both files into a single file for this batch, click **Create New**.

4. When you are finished with the Calibration and Compound Selection page, click **Next**.

   The Finish page opens. See "Submitting the Batch" on page 340.

❖ **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 340.

Figure 86. Calibration and Compound Selection Page
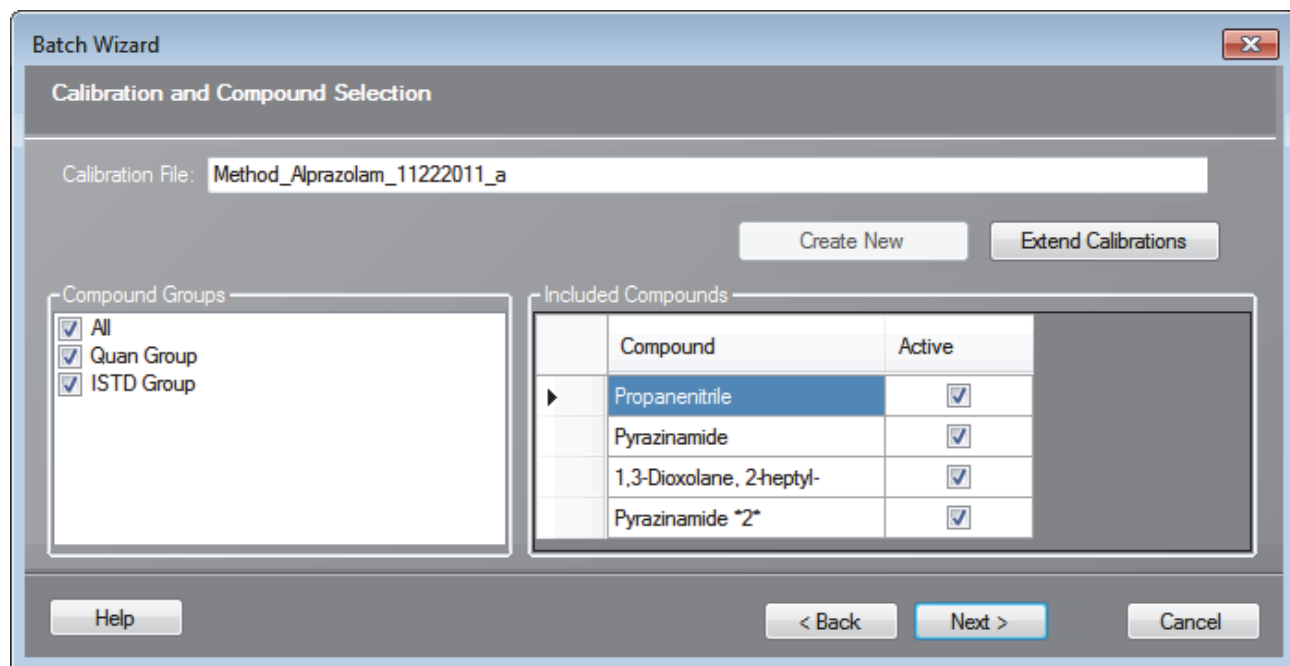
Table 71. Calibration and Compound Selection parameters (Sheet 1 of 2)

Parameter	Description
Calibration File	Name of the current batch in this form: *MasterMethodName_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.

Table 71. Calibration and Compound Selection parameters (Sheet 2 of 2)

Parameter	Description
Compound Groups	Displays all available groups defined in the Groups page of the Master Method View. See "Editing the Groups Page" on page 126.
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 335.
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 340.
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.

Working in Data Review View

In the Data Review view, you can view the data generated by the master method. Use the Data Review view to verify the data for a sample-specific compound before you generate reports. You can use the functions in the Data Review view to investigate and edit the quantification or qualification values in a batch.

❖ **To open the Data Review view**

1. Do one of the following:

   From the dashboard, click **Analysis**.

   –or–

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

2. In the Analysis navigation pane, click **Data Review**.

   The Data Review view for the currently selected batch opens.

The Data Review view uses a sample list and one of two modes: Quan Mode or Qual Mode. The Qual Mode is available only for Unknown/TIC sample types. When you view the data for an Unknown/TIC sample type, you can switch between Qual Mode and Quan Mode.

> **Note** In the Qual Mode, the application displays peak information for compounds with mass spectral data only. The Qual Mode is not available for batches that have analog data only (no mass spectra compounds).

This section includes the following topics:

- Data Review Sample List

- Quan Mode

- Qual Mode

Data Review Sample List

Use the sample list to select a particular sample. To see the columns in a sample list and view their descriptions, see "Data Review sample list."

Status indicators for each sample indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The sample list includes the following features:

- Column Display

- Status Indicators

- Caution Flags

- Compound Flags

- Inactive and Excluded Compounds

The sample list is the same in both Quan Mode and Qual Mode and displays all the quantitative data for the samples of a batch.

- In Quan Mode, the sample list works with the Compounds pane to select a unique sample and compound combination, which then has its textual and graphical values displayed in the Quan Mode pane. The list of compounds that are available for a specific method is displayed in the Compounds pane.

  From the sample list, you can make a compound active or inactive.

  - Switching a compound to inactive status does not remove its data and calculated values from the result set. Instead, the TraceFinder application masks the appearance of that compound for that particular sample and grays the compound in the compounds list.

  - For a calibration standard, the application stops using the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. It is no longer part of the result set.

- In Qual Mode, the sample list works with the peak list to select a unique sample and peak combination, which then has its textual and graphical values displayed in the Qual Mode pane.

Figure 87. Data Review sample list

Cells in the sample list that should not have a value, such as the theoretical concentration for an unknown, are shaded and empty. Cells that should have a value, but none exists, report N/A (not available). Results for compounds that are not detected display N/F (not found).

Table 72. Data Review sample list columns (Sheet 1 of 3)

Column	Description
Status	● Sample is not acquired.
	● Sample is acquired but not processed.
	● Sample is acquired and processed.
	● Sample is currently acquiring.
Flags	Caution flag displayed when a compound within the sample has an error.
Filename	Name of the raw data file that contains the sample data.
Sample Type	Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types:
	Matrix Blank, Solvent, Cal Std, Chk Std, Unknown, Unknown/TIC, LCS, LCSD, MDL, MS, MSD, Method Val, Tune, Tune/Breakdown, or Breakdown
Level	The level defined for a calibration sample or quality control sample.

Table 72. Data Review sample list columns (Sheet 2 of 3)

Column	Description
Sample ID	A user-defined, alphanumeric string that identifies a sample.
Sample Name	A user-defined name that identifies a sample.
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
Integration Mode	Indicates whether the peaks have been manually integrated or integrated from the original method.
Height	The distance from the peak maximum to the peak base, measured perpendicular to the ordinate. When the Resp Ratio is specified as Height, this column displays an asterisk (*Height).
Area	The area obtained by integrating peak intensities from the start to the end of the peak. When the Resp Ratio is specified as Area, this column displays an asterisk (*Area).
Actual RT	Actual retention time for the compound. Retention time is the time after injection when a compound elutes and the total time that the compound is retained on the chromatograph column.
Expected RT	Expected retention time for the compound.
Calc Amt	The amount present in the sample, as determined using the calibration curve and the response ratio.
Theo Amt	Theoretical amount of the compound expected in the sample.
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.
Resp Ratio	The ratio of the Response value to the IS Response value. If the Response is specified as Area in the processing method, the units of both Response and IS Response are counts-sec. If the Response is specified as Height in the processing method, the units of both Response and IS Response are counts.
IS Amt	Amount of internal standard.
IS Resp	Response of the internal standard.

Table 72. Data Review sample list columns (Sheet 3 of 3)

Column	Description
Active	Displays or hides a compound for a particular sample. When a calibration standard is marked inactive, the application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. It is no longer part of the result set.
Excluded	Turns a compound on or off in the calibration curve of the Qualification pane.
%Diff	The calculated amount minus the expected amount, divided by the expected amount, and then multiplied by 100.
%RSD	Standard deviation of the multiple samples of one level, multiplied by 100, and divided by the average of the multiple samples of that level. This calculation is based on the calculated amounts.
%CV	Coefficient of Variance. Standard deviation of the multiple samples of one level, multiplied by 100, and divided by the average of the multiple samples of that level. This calculation is based on the areas of the peaks.
Channel	Specifies the channel on which the sample was run. If the sample is not acquired, the value is Pending. The Channel column is available only when you have enabled multiplexing in the Configuration mode. See "Multiplexing" on page 92.
Comment	A user-defined comment for the sample.

Column Display

The sample list can contain 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, Flags, Filename, and Sample Type columns stay fixed while the other columns scroll right and left.

❖ **To customize the column display**

1. Right-click the Data Review sample list and choose **Modify Columns** from the shortcut menu.

   The Modify Columns dialog box opens. See "Modify Columns dialog box."

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

   All the columns you select are displayed after the Status, Flags, 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 Data Review sample list, and the last column in the list represents the rightmost column in the Data Review sample list.

      > **Note** You cannot move the Status, Flags, Filename, or Sample Type column.

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

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

   b. Type a new value for the width.

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

The columns in the sample list immediately reflect your changes. The application uses these settings for all sample lists in the Data Review view.

Figure 88. Modify Columns dialog box

Modify Columns						
Available Columns				**Displayed Columns**		
	Column Name	Column Width			Column Name	Column Width
1	RR/RF	80	>>	1	Status	40
2	IS Amt	80	>	2	Flags	40
3	IS Resp	80		3	Filename	100
4	Active	100	<	4	Sample type	100
5	Excluded	100	<<	5	Level	100
6	% Diff	100		6	Sample ID	100
7	% RSD	100	Up	7	Sample name	100
8	% CV	100	Down	8	Comment	100
9	Channel	100		9	Vial position	100
10	Final Units	100		10	Injection volume	110
11	Calc Amt	125		11	Expected RT	100
12	Theo Amt	80		12	Actual RT	100
13	Sample Amt	100		13	Integration mode	100
				14	Height	100
				15	Area	100

Table 73. Modify Column 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, Flags, Filename, and Sample Type columns.
<<	Moves all columns except Status, Flags, 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, Flags, Filename, and Sample Type columns.
Down	Moves the selected column name in the Displayed Columns pane one row down in the column order. You cannot move the Status, Flags, Filename, and Sample Type 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	Flags	Filename	Sample type	Sample ID	Sample name
1	●	⚠	UnknownA2	Unknown	A2	Sample2
2	●	⚠	UnknownA3	Unknown	A3	Sample3

Status indicators

Caution Flags

The Flags column in the sample list displays a caution flag if the sample is not in compliance with the method criteria.

Sample caution flags remain static when you switch between compounds for chromatogram review until a change is completed, for example, when a compound is manually integrated and no longer falls outside the accepted criteria.

	Status	Flags	Filename	Sample type	Sample ID	Sample name
1	●	⚠	UnknownA2	Unknown	A2	Sample2
2	●	⚠	UnknownA3	Unknown	A3	Sample3

Sample caution flags

To display a summary of problems found in the sample, click the caution flag. The summary does not list compounds that are not found in Unknown sample types.

	Status	Flags	Filename	Sample type	Level	Sample ID
▶ 1	●	⚠				
2	●	⚠				
3	●	⚠				

UnknownA1 Flag Details

Propanenitrile
3.167:Peak area 23486986.169 is out of bounds (ISTD Minimum Recovery 0.000 and ISTD Max Recovery 0.000)

Compound Flags
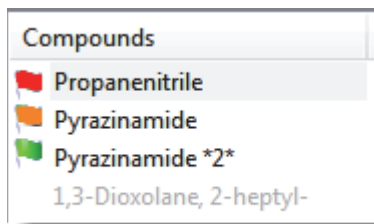
Flags are displayed in these situations:

- When a compound has violated (or is activated by) any of the values set in the method (See "Editing the QAQC Page" on page 183.)

- For compounds that are not found

- For compounds that are not found in Cal Std or Chk Std sample types

- For compounds that are outside the specified ion ratio range

These criteria do not apply to Matrix Blank sample types when the compound is an internal standard.

The compounds list is sorted first by flag indicators and then by compound names. Compound flags indicate the following:

- Red flags for compounds that have ion ratio failures or method validation failures

- Orange flags for compounds that are below the LOQ, below the LOD, or between the LOD and LOQ values specified in the method

- Green flags for compounds that are over the LOR amount specified in the method

- No flag for compounds that have no errors or where no report options are selected

Inactive and Excluded Compounds

Use the Active and Excluded columns to control which compounds are used for calculating the calibration curve and for reporting.

Follow these procedures:

- To make a sample active or inactive

- To exclude a calibration point

❖ **To make a sample active or inactive**

1. Select the sample in the sample list.

   All compounds in the selected sample are displayed in the Compounds pane. Inactive compounds are grayed out.

2. In the Compounds pane, select the compound whose active/inactive status you want to change.

3. In the sample list, select or clear the **Active** check box.

   Use the horizontal scroll bar at the bottom of the table to scroll to the Active column.

Inactive compound

❖ **To 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.

The application displays a value that is no longer used for calibration as an empty box in the graphical view of the calibration curve.

Excluded calibration point
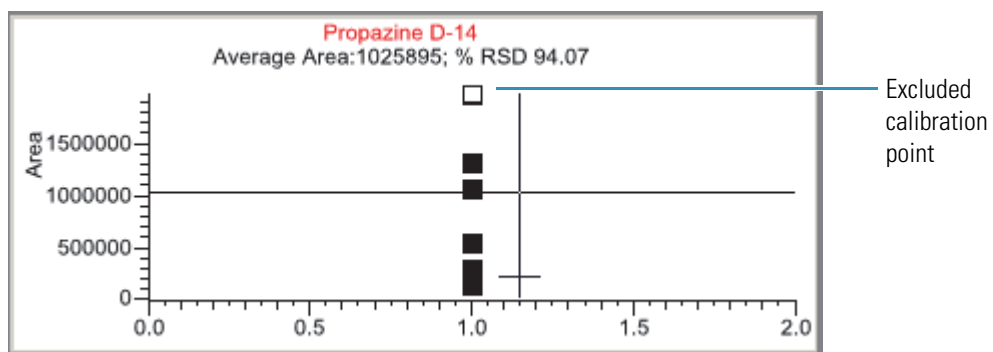
Quan Mode

Use the Quan Mode and the associated Compounds pane to view quantitative information to complement the textual information for the selected sample. The Quan Mode displays peak information for selected compounds that are found in the processed samples.

Sample list   Compounds pane

Peak display panes

In addition to the Data Review Sample List, the Quan Mode view uses the following panes:

- Compounds Pane

- Peak Display Panes

Compounds Pane

The Compounds pane works with the sample list pane to display textual and graphical values for a unique file and compound combination.

❖ **To sort the compounds list**

In the Compounds pane, right-click and choose one of the following sort styles from the shortcut menu.

Command	Description
Sort by Flag and Alphabetical	Sorts the compounds first by flag and then, within each flag group, sorts the compounds alphabetically.
Sort by Flag and Retention Time	Sorts the compounds first by flag and then, within each flag group, sorts the compounds by retention time.
Sort by Alphabetical	Sorts the compounds alphabetically (1–*n* followed by *a–z*).
Sort by Retention Time	Sorts the compounds from shortest retention time to longest retention time.

❖ **To display specific problems with a compound**

Hold the cursor over the flag to view a description of the problems with the compound.

Peak Display Panes

In the peak display panes, you can display multiple panes of data for each compound.

You can display any of the following types of data:

- Quan Peak

- Confirming Ions

- Calibration Curve

- Ion Overlay

- ISTD

- Reference Peak

- Spectra

❖ **To display peaks for a specific compound**

1. In the sample list, select a sample.

   The Compounds pane lists all compounds specified in the method and found in the sample.

2. In the Compounds pane, select a compound that was found in the sample.

   By default, the first display pane shows the quantitative peak for the selected compound.

3. In the second pane, select the additional type of data that you want to display.

Figure 89. Displaying a compound peak

1. Select a sample.   2. Select a compound. 3. Select a data type.

Follow these procedures to change the display of the peak data:

- To change the peak panes

- To zoom in on a peak

❖ **To change the peak panes**

In any of the peak panes, right-click the header bar or click the ⌄ icon.
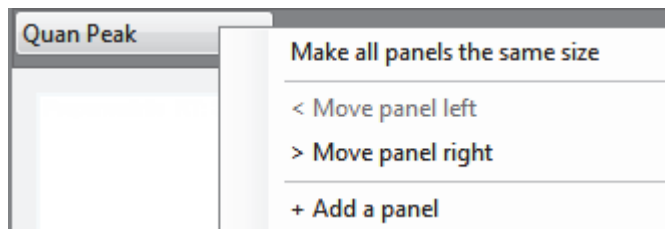
Command	Description
Make All Panels the Same Size	Evenly divides the area to make all panes the same width. This command does not change the pane height.
Move Panel Left	Moves the current panel one space to the left. This command is not available when the current pane is the leftmost pane.
Move Panel 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 364.

Figure 90. Quantitative peak pane with multiple quantitative peaks
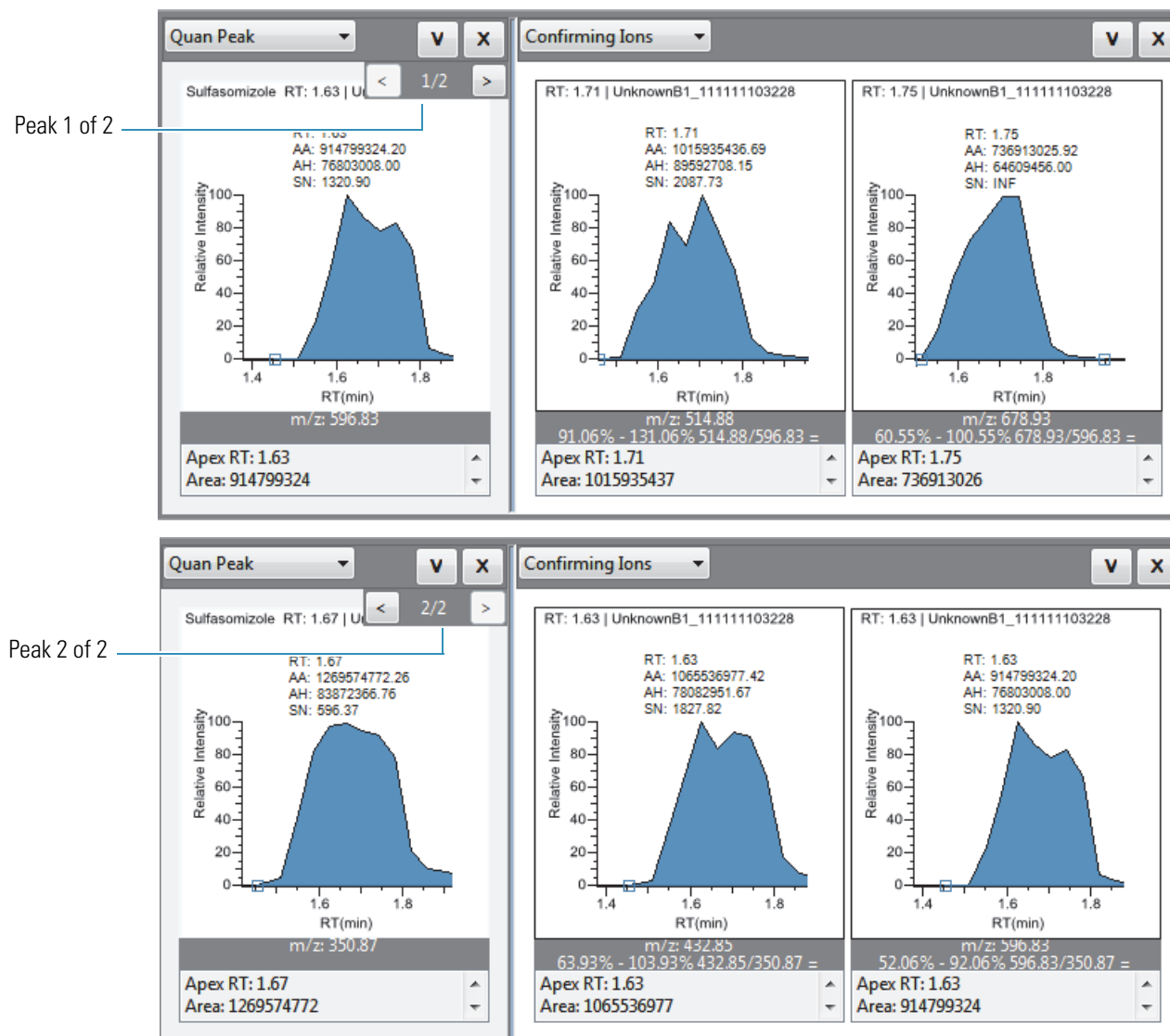
Follow these procedures to modify the quantitative peak data:

- 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.

    The Add Peak command is available only when the application has not detected a peak.

2. Click to indicate the left and right base points for the peak.

    The application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.

Manually added base points
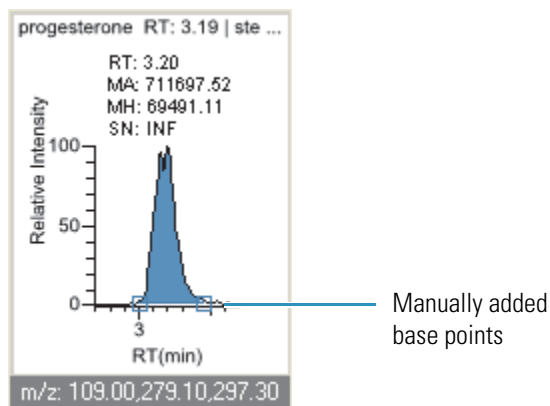
Note The Add Quan Peak command is also available on the Confirming Ions pane.

❖ **To remove a manually created peak**

Right-click the pane, and choose **Remove Quan Peak** from the shortcut menu.

The application removes the manually added peak.

Note The Remove Quan Peak command is also available on the Confirming Ions pane.

❖ **To manually integrate a quantitative peak**

1. Hold your cursor over one of the two peak delimiter tags in the peak pane.

    When the tag can be selected, the cursor changes to a crosshair-style cursor. You can zoom in on the baseline to make it easier to select the tag.

2. Drag the peak delimiter tag to another location and automatically update the peak values (area, height, and so forth) into the result set.

    The generated reports for these data identify the manual modifications.

    You can store two peak value sets (method and manual integration settings) with each compound in each file. These settings can result in a different set of stored values. The application originally calculates the method values based on the processing method parameters. The manual values are a result of what you have edited.

❖ **To switch between method and manual integration modes**

Right-click the chromatogram view and choose **Method Integration Settings** or **Manual Integration Settings** from the shortcut menu.

Initially, the method and manual integration settings that are stored for a compound and file are identical. When you switch modes, the saved result set does not change. However, when manual data are available, the chromatogram plots and the result set update as you switch between method and manual modes.

As you switch between modes, each pane reflects the changes. The generated reports for these data identify the manual modifications.

> **Note** The Method Integration Settings and Manual Integration Settings commands are also available on the Confirming Ions pane.

❖ **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.

> **Note** The Peak Labels command is also available on the Confirming Ions pane.

> **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 91. Peak Detection Settings dialog box

Editing all samples in the batch

Editing only the selected sample
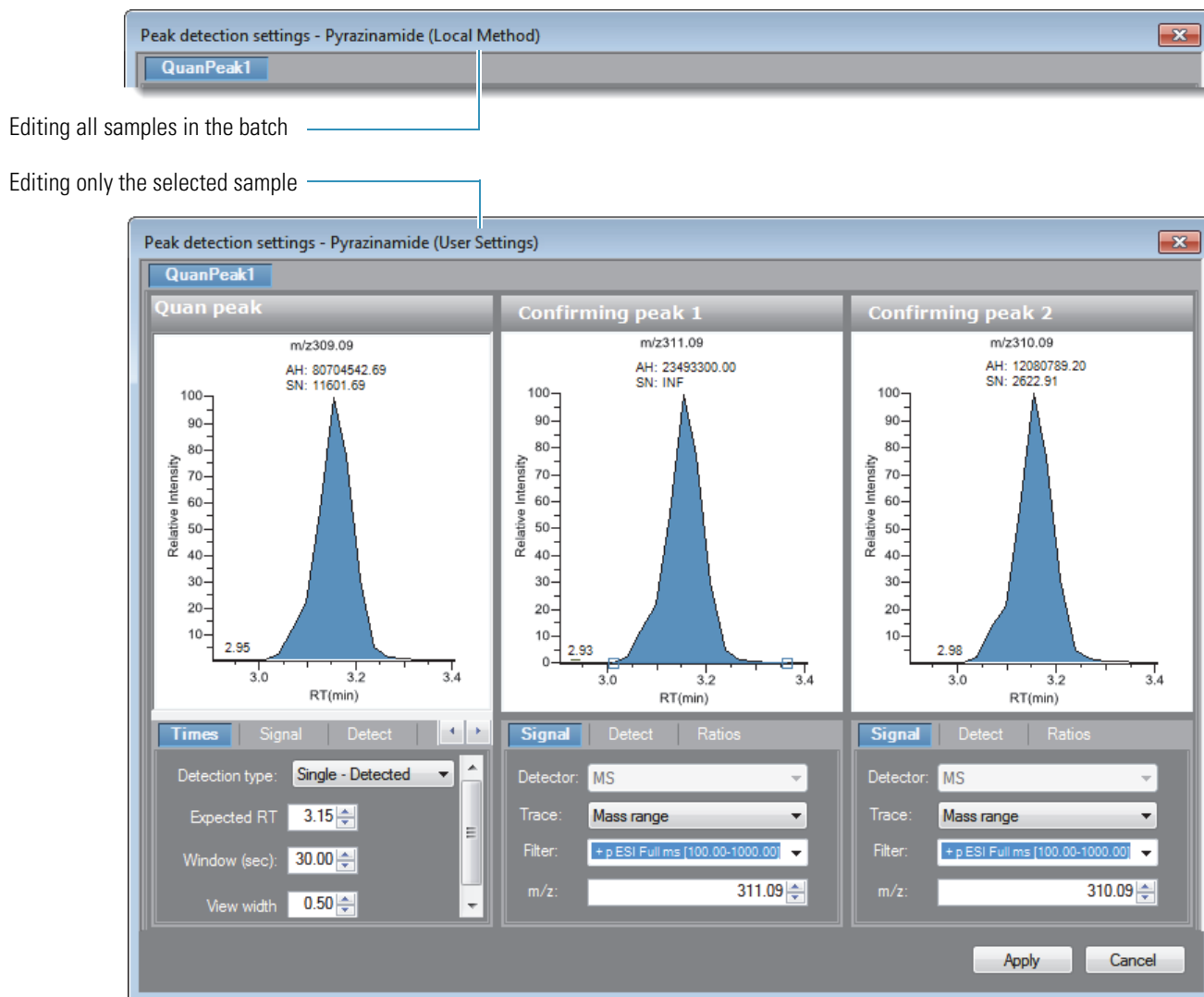
2. Edit any of the detection settings.

   For detailed descriptions of all detection settings, see "Detection" on page 135.

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 74. 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 74. Quan Peak pane shortcut menu commands (Sheet 2 of 2)

Command	Description
Show Peak Info	Displays peak information for the selected compound. For example

> **Acetamide, N-(2-hydroxyphenyl)-**
>
> Quan ion m/z: 295.18
>
> Integration mode: Method
>
> Left RT: 1.31 Area: 215213
>
> Apex RT: 1.40 Height: 69178
>
> Right RT: 1.51 Noise: 690.16
>
> Data file: steroids03_111115163458
>
> Filter: + c Full ms2 331.30@cid40.00
>
> Detector: MS
>
> Trace: Mass range

Command	Description
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 92. Quantitative peak with multiple confirming ions
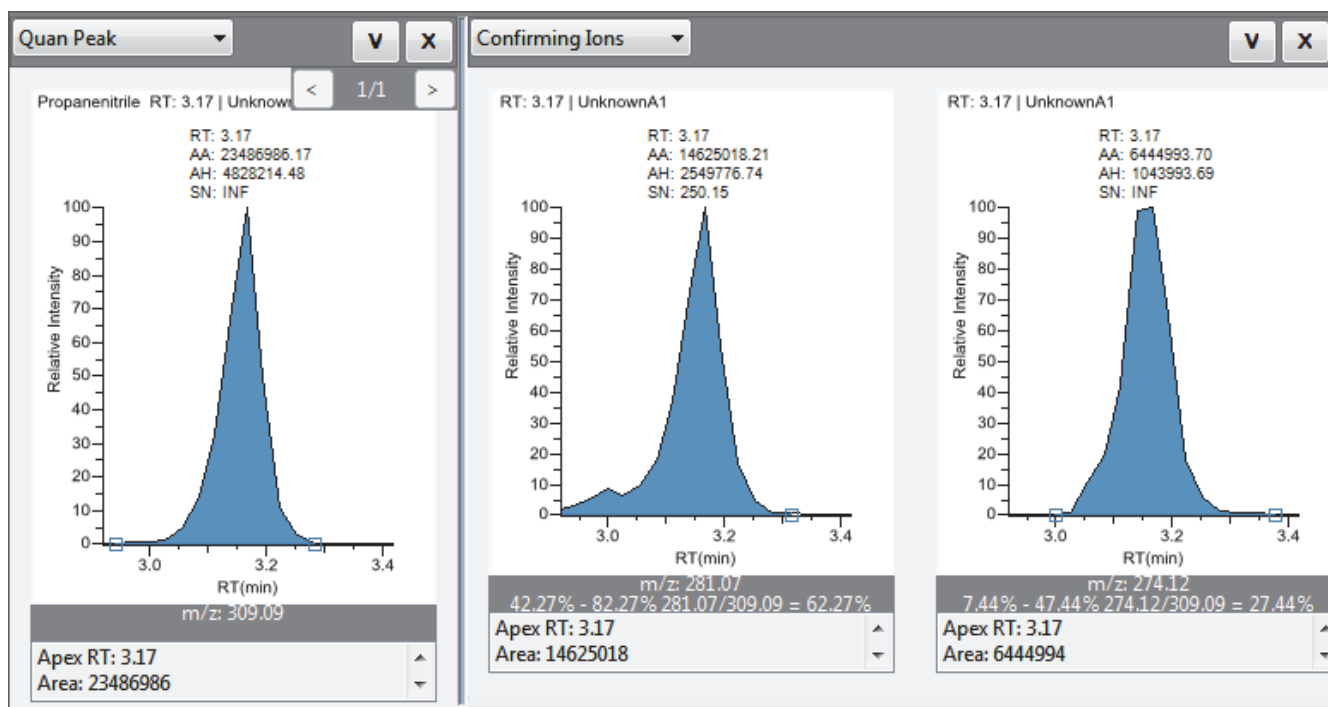
Figure 93. Confirming ion with coelution failure
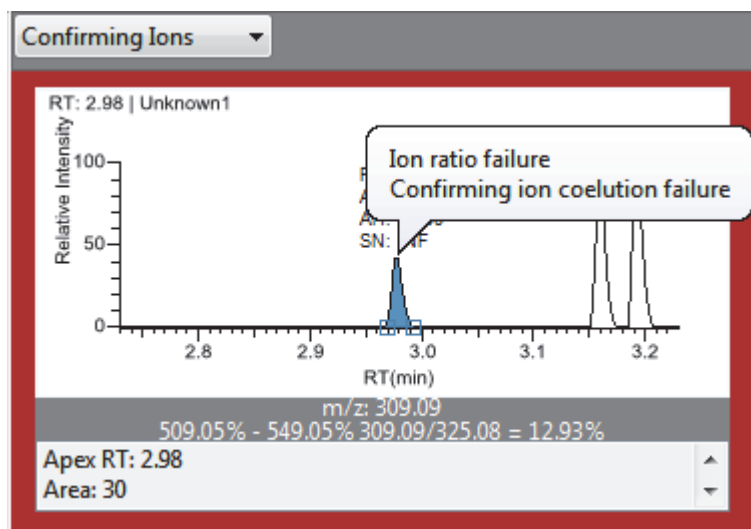
❖ **To manually integrate a confirming ion peak**

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 75. Confirming Ions pane shortcut menu commands (Sheet 1 of 2)

Command	Description
Method Integration Settings	Displays the method integration settings.
Manual Integration Settings	Displays the manual integration settings.
Add Quan Peak –or– Remove Quan Peak –or– Cancel Add 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.

Table 75. Confirming Ions pane shortcut menu commands (Sheet 2 of 2)

Command	Description
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 94. Quantitative peak with a calibration curve plot
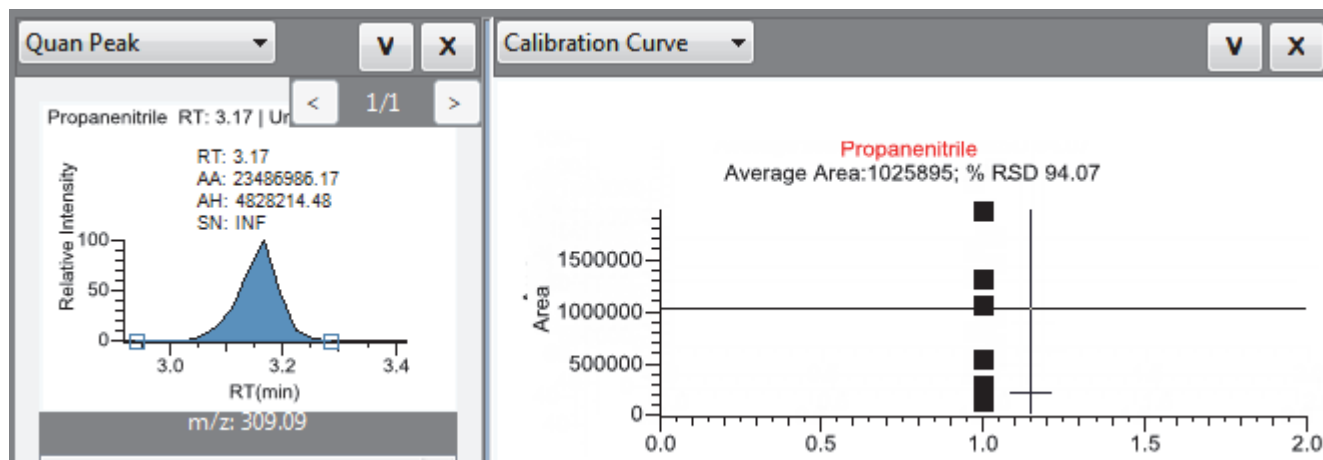
❖ **To manually exclude a calibration point**

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.

Excluded calibration point
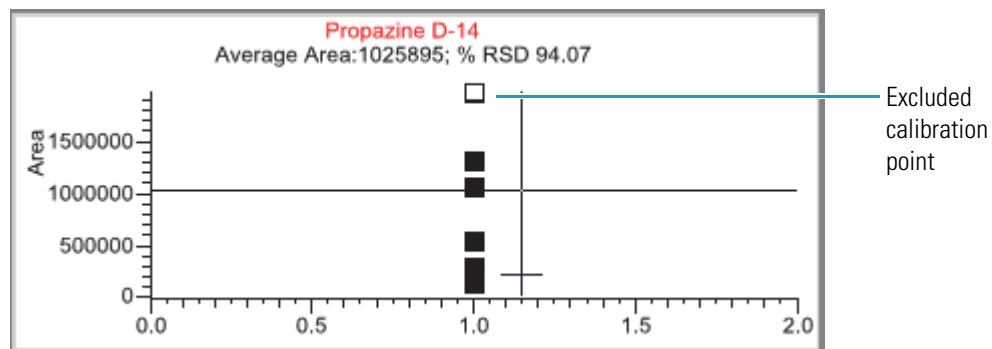
Table 76. Calibration Curve pane shortcut menu commands

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 sample and compound. Use this pane to graphically review the peak apex alignment and co-eluting peak profiles.

> **Note** For compounds with an analog detection type, the application displays "No Data" in the Ion Overlay pane.

Figure 95. Quantitative peak with confirming ion overlay
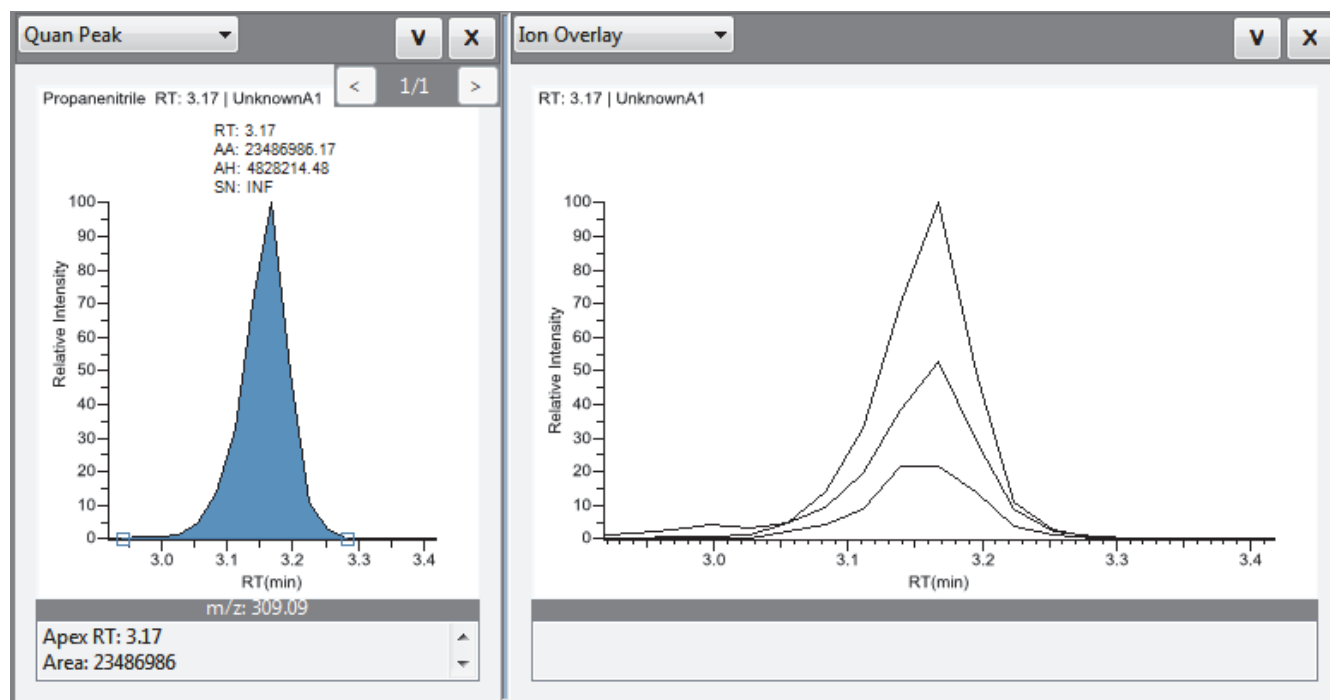
ISTD

The ISTD pane displays the internal standard specified for the compound in the method. See "To specify an internal standard for a compound" on page 173.

Figure 96. Quantitative peak with an internal standard
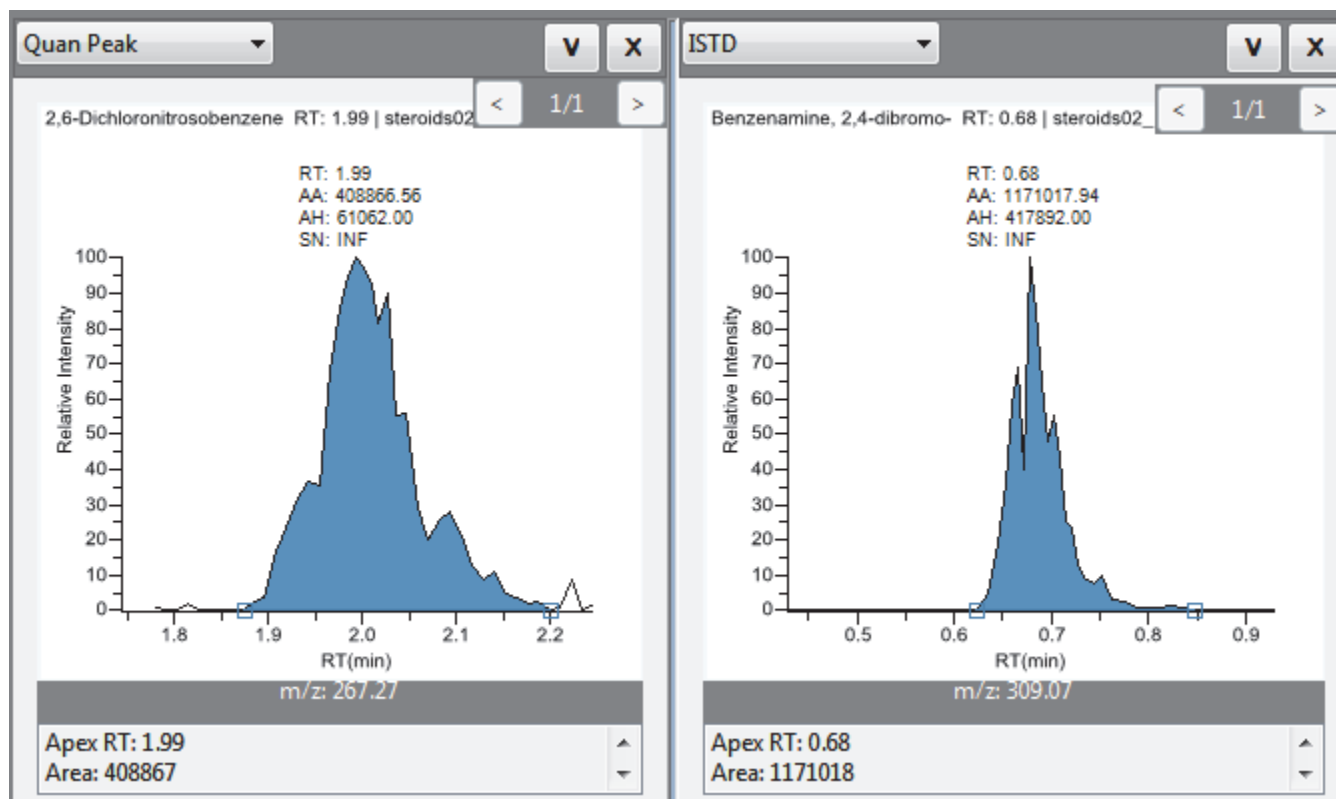
Reference Peak

The Reference Peak pane displays the reference peak as specified in the method. See "To specify a chromatogram reference sample" on page 124.

Figure 97. Quantitative peak with a reference peak
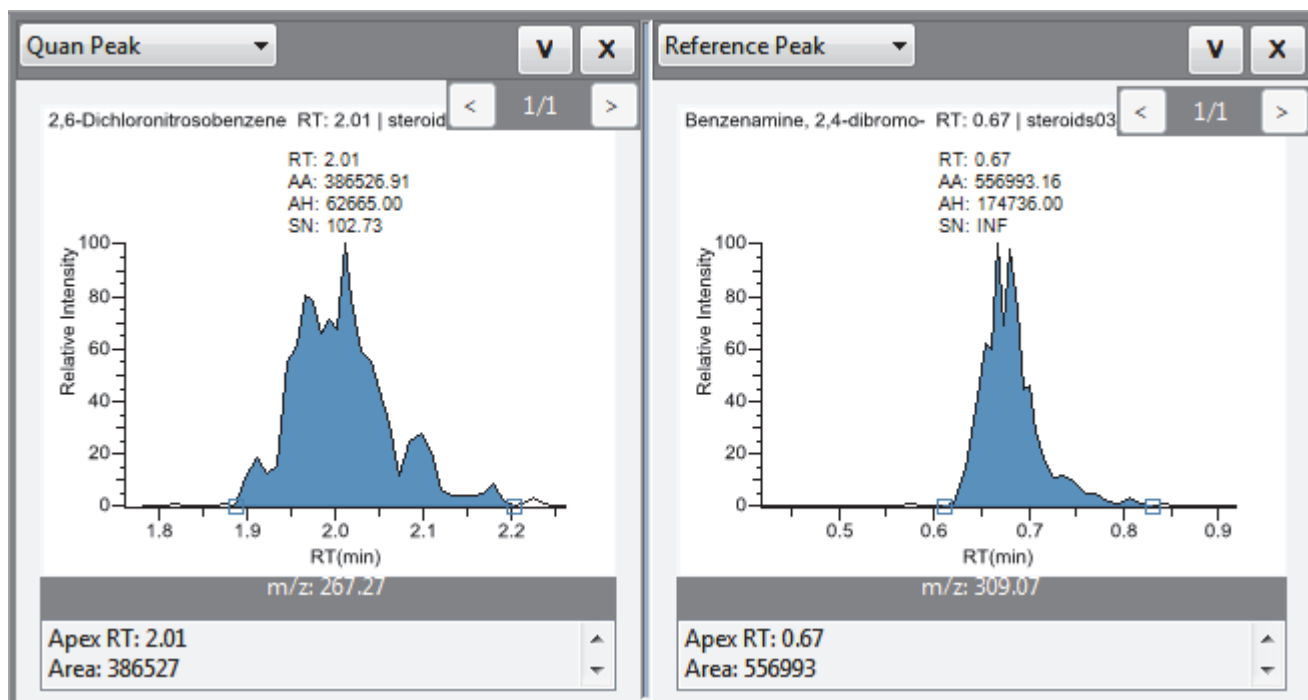
Spectra

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 98. Quantitative peak with data and reference spectra
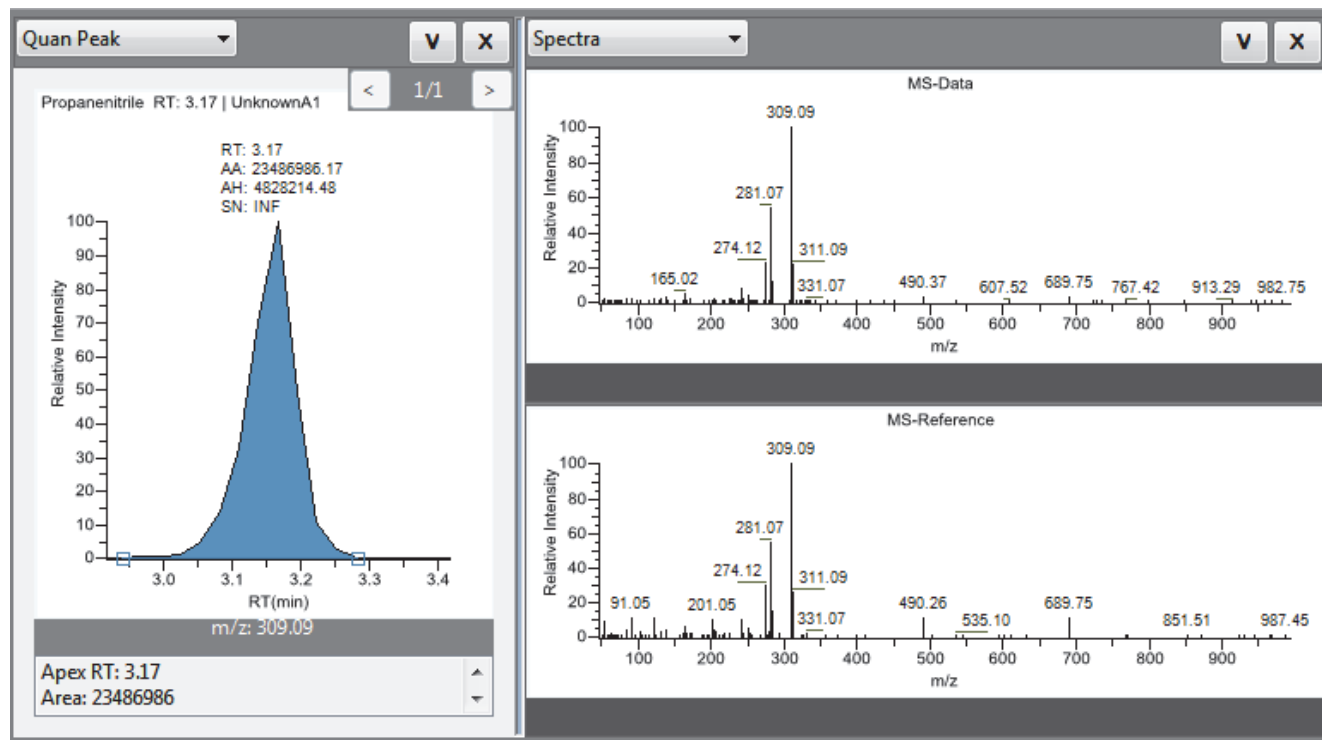
Qual Mode

Use the Qual Mode and the associated peak list to view qualitative information that complements the textual information for the selected Unknown/TIC sample. The Qual Mode view displays detected peaks for the selected sample. From the Qual Mode view, you can manually add peaks. The Qual Mode view is available only for Unknown/TIC sample types.

Sample list

Peak list

Chromatogram navigation pane

Qualitative peak pane

Spectra pane

Ranking pane

Tip To resize the panes, drag the separators that divide the panes.

In addition to the Sample List, the Qual Mode view displays data in the following panes:

- Peak List

- Chromatogram Navigation Pane

- Qualitative Peak Pane

- Spectra Pane (Reference and Selected)

- Ranking Pane

Peak List

The peak list works with the sample list to display graphical values for a unique sample and peak combination. For detailed descriptions of parameters on the peak list, see "Peak list parameters" on page 378.

❖ **To display peaks for a specific compound**

1. From the sample list, select a sample.

> **Note** If you select a sample type other than Unknown/TIC, the TraceFinder application returns you to Quan Mode.

The peak list displays the retention times for peaks identified in the selected sample, the values for the best match methods for each peak, and the compound match.

The number of peaks that are listed is specified in the method. You can change the number of identified peaks in the Method Template Editor. See "Creating a Method Template" on page 216.

2. From the peak list, select a peak in the sample.

Peak RT	SI	RSI	MP	Est Amt	Compound
7.95	370	892	0	0.000	Hydrogen bromide
9.60	341	857	0	0.000	2,5-Cyclohexadien-1-one,
11.18	910	915	52	0.000	Pyrene

The TraceFinder application displays the selected peak in the qualitative peak pane.

When you select a data-dependent sample, the peak can be from either a full scan or a QED spectrum of an SRM-filtered chromatogram.

The TraceFinder application displays the Spectra pane with two sections:

- The Qual Data pane shows spectra data for the peak in the raw data file.

- The Qual Library pane shows actual spectra for the identified library compound.
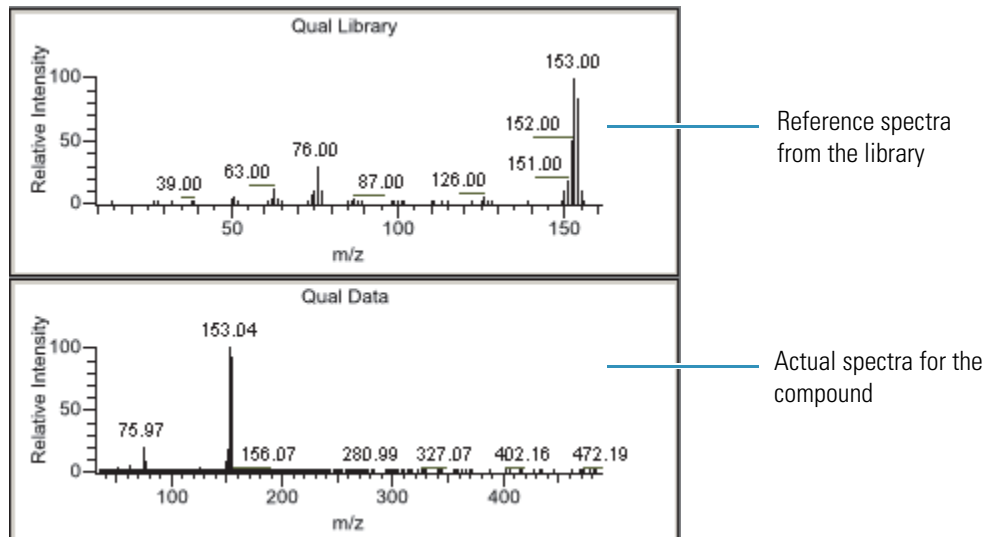
The TraceFinder application locates the selected peak in the navigation chromatogram.
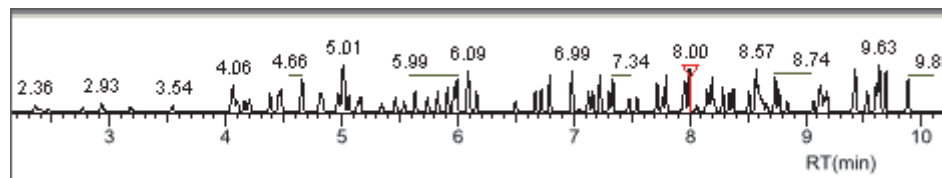
❖ **To remove a peak**

1. Select a peak in the peak list.

2. Right-click and choose **Remove Selected Peak** from the shortcut menu.
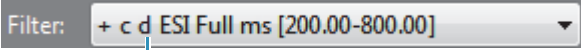
   The TraceFinder application removes the selected peak from the peak list.

   Note There is no undo for this action, but you can manually add a peak to redefine a removed peak. See "Chromatogram Navigation Pane" on page 379.

Figure 99. Peak list

Table 77. Peak list 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 method used to search the NIST library.
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.

Chromatogram Navigation Pane

The chromatogram navigation pane displays all peaks in the selected sample. The peak selected in the peak list displays a red marker. See "Chromatogram navigation pane" on page 380.

For a description of commands on the shortcut menu, see "Chromatogram navigation pane shortcut menu commands" on page 380.

❖ **To zoom in on a peak**

1. In the chromatogram navigation pane, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the default view, right-click the chromatogram navigation pane and choose **Reset Scaling** from the shortcut menu.

❖ **To manually add a peak**

1. Zoom in to better identify which peak to add to the results set.
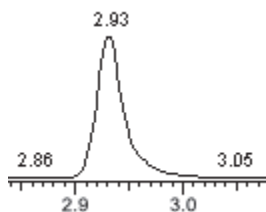
2. Right-click the chromatogram navigation pane, and choose **Add Qual Peak** from the shortcut menu.

3. Click to indicate the left and right base points for the peak.

   The TraceFinder application marks the peak in the chromatogram navigation pane.
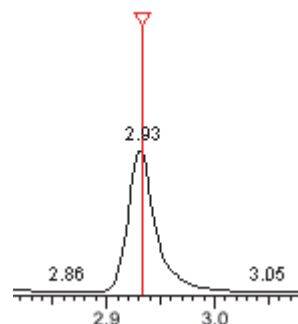
   The TraceFinder application places the peak delimiter tags at the base point locations and automatically updates the peak values in the peak list and qualitative peak pane.

Figure 100. Qualitative peak pane with a manually added peak

Manually added
base points
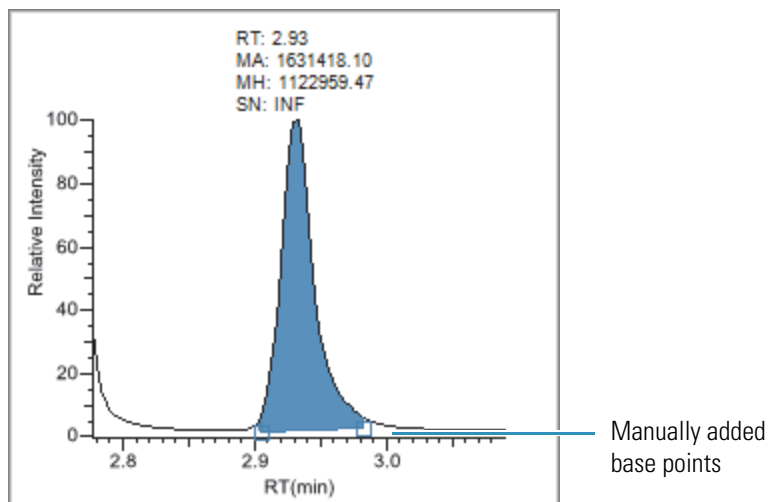
	Peak RT	SI	RSI	MP	Est Amt	Compound
▶	2.93	235	870	0	0.000	Benzene, nitro-
	3.01	213	944	0	0.000	Benzene, nitro-
	3.15	102	792	0	0.000	Pyrazinamide

Figure 101. Chromatogram navigation pane
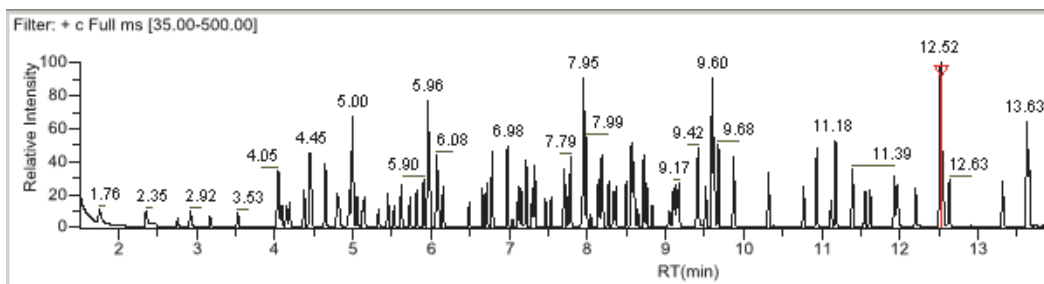
Table 78. Chromatogram navigation pane shortcut menu commands

Command	Description
Add Qual Peak	Select the beginning and ending base points for a new qual peak.
Reset Scaling	Resets the original scaling after a zoom operation.

Qualitative Peak Pane

The qualitative peak pane displays the selected peak. See "Qualitative peak pane" on page 383.

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

For a description of commands on the shortcut menu, see "Qualitative peak pane shortcut menu commands" on page 383.

❖ **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 qualitative peak pane, and choose **Add Peak** from the shortcut menu.

   If a peak is already detected, the Add Peak command is not enabled.

2. Click to indicate the left and right base points for the peak.

   The TraceFinder application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.

Manually added base points
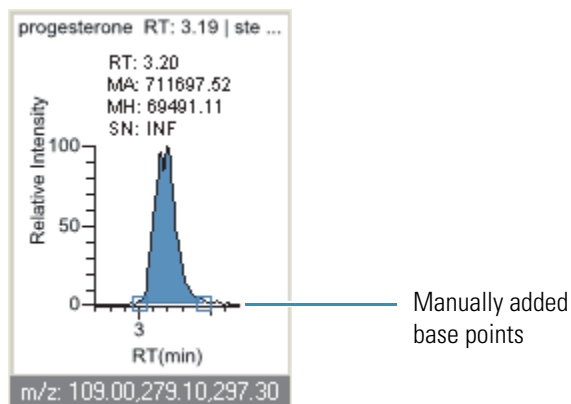
❖ **To remove a peak**

Right-click the chromatogram plot, and choose **Remove Peak** from the shortcut menu.

The TraceFinder application removes the peak displayed in the qualitative peak pane. All data for this peak are removed from the Qual Mode panes.

❖ **To switch between method and manual integration modes**

Right-click the chromatogram view and choose **Method Integration** or **Manual Integration** from the shortcut menu.

Initially, the method and manual integration settings that are stored for a compound and file are identical. 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 chromatogram plot and hold the cursor over **Peak Labels**.

2. Choose to display labels for the peak retention time, peak height, peak area, or signal to noise.

   The label types in the list are selected for displayed labels and cleared for labels that are not displayed.

3. To remove a label, select the label type again and clear it.

   Label settings are globally applied to qualitative peaks, confirming peaks, and internal standard peaks.

   > **Tip** The labels do not always update on all peak displays. To update all labels, select a different compound, and then reselect the compound whose labels you changed.

Figure 102. Qualitative peak pane
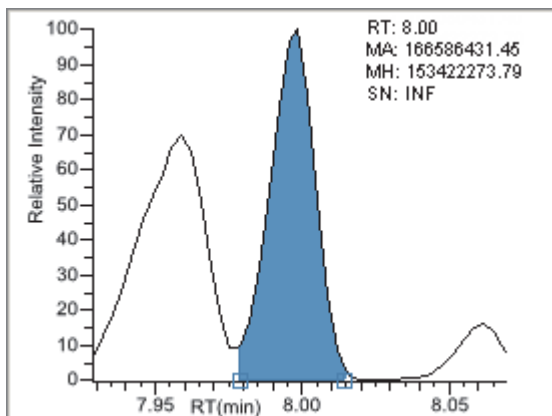
The qualitative peak pane shortcut menu includes the following commands:

Table 79. Qualitative peak pane shortcut menu commands

Command	Description
Reset Scaling	Resets the original scaling after a zoom operation.
Method Integration	Displays method integration settings.
Manual Integration	Displays manual integration settings.
Peak Labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).
Remove Qual Peak	Removes the qualitative peak displayed in the Qual pane.

Spectra Pane (Reference and Selected)

The spectra pane displays the reference spectra and the spectra for the selected sample. The top pane displays the reference spectra for the identified compound from the library; the bottom pane displays the spectra for the selected peak.

Figure 103. Spectra pane
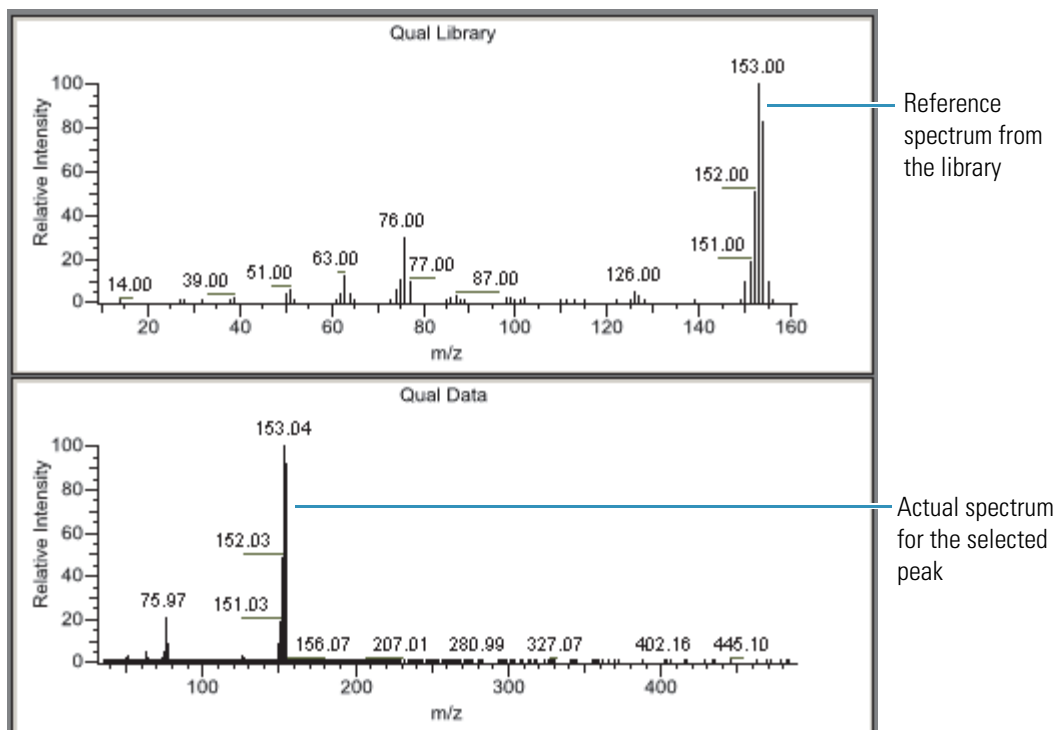
❖ **To zoom in on a peak**

1. In the spectra plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

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

Ranking Pane

The ranking pane displays the three best library matches for the selected peak. Use this pane to select a different library entry for the peak. See "Ranking 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

For detailed descriptions of ranking pane parameters, see "Ranking pane parameters."

❖ **To change the library entry for a selected peak**

In the ranking pane, select the check box for the library entry that you want to use to identify the selected peak.

- In the Spectra pane, the reference spectra change to show the spectra for the selected library entry.
- In the peak list, the SI, RSI, MP, and Compound values update to reflect the selected library entry.

	Rank	SI	RSI	MP	Library entry
☑	1	102	792	0	Pyrazinamide
☐	2	183	791	3	Methanesulfonic acid, 1-methylethyl ester
☐	3	174	760	2	2-Pyrimidinamine, 4,6-dimethyl-
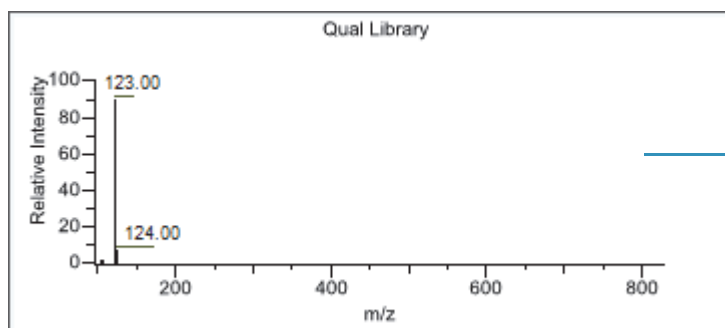
Selected library entry in the ranking pane

Qual Library

Reference spectra for Pyrazinamide

	Peak RT	SI	RSI	MP	Est Amt	Compound
	3.01	213	944	0	0.000	Benzene, nitro-
▶	3.15	102	792	0	0.000	Pyrazinamide
	3.67	242	923	2	0.000	1,3-Dioxolane, 2-heptyl-

Peak list for Pyrazinamide

Figure 104. Ranking pane

Table 80. Ranking 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 method used to search the NIST library.
RSI	Reverse search index method used to search the NIST library.
MP	Match probability.
Library Entry	Library compound that matches the identified peak.

Working in the Report View

Use the Report View to display or generate reports for the currently selected batch in the 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**.

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**.
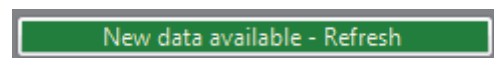
This section includes the following topics:

- Viewing Reports
- Generating Reports
- Working with Reports
- Working with the Active View

Figure 105. Report View in Analysis mode
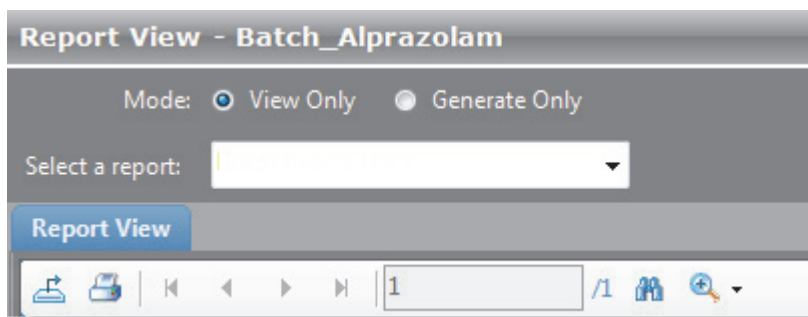
- **View Only**: Displays a PDF or Excel spreadsheet preview of the selected report type for the batch, sample, or compound. See "Viewing Reports."

  Preview reports for all Standard report types are always available. You must generate Custom and Target Screening report types before they are available in this list.

The Report View page displays one of the following report outputs:

– Standard reports as PDF files

– Custom reports in XLSM format

– Target Screening reports as PDF files

• **Generate Only**: Creates all specified report output formats for the selected sample- or batch-level report. See "Generating Reports" on page 392.

Viewing Reports

Use the View Only features to view all configured standard reports and any custom or target screening reports that you have generated. After you generate a report, the application displays the report in the View Only report list.

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.

Report Name	Type	Requires
Batch Report	Standard	
Blank Report	Standard	Sample
Compound Calibration Report	Standard	Compound
Confirmation Report	Standard	Sample, Compound

Filter Reports
☐ Only show automated batch reports
☑ Standard reports   ☑ Custom reports   ☑ Target Screening reports

These reports reflect the Displayed Reports selections in the Configuration mode. To change the configured reports that are available in this view, see "Specifying the Reports Configuration" on page 68.

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 81. Filter Reports options

Option	Behavior
Only Show Automated Batch Reports	Displays only reports that have an output format specified in the Automated Batch Reports area in the Batch View. See "Editing Report Output Formats" on page 320.
Standard Reports	Displays Standard report types.
Custom Reports	Displays all generated Custom report types. Custom reports are not available for viewing until you have generated the report.
Target Screening Reports	Displays all generated Target Screening reports. Target Screening reports are not available for viewing until you have generated the report.

Note When you make changes to the method in the Local Method view, to the peaks in the Data Review view, or to the samples in the Batch View, you must regenerate the custom or target screening reports 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: | TIC Summary Report ▼ | Sample file: | ▼ |

Follow the procedure "To select a sample" on page 390.

- 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 390.

- 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 and a compound" on page 391.

❖ **To select a sample**

1. Open the Sample File list to display all samples in the batch.

Sample Name	Sample ID	Sample Type
UnknownA1	1	Unknown
UnknownA2	2	Unknown
UnknownA3	3	Unknown

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 Check Standard Report, the sample list displays only Chk Std samples.

   > **Note** Click the column headers to sort the samples. The application maintains this sort order each time you open the Report View for this batch.

3. Double-click the name of the sample.

   The sample list closes. The Report View page displays the sample-level report.

❖ **To select a compound**

1. 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
3.67	1,3-Dioxolane, 2-heptyl-

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	Unknown
UnknownA2	2	Unknown
UnknownA3	3	Unknown

─ 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 Check Standard Report, the sample list displays only Chk Std 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 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
3.67	1,3-Dioxolane, 2-heptyl-

5. Double-click a single compound or **All Compounds.**

   The compound list closes.

   The Report View page displays the compound-level report for the selected sample and compound.

Generating Reports

Use the Generate Only features to create sample-level reports. You cannot use the View Only features to view custom or target screening reports until you generate the report. When you make changes to the method in the Local Method view or to the peaks in the Data Review view, you must regenerate the custom or target screening reports to see the effects of those changes.

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.

Report Name	Type	Requires
Blank Report	Standard	Sample
Chromatogram Report	Standard	Sample
ConfirmationReport	Custom	Sample
ConfirmationReport2	Custom	Sample

Filter Reports
☐ Only show automated batch reports

☑ Standard reports   ☑ Custom reports   ☑ Target Screening 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 Configuration" on page 68.

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	Behavior
Only Show Automated Batch Reports	Displays only sample-level reports that have an output format specified in the Automated Batch Reports area in the Batch View. See "Editing Report Output Formats" on page 320.
	If you have only batch-level reports specified in the Batch View, selecting this option excludes all reports in the Report Name list.
Standard Reports	Displays sample-level Standard report types.
Custom Reports	Displays sample-level Custom report types.
Target Screening Reports	Displays sample-level Target Screening report types.

Note Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

4. Double-click the name of the report.

The report list closes. You must select a sample file for the selected report.
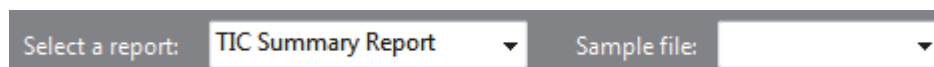
❖ **To select a sample**
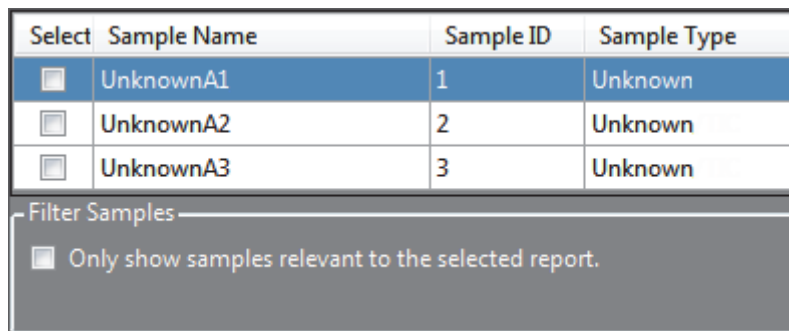
1. Open the Sample File list to display all samples in the batch.

2. To show only samples that would be included in the selected report, select the **Only Show Samples Relevant…** check box.

For example, if you selected the Check Standard Report, the sample list displays only Chk Std samples.

> **Note** Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

3. Select the check box for each sample that you want to include in the report.

4. Click **Generate**.

The Report Selection Confirmation dialog box opens.
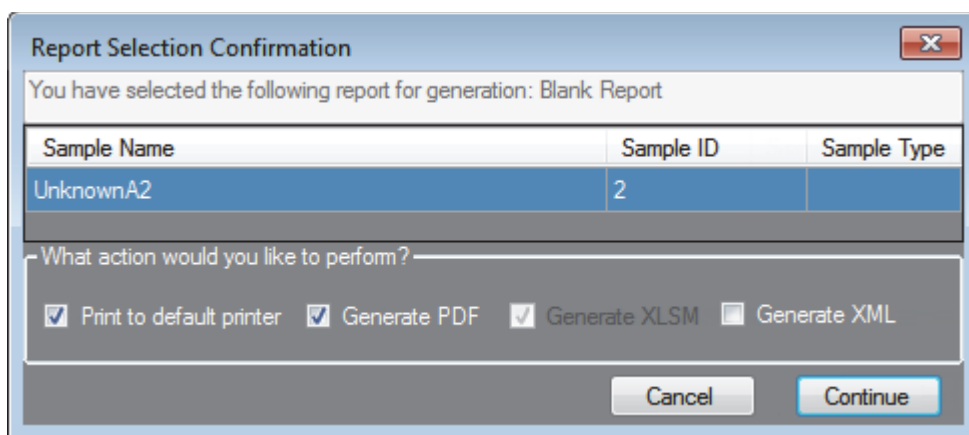
5. In the What Action Would You Like to Perform area, select the types of reports that you want to create.

> **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.
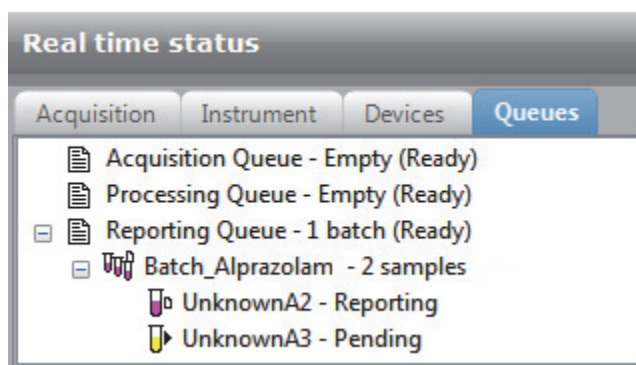
When you have already generated this report in the Batch View or Acquisition mode, the application time-stamps the new report to differentiate it from the original report.

7. To view the report you generated, follow the instructions in "Viewing Reports" on page 388.

> **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.

- A PDF report view is available for all Standard and Target Screening report types.

- An Excel Macro-Enabled Workbook report view is available for any Custom report types that you have generated with the Generate XLSM option selected.

Follow these procedures:

- To print a standard or target screening report

- To export a standard report

- To search for text

- To enlarge the report text

❖ **To print a standard or target screening report**

1. Select the report 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:
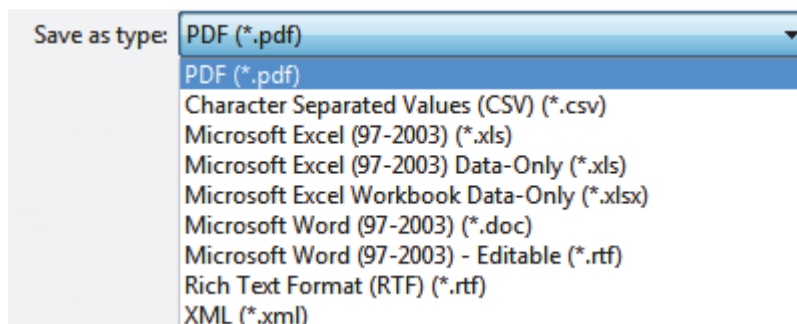
7. Click **Save**.

   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.

   Sample ID
   APN001
   APN002
   APN003

❖ **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.

   Page Width
   Whole Page
   400%
   300%
   200%
   150%
   100%
   75%
   50%
   25%
   Customize...
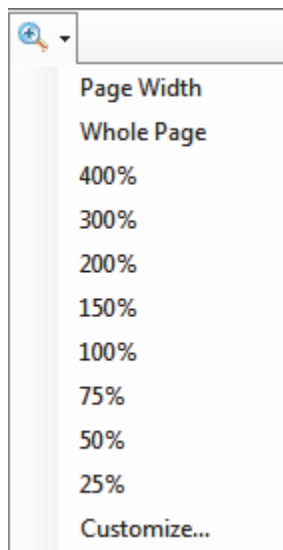
Working with the Active View

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.
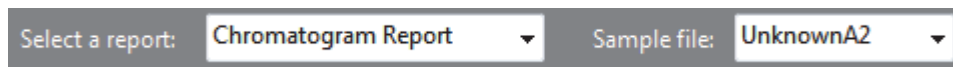
The Active View page displays quantitative data and QAQC error flags for each sample. See "Active View page."

❖ **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.

   | Select a report: | Chromatogram Report ▼ | Sample file: | UnknownA2 ▼ |

❖ **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.

| Showing: | All Compounds | | Showing: | Flagged Compounds Only |

Figure 106. Active View page
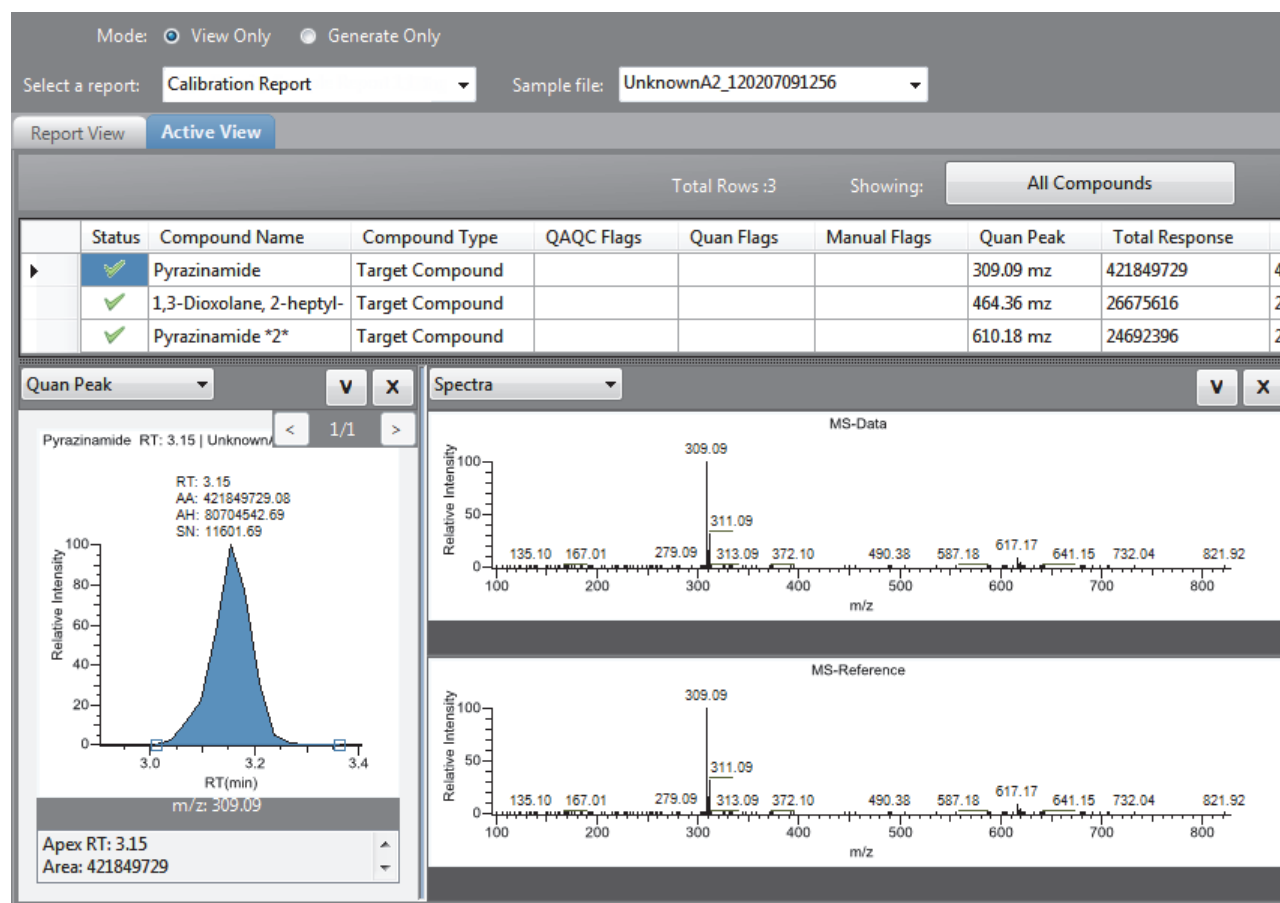
Table 82. Active View parameters (Sheet 1 of 4)

Parameter	Description
View Only	Makes the Active View pane available.
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 82. Active View parameters (Sheet 2 of 4)

Parameter	Description
Column headings	Many column headings are specific to individual reports. See "Active View Report Contents" on page 404.
Status	Indicates the status of the reported compound.

	• A yellow check mark indicates one of the following conditions:
	     – The compound was manually integrated.
	     – Any of the confirming peaks was manually integrated.
	     – The compound has quantitation flags.
	   • A red check mark indicates that the QAQC checks failed.
	   • A green check mark indicates that none of these conditions exist.

	When the compound is an internal standard, warnings are displayed only on the internal standard report. The Status column is blank for Manual Integration reports.
Compound Name	Alphanumeric name assigned to the compound.
Compound Type	Target Compound, Internal Standard, Surrogate, MSTune, Native, or Breakdown.
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)
	
	Quan flags do not apply to these sample types: Cal Std, Chk Std, Matrix Blank, 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.
Concentration	
Confirming *n* Mass	Mass of the confirming peak.

Table 82. Active View parameters (Sheet 3 of 4)

Parameter	Description
Confirming *n* Response	Response of the confirming peak.
Confirming *n* Manual Flag	Indicates a manually integrated confirming peak.
Confirming *n* Ion Ratio Flag	Indicates that the ion ratio is out of range. 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 173.
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 173.
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 150.
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.
Manual Peak Area	Area of the manually integrated peak.

Table 82. Active View parameters (Sheet 4 of 4)

Parameter	Description
Internal Standard reports	
Std Response	Average of the internal standard's response as found in the calibration file.
Minimum Response	Minimum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 190.
Maximum Response	Maximum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 190.
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 190.
Max RT	Maximum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 190.
Sample RT	Retention time found in the sample.
Graphical data	
Quan Peak 1	
Calibration curve	Displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration.
Spectra	Displays a comparison of the spectra found in the data and the method reference.
QED Spectra	Displays the averaged QED spectra from the raw data file and the datastore match. If the sample contains no QED data, the page is blank.
Confirming Ions	Displays a graphical view of all qualifying/confirming ions for the selected sample and compound, and displays calculated ion ratios and ion ratio acceptance windows.

Active View Report Contents

Each standard report that uses the Active View displays values that are common to all reports. See "Common Active View report columns" on page 405.

In addition to the common values, the following reports display additional active view features:

- Blank Report Active View columns

- Calibration Report Active View columns

- High Density Sample Report 1 and High Density Sample Report 1 Long Active View columns

- High Density Sample Report 2 and High Density Sample Report 2 Long Active View columns

- High Density Sample Report 3 and High Density Sample Report 3 Long Active View columns

- Internal Standard Summary Report Active View columns

- Ion Ratio Failure Report Active View columns

- Manual Integration Report Active View columns

- LCSLCSD Report Active View columns

- Method Detection Limit Report Active View columns

- Method Validation Report Active View columns

- MSMSD Report Active View columns

- Quantitation Report Active View columns

- Solvent Blank Report Active View columns

Table 83. 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, Internal Standard, Surrogate, MSTune, Native, or Breakdown.
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) Quan flags do not apply to these sample types: Cal Std, Chk Std, Matrix Blank, or Solvent. The Calibration report does not use the Quan Flags column. The Method Validation, Method Detection Limit, and LCSLCSD reports do 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 84. 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.
Inj Conc	Calculated amount as the sample was injected, with no conversion applied.

Table 84. Blank Report Active View columns (Sheet 2 of 2)

Column	Description
Inj Units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 173.
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 173.

Table 85. 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.

Table 86. High Density Sample Report 1 and High Density Sample Report 1 Long Active View columns

Column	Description
m/z	Mass-to-charge ratio for the 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.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.

Table 87. High Density Sample Report 2 and High Density Sample 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 88. High Density Sample Report 3 and High Density Sample 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.
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.

Table 88. High Density Sample Report 3 and High Density Sample Report 3 Long Active View columns (Sheet 2 of 2)

Column	Description
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 89. 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 190.
Maximum Response	Maximum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 190.
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 190.
Max RT	Maximum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 190.
Sample RT	Retention time found in the sample.

Table 90. 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 91. Manual Integration Report Active View columns (Sheet 1 of 2)

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.

Table 91. Manual Integration Report Active View columns (Sheet 2 of 2)

Column	Description
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 92. LCSLCSD Report Active View columns

Column	Description
Spike Amount	Lab control theoretical concentration.
LCS Concentration	Lab control spike concentration.
LCS % Received	Lab control concentration percentage.
Lower Limit %	Recovery lower limit as specified in the master method. See the Limits section in "Editing the QAQC Page" on page 183.
Upper Limit %	Recovery upper limit as specified in the master method. See the Limits section in "Editing the QAQC Page" on page 183.
LCSD Concentration	Lab control spike duplicate concentration.
LCSD % Received	Lab control spike duplicate concentration percentage.
RPD	Lab control relative percentage difference.
Max RPD	Lab control spike maximum relative percentage difference (set in method).
Number of Rec Failures	Number of recovery failures for lab control spike concentration and lab control spike concentration duplicate.
Number of RPD Failures	Number of relative percentage difference failures for lab control spike concentration and lab control spike concentration duplicate.

Note For LCSLCSD batch reports, the application displays the active view peak graphics only when you click a field pertaining to a sample, such as the LCS or LCSD concentration fields.

Table 93. Manual Integration Report Active View columns (Sheet 1 of 2)

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.

Table 93. Manual Integration Report Active View columns (Sheet 2 of 2)

Column	Description
Manual Peak Height	Height of the manually integrated peak.
Manual Peak Area	Area of the manually integrated peak.

Table 94. Method Detection Limit Report Active View columns

Column	Description
Avg Conc	The average of the concentration for the compound across all samples.
Std Dev	The standard deviation of the concentration.
t-stat	The t-statistic value defined as the ratio of a coefficient to its standard error.
% RSD	%RSD of concentrations
MDL	Method detection limits. The calculated limit of detection.

Note For Method Detection Limit batch reports, the application displays the active view peak graphics only when you click a field pertaining to a sample. These numbered fields are to the right of the MDL column.

Table 95. Method Validation Report Active View columns

Column	Description
Avg Conc	The average of the concentration for the compound across all samples.
Theo Conc	Values for each compound that represent the expected theoretical concentration of that compound in the sample as defined in the master method. See the Meth Val section in "Editing the QAQC Page" on page 183.
% Diff	The percentage difference calculated as ([MethodValidationMeanValue minus the Theo Conc] divided by the Theo Conc) multiplied by 100.
Min Conc	Calculated by (Min recovery percent * Theo Conc) divided by 100.
Max Conc	Calculated by (Max recovery percent * Theo Conc) divided by 100.
% RSD	%RSD of concentrations
Max % RSD	The maximum relative standard deviation (RSD) of the set of observed concentrations for a component across the set of method validation samples (when in average RF mode) as defined in the master method. See the Meth Val section in "Editing the QAQC Page" on page 183.
Calculated Amount <*Sample Name*>	This field is reproduced for every Method Val sample.

Table 96. MSMSD Report Active View columns

Column	Description
Unknown Concentration	Concentration of the unknown sample.
Spike Amount	Matrix spike theoretical concentration.
MS Concentration	Matrix spike concentration.
MS % Received	Matrix spike concentration percentage.
Lower Limit %	Recovery lower limit as specified in the master method. See the Limits section in "Editing the QAQC Page" on page 183.
Upper Limit %	Recovery upper limit as specified in the master method. See the Limits section in "Editing the QAQC Page" on page 183.
MSD Concentration	Matrix spike duplicate concentration.
MSD % Received	Matrix spike duplicate concentration percentage.
RPD	Matrix spike relative percentage difference.
Max RPD	Maximum relative percentage difference as specified in the master method. See the Lab Control section in "Editing the QAQC Page" on page 183.
Number of Rec Failures	Number of matrix spike and matrix spike duplicate failures.
Number of RPD Failures	Number of relative percentage difference failures.

Note For MSMSD batch reports, the active view peak graphics are shown only when you click a field pertaining to a sample, such as Unknown, MS, or MSD concentration fields.

Table 97. Quantitation Report Active View columns (Sheet 1 of 2)

Column	Description
RT	Retention time for the peak. The time after injection when the compound elutes. The total time that the compound is retained on the column.
QIon	Mass range for the 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 150.
Response	Sum of all quantitative peak response values for the compound.

Table 97. Quantitation Report Active View columns (Sheet 2 of 2)

Column	Description
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 173.
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 173.

Table 98. 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 150.
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. See Local Method View. A local method is a copy of a master method associated with a batch. Local methods are named *BatchName_MasterMethodName*.

❖ **To open the Local Method View**

1. Do one of the following:

   From the dashboard, click **Analysis**.

   –or–

   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 100.

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**.
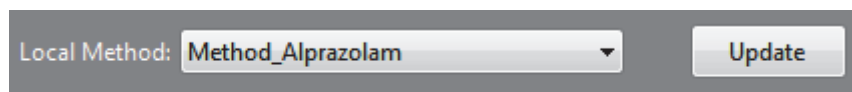
The application overwrites the local method with the master method of the same name. You can use this feature to overwrite an edited local method with the original master method or to overwrite the local method with an updated master method.

Figure 107. Local Method View

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 421. 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 331.

Follow these procedures:

- To create a new batch template
- To specify active compounds
- To specify template method information
- To specify active compounds
- 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 report options
- To specify active compounds

❖ **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.
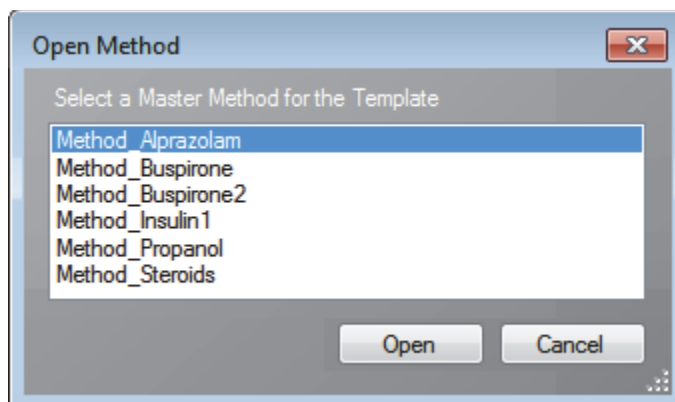
2. Select a master method and click **Open**.

   The Batch Template Editor opens. For detailed descriptions of all parameters, see "Batch Template Editor" on page 421.

   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.
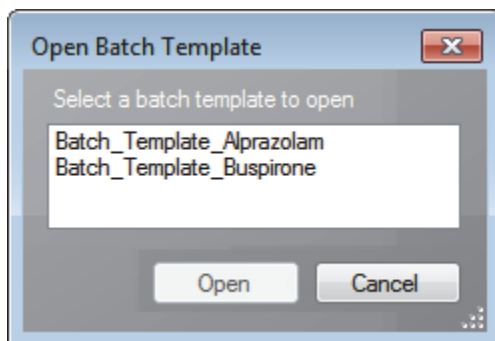
2. Select a batch template and click **Open**.

   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 421.

❖ **To specify template method information**

1. From the Project list, select a project name.

2. From the Subproject list, select a subproject name.

   Tip If there are no projects or subprojects to select, go to the Project Administration view of the Configuration mode and create a new subproject. See "Project Administration" on page 49.

3. To change the current method, click **Select Method** and select a new method.
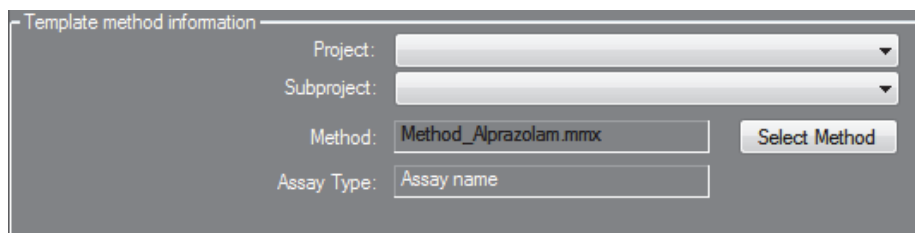
❖ **To add a sample to the batch**

Right-click and choose **Add Sample** from the shortcut menu, or click the add sample icon, ![add sample icon].

The application adds a new, Unknown 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, Unknown sample.

2. Right-click and choose **Insert Sample** from the shortcut menu.

   The application inserts a new, Unknown sample above the selected sample.

	Sample type	Level	Sample ID	Sample name	Comment	Repeat sample count
	Unknown ▼					1
✏	Matrix Blank ▼					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, ![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		
Matrix Blank	Solvent	Unknown/TIC
Cal Std	Chk Std	Unknown
LCS	MDL	MS
LCSD	Method Val	MSD
Tune	Tune/Breakdown	Breakdown

2. For each Chk Std or Cal Std 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 Master Method" on page 119.

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 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.
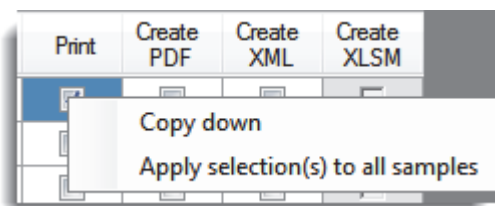
   All check boxes in the column below the selected cell duplicate the selected or cleared state of the selected cell.

   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.

Example

The application copies selected report output formats from the first sample.

	Sample type		Level	Sample ID	Sample name	Comment
▶	Unknown	▼				
	Matrix Blank	▼				
	Solvent	▼				

Automated Batch Reports

Sample Level	Batch Level

	Report Name	Type	Print	Create PDF	Create XML	Create XLSM
1	Blank Report	Standard	☑	☐	☐	☐
2	Chromatogram Report	Standard	☑	☐	☐	☐
▶ 3	Confirmation Report	Standard	☑	Apply selection(s) to all samples		

The application duplicates the selected report output formats to all samples in the batch.

	Sample type		Level	Sample ID	Sample name	Comment
	Unknown	▼				
▶	Matrix Blank	▼				
	Solvent	▼				

Automated Batch Reports

Sample Level	Batch Level

	Report Name	Type	Print	Create PDF	Create XML	Create XLSM
1	Blank Report	Standard	☑	☐	☐	☐
2	Chromatogram Report	Standard	☑	☐	☐	☐
▶ 3	Confirmation Report	Standard	☑	☐	☐	☐

❖ **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
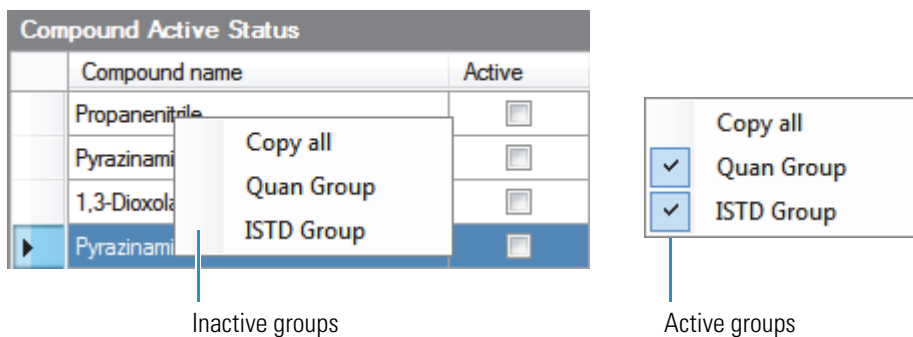
Figure 108. Batch Template Editor

Table 99. Batch Template Editor parameters (Sheet 1 of 2)

Parameter	Description
Template Method Information	
Project	The top-level project for the batch.
Subproject	The lower-level project for the batch.
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.

Table 99. Batch Template Editor parameters (Sheet 2 of 2)

Parameter	Description
Column values	
Sample Type	Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, Solvent, Cal Std, Chk Std, Unknown, Unknown/TIC, LCS, LCSD, MDL, MS, MSD, Method Val, Tune, Tune/Breakdown, or Breakdown
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.

Reports

This appendix contains information about standard and custom reports.

> **Contents**
>
> - Specifying Reports
> - Report Flags
> - Sample Standard Reports

The report engine can generate several different types of reports designed to meet the needs of the laboratory, the laboratory's customers, and key regulatory agencies that might review the results. The 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 both standard reports and custom reports.

Specifying Reports

As a user in the ITAdmin or LabDirector role, you can configure a list of reports that are available for the Method Development or Acquisition mode.

For detailed information about configuring reports in the Configuration mode, see "Specifying the Reports Configuration" on page 68.

For detailed information about specifying reports when you create a method in the Method Development mode, see "Editing the Reports Page" on page 202.

For detailed information about viewing batch reports in the Acquisition mode, see "Selecting and Reviewing Reports" on page 265.

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

The TraceFinder application can generate the following types of standard reports:
- Batch Report
- Batch Report Rev 1
- Blank Report
- Breakdown Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- Confirmation Report 2
- High Density Calibration Report
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary Report
- Tune Report

To view an example of each type of standard report, see "Sample Standard Reports" on page 430.

Custom Reports

For each custom report you generate, you can create a hardcopy printout or an Excel Macro-Enabled Workbook (.xlsm) output file. The default report description is the report name.

A user in the ITAdmin or LabDirector role can configure custom reports to generate a single report for an entire batch or 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 Long Report
- Target Screening Summary Report

Figure 109. Reports page showing standard reports

Figure 110. Reports page showing custom reports
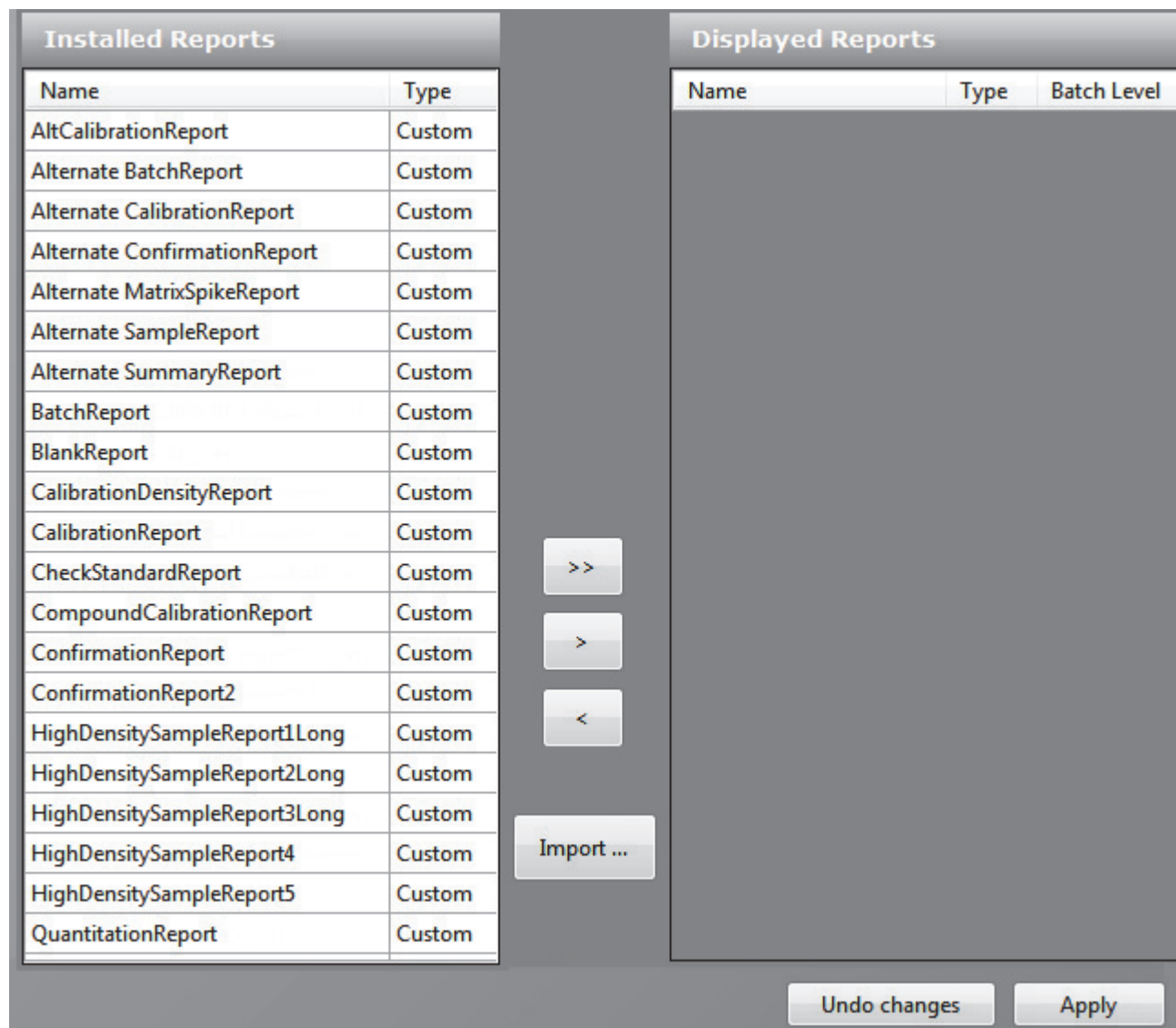
Figure 111. Reports page showing target screening reports
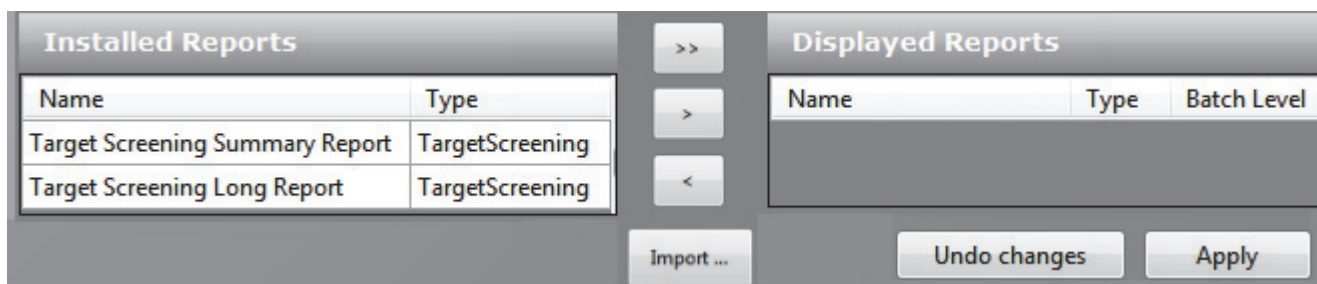
> **Note** Target screening reports are available only when you install the ToxID software and enable the target screening features. See "Enabling Optional Features" on page 88.

Report Flags

When generating or viewing a report, you might see one of the following quantification or calibration flags listed on the page.

Table 100. 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 101. 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
- Blank Report
- Breakdown Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- Confirmation Report 2
- High Density Calibration Report
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary Report

Tip To easily view reports in landscape format, choose **View > Rotate View > Clockwise** from the Adobe Acrobat™ viewer menu.

Batch Report

Batch Report

Lab Names:	Thermo Lab
Instrument:	TQU00637
User:	TQU00637\RPC
Batch:	011HPLR1

Method:	011HPLR1_PDP_040511
	PDP_040511
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
Cal File:	PDP_040511
	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	

Blank Report

Blank Report

Lab Name:	Thermo Lab
Instrument:	TQU00637
User:	TQU00637\RPC
Batch:	011HPLR1

Method:	011HPLR1_PDP_040511
	PDP_040511
Call File:	011HPLR1.calx

| Sample Name | File Date | Comment |
| LLOD_HP031711 | 3/17/2011 5:46:30 PM | |

| Vial Pos | Sample ID | File Name | Level |
| 5 | 1 | LLOD_HP031711 | N/A |

Surrogates

	RT	Qion	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units	Max Conc		Flags
Propoxur_(S)	7.69	111.10	1553885	Quadratic	0.00	5.89	PPB	5.89	PPB	3.00	Fail	b

Target Compounds

	RT	Qion	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units	Max Conc		Flags
Oxamyl_Oxime	4.32	72.10	1291350	Quadratic	0.00	12.67	PPB	12.67	PPB	6.00	Fail	b
Omethoate	4.34	183.04	540508	Quadratic	0.00	1.57	PPB	1.57	PPB	0.75	Fail	b
Formetanate	4.35	165.10	4408552	Quadratic	0.00	6.27	PPB	6.27	PPB	3.00	Fail	b
Dinotefuran	4.52	129.14	608336	Quadratic	0.00	6.80	PPB	6.80	PPB	3.00	Fail	b
Aldicarb_SO	4.51	132.05	538697	Quadratic	0.00	6.39	PPB	6.39	PPB	3.00	Fail	b
Propamocarb	4.53	102.00	750180	Quadratic	0.00	2.54	PPB	2.54	PPB	3.00	Pass	
Pymetrozine	4.56	105.10	231305	Quadratic	0.00	1.59	PPB	1.59	PPB	0.75	Fail	b
Aldicarb_SO2	4.68	148.04	842061	Quadratic	0.00	6.46	PPB	6.46	PPB	3.00	Fail	b
Oxamyl	4.77	90.00	408081	Quadratic	0.00	6.44	PPB	6.44	PPB	3.00	Fail	b
Methomyl	4.98	88.10	973424	Quadratic	0.00	17.35	PPB	17.35	PPB	6.00	Fail	b
Flonicamid	5.05	203.00	121206	Quadratic	0.00	17.91	PPB	17.91	PPB	9.00	Fail	b
ODMS	5.07	169.00	495002	Quadratic	0.00	3.18	PPB	3.18	PPB	1.50	Fail	b
5-OH_TBZ	5.12	147.10	427244	Quadratic	0.00	2.75	PPB	2.75	PPB	1.50	Fail	b
Thiamethoxam	5.12	181.10	149534	Quadratic	0.00	1.62	PPB	1.62	PPB	0.75	Fail	b
Monocrotophos	5.26	193.00	820046	Quadratic	0.00	3.22	PPB	3.22	PPB	1.50	Fail	b
Imidacloprid	5.66	209.06	611636	Quadratic	0.00	6.51	PPB	6.51	PPB	3.00	Fail	b
Clothianidin	5.71	169.10	216332	Quadratic	0.00	3.14	PPB	3.14	PPB	1.50	Fail	b
Thiabendazole	5.87	131.10	692435	Quadratic	0.00	2.99	PPB	2.99	PPB	1.50	Fail	b
3-OH_Carbofuran	6.03	163.08	1717688	Quadratic	0.00	6.43	PPB	6.43	PPB	3.00	Fail	b

Flag legend: LOD=<i<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Manually integrated ☐

Breakdown Report

Lab name:	Thermo Fisher Laboratory				Page 1 of 1
Instrument:	Thermo Scientific Instrument	**Method:**	2_bkdn1		
User:	DGT4K5D		bkdn1		
Batch:	2	**Cali File:**	2.calx		

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	level 2 = 10 ng/uL	level2	N/A		2/22/2008 9:37:36 AM	

Group name	Type	Response	% Breakdown	Max % Breakdown	Results
grp1			94.81%	80.00%	Fail
Peak@6.07	Native	5070111			
Peak@4.44	Breakdown	23600215			
Peak@4.99	Breakdown	13048952			
Peak@5.96	Breakdown	55935361			

Group name	Type	Response	% Breakdown	Max % Breakdown	Results
grp2			73.95%	20.00%	Fail
Peak@6.07	Native	5070111			
Peak@6.78	Breakdown	9920308			
Peak@6.98	Breakdown	4475695			

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	6.852e1	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	1.333e5	-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
User:	TQU00637\RPC
Batch:	011HPLR1

Method:	011HPLR1_PDP_040511
	PDP_040511
Cal 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

Calibration Report

| Lab Name: | Thermo Lab | | | | | | Page 7 of 7 |

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	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

Lab name:	Thermo Fisher Laboratory		
Instrument:	Thermo Scientific Instrument	**Method:**	Preview2_EPA536-Triazines
User:	AMER\jamie.humphries		EPA536-Triazines
Batch:	Preview2	**Cali File:**	Preview2.calx
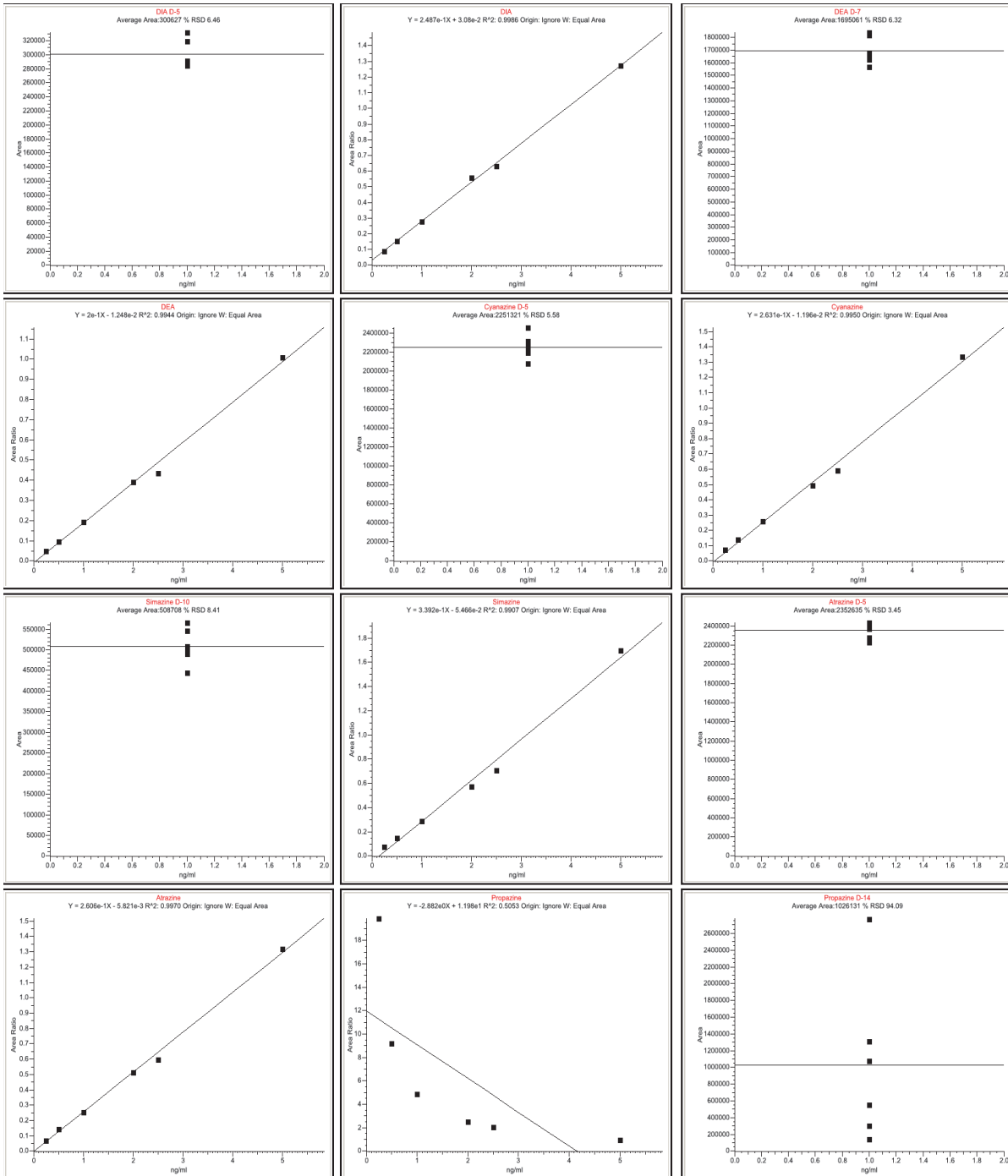
Check Standard Report

Check Standard Report

Lab Name:	Thermo 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	25	L2XLOQ_HP031711_02	2XLOQ	L2XLOQ_HP031711	3/18/2011 1:45:29 AM	

Compound	Curve Type	Daily RF	Mean RF	Min RF	RF %D	Max RF %D	QC Amt	Calc Amt	Amt %D	Max Amt %D	Flag
Oxamyl_Oxime	Q			0.000			80.00	79.12	-1.11	20.00	**Pass**
Omethoate	Q			0.000			9.91	9.90	-0.08	20.00	**Pass**
Formetanate	Q			0.000			40.10	39.56	-1.34	20.00	**Pass**
Dinotefuran	Q			0.000			40.00	41.32	3.31	20.00	**Pass**
Aldicarb_SO	Q			0.000			40.00	39.04	-2.40	20.00	**Pass**
Propamocarb	Q			0.000			40.00	31.53	-21.18 *	20.00	**Fail**
Pymetrozine	Q			0.000			10.00	10.38	3.81	20.00	**Pass**
Aldicarb_SO2	Q			0.000			40.20	39.44	-1.88	20.00	**Pass**
Oxamyl	Q			0.000			40.00	39.28	-1.80	20.00	**Pass**
Methomyl	Q			0.000			80.00	85.06	6.33	20.00	**Pass**
Flonicamid	Q			0.000			120.00	112.98	-5.85	20.00	**Pass**
ODMS	Q			0.000			20.00	19.88	-0.58	20.00	**Pass**
5-OH_TBZ	Q			0.000			20.00	19.03	-4.83	20.00	**Pass**
Thiamethoxam	Q			0.000			10.00	9.86	-1.41	20.00	**Pass**
Monocrotophos	Q			0.000			20.00	19.81	-0.95	20.00	**Pass**
Imidacloprid	Q			0.000			40.00	39.44	-1.41	20.00	**Pass**
Clothianidin	Q			0.000			20.00	19.84	-0.81	20.00	**Pass**
Thiabendazole	Q			0.000			20.00	19.59	-2.04	20.00	**Pass**
3-OH_Carbofuran	Q			0.000			40.00	38.93	-2.68	20.00	**Pass**
Acetamiprid	Q			0.000			10.00	9.75	-2.53	20.00	**Pass**
Cymoxanil	Q			0.000			40.00	39.53	-1.18	20.00	**Pass**
Thiacloprid	Q			0.000			10.00	9.90	-1.01	20.00	**Pass**
Methidathion_OA	Q			0.000			40.00	39.14	-2.15	20.00	**Pass**
Aldicarb	Q			0.000			40.00	38.68	-3.31	20.00	**Pass**
Azinphos_Me_OA	Q			0.000			40.00	39.52	-1.20	20.00	**Pass**
Metribuzin	Q			0.000			20.00	19.88	-0.59	20.00	**Pass**
Simazine	Q			0.000			20.00	20.38	1.88	20.00	**Pass**
Propoxur_(S)	Q			0.000			40.00	40.08	0.19	20.00	**Pass**
Pirimicarb	Q			0.000			80.00	79.60	-0.50	20.00	**Pass**
Bendiocarb	Q			0.000			20.00	19.71	-1.43	20.00	**Pass**
Carbofuran	Q			0.000			20.00	19.76	-1.19	20.00	**Pass**
Fenamiphos_SO	Q			0.000			20.00	18.77	-6.16	20.00	**Pass**

Manually Integrated [ ]   * = Fail;Curve Type: A=Average RF; L=Linear; Q=Quadratic;R=Recovery limits exceeded

Chromatogram Report

Lab Name:	Thermo Lab				Page 1 of 1	
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:	TQU00637.RPC
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
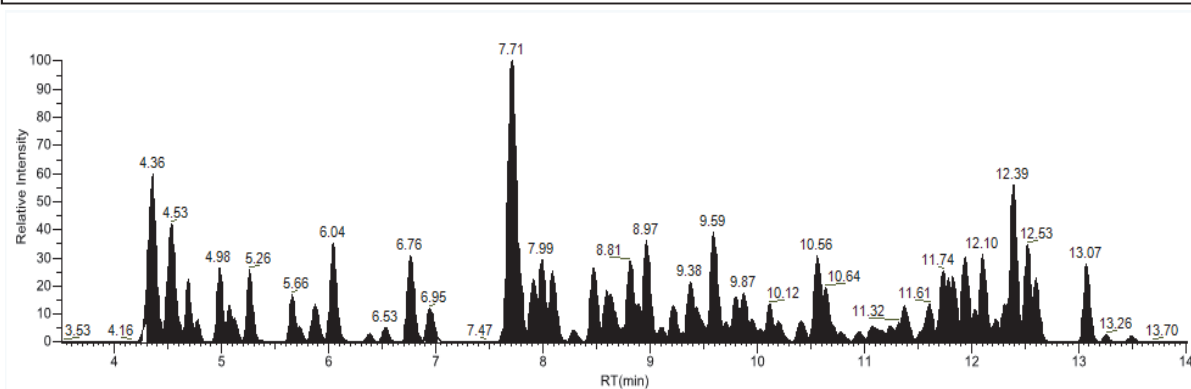
Level	Std Amount	Std Area	IS Amount	IS Area	Response factor	Calc Amt	Units	% CV	% RSD
1XLOQ	20.00	1957462			97873.106	22.01	PPB	N/A	N/A
2XLOQ	40.00	3754131			93853.284	42.58	PPB	N/A	N/A
4XLOQ	80.00	7124741			89059.260	82.22	PPB	N/A	N/A
6XLOQ	120.00	10430815			86923.457	122.54	PPB	N/A	N/A
10XLOQ	200.00	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

Compound Calibration Report

Lab Name:	Thermo Lab		
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	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	

Calibration Flags: D =RSD, F = Response factor, R = R Squared, A = Amount

Manually Integrated:

Compound Calibration Report - Alternate

Lab Name: Thermo Lab
Instrument: TQU00637
User: TQU0637\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	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	

Dinotefuran

	Injected	Sample
Conc:	642.34 PPB	642.34 PPB

Retention Time:	4.52
Area:	41994838
Height:	8893885

Quan Ion: 203.11->129.14
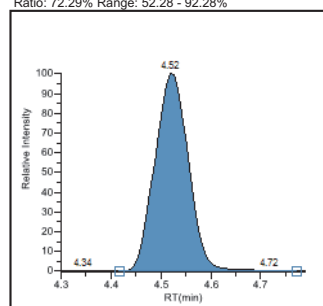
Qual Ion 1: 203.11->114.15
Ratio: 72.29% Range: 52.28 - 92.28%

Calibration Curve

Dinotefuran
$Y = -3.798e1X^2 + 8.978e4X; R^2: 0.9995;$ Origin: Force; W: Equal; Area

MS-Data

L32XLOQ_HP031711 - Dinotefuran 4.52

MS-Reference   X:\Thermo\TraceFinder\1.1\Projects\Default\Default\011HPLR1\Data\L32XLOQ_HP031711.raw

MS - Method

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					Page 1 of 1
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	

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
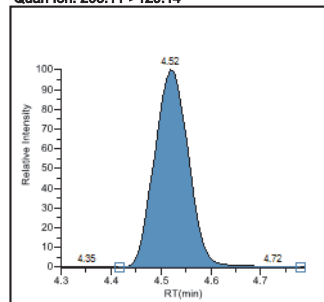
Qual Ion 1: 203.11->114.15
Ratio: 72.29% Range: 52.28 - 92.28%
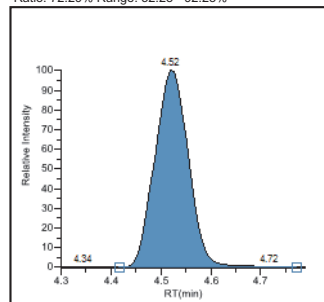
MS-Data
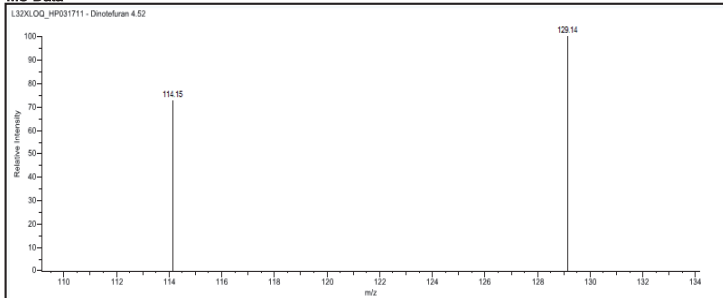
MS-Reference   hermo\TraceFinder\1.1\Projects\Default\Default\011HPLR1\Data\L32XLOQ_HP031711.raw
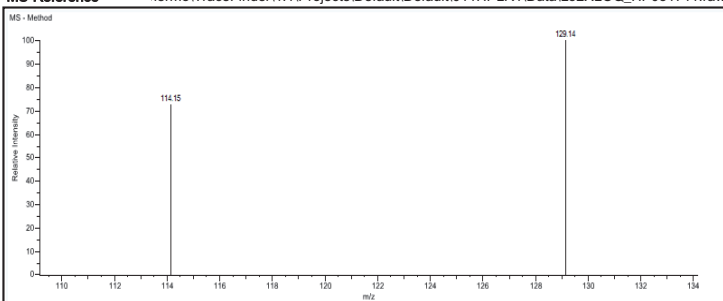
Overlay

High Density Calibration Report

High Density Calibration Report

Lab Name: Thermo Lab

Instrument: TQU00637

User: TQU00637\RPC

Batch: 011HPLR1

Method: 011HPLR1_PDP_040511

PDP_040511

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

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
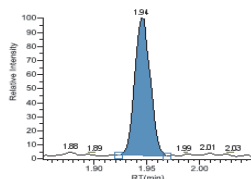
Qual m/z: 473.20
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %

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	**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	

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
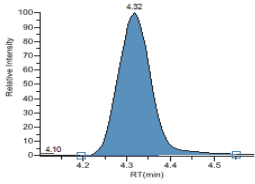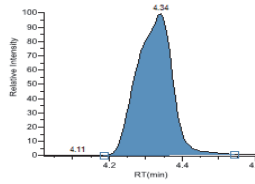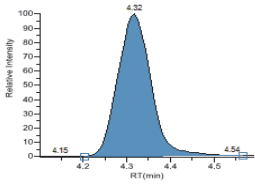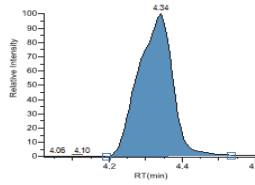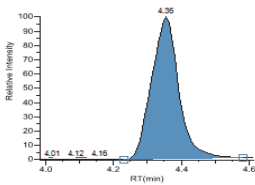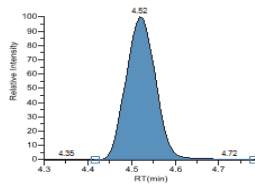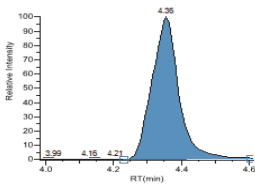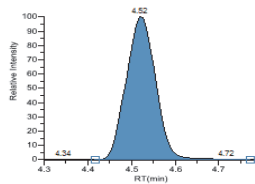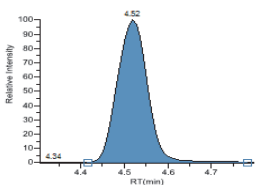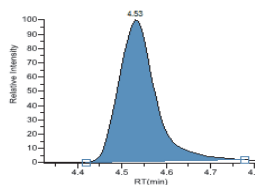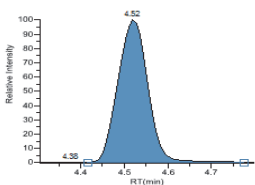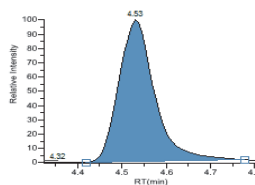
High Density Sample Report 2 Long

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: 4.32min (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 %

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
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 Long

Lab Name:	Thermo Lab			Page 1 of 40
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

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						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	

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:	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	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

LCSLCSD Report

> **IMPORTANT** When the Sample ID is the same for an unknown sample and an LCS or LCSD sample, the unknown sample is included in the LCSLCSD report. The report information for the unknown sample is displayed as zeros.

LCSLCSD Report

Page 1 of 1

Lab name:	Thermo Fisher Laboratory
Instrument:	Thermo Scientific Instrument
User:	AMER\jamie.humphries
Batch:	Preview2

Method:	Preview2_EPA536-Triazines
	EPA536-Triazines
Cali File:	Preview2.calx

Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
Tray1:16	SampleID002	5ppb-002	N/A	D008	6/27/2007 1:25:44 AM	New Dilutions 6/26/2007 l
Tray1:9	SampleID002	500ppt-002	QC	D002	6/26/2007 9:47:43 PM	New Dilutions 6/26/2007 l
Tray1:3	SampleID002	Cal002	c2	D002	6/26/2007 6:09:47 PM	New Dilutions 6/26/2007 l
Tray1:15	SampleID008	5ppb-001	N/A	D008	6/27/2007 12:54:35 AM	New Dilutions 6/26/2007 l
Tray1:8	SampleID008	500ppt-001	QC	D008	6/26/2007 9:16:35 PM	New Dilutions 6/26/2007 l

SampleID002

Compound	Spike Amt	Lower Limit %	Upper Limit %	LCSD Conc	% Rec	RPD	Max RPD	Rec Fails	RPD Fails
DIA	0.500	50.00	150.00	4.712	0.00	50.00	50.00	0	0
DEA	0.500	50.00	150.00	5.065	0.00	50.00	50.00	0	0
Cyanazine	0.500	50.00	150.00	5.127	0.00	50.00	50.00	0	0
Simazine	0.500	50.00	150.00	4.862	0.00	50.00	50.00	0	0
Atrazine	0.500	50.00	150.00	5.184	0.00	50.00	50.00	0	0
Propazine	0.500	50.00	150.00	3.829	0.00	50.00	50.00	0	0

SampleID008

Compound	Spike Amt	LCS Conc	% Rec	Lower Limit %	Upper Limit %	LCSD Conc	% Rec	RPD	Max RPD	Rec Fails	RPD Fails
DIA	0.500	4.754	0.00	50.00	150.00	4.712	0.00	0.00	50.00	0	0
DEA	0.500	4.960	0.00	50.00	150.00	5.065	0.00	0.00	50.00	0	0
Cyanazine	0.500	5.218	0.00	50.00	150.00	5.127	0.00	0.00	50.00	0	0
Simazine	0.500	4.839	0.00	50.00	150.00	4.862	0.00	0.00	50.00	0	0
Atrazine	0.500	5.178	0.00	50.00	150.00	5.184	0.00	0.00	50.00	0	0
Propazine	0.500	3.829	0.00	50.00	150.00	3.829	0.00	0.00	50.00	0	0

Manually integrated

Manual Integration Report

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	

3-OH_Carbofuran
m/z: 163.08
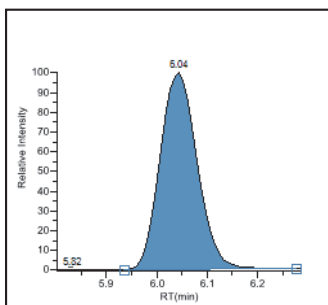
Method Integration

Apex RT:	6.04
Height:	30046630
Area:	148721201
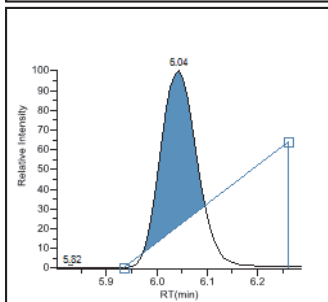
Manual Integration

Apex RT:	6.04
Height:	23956657
Area:	94907912

Method Detection Limit Report

Lab name:	Thermo Fisher Laboratory
Instrument:	Thermo Scientific Instrument
User:	AMER\jamie.humphries
Batch:	Preview2

Method: Preview2_EPA536-Triazines
EPA536-Triazines
Cali File: Preview2.calx

Method Detection Limit Summary

Compound	Avg Conc	Std Dev	t-stat	% RSD	MDL	
DIA D-5	290218	0		0.00		IS
DIA	0.095	0.000	0.000	0.00	0.000	<<<
DEA D-7	1704578	0		0.00		IS
DEA	0.065	0.000	0.000	0.00	0.000	<<<
Cyanazine D-5	2204710	0		0.00		IS
Cyanazine	0.062	0.000	0.000	0.00	0.000	<<<
Simazine D-10	513521	0		0.00		IS
Simazine	0.168	0.000	0.000	0.00	0.000	<<<
Atrazine D-5	2292164	0		0.00		IS
Atrazine	0.023	0.000	0.000	0.00	0.000	<<<
Propazine	-1069.216	0.000	0.000	0.00	0.000	<<<
Propazine D-14	826	0		0.00		IS

Manually integrated [   ]

Method Detection Limit Report

Lab name:	Thermo Fisher Laboratory
Instrument:	Thermo Scientific Instrument
User:	AMER\jamie.humphries
Batch:	Preview2

Method:	Preview2_EPA536-Triazines
	EPA536-Triazines
Cali File:	Preview2.calx

Method Validation Report Data

Compound	1
DIA D-5	290218
DIA	0.095
DEA D-7	1704578
DEA	0.065
Cyanazine D-5	2204710
Cyanazine	0.062
Simazine D-10	513521
Simazine	0.168
Atrazine D-5	2292164
Atrazine	0.023
Propazine	-1069.216
Propazine D-14	826

Manually integrated ⬜

Method Detection Limit Report

Lab name:	Thermo Fisher Laboratory		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
Tray1:1	SampleID007	Cal007	N/A	D007	6/26/2007 8:45:28 PM	New Dilutions 6/26/2007 F

Manually integrated

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 1 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

Compound Identification:

Compound	Quan mass	RT	Window	View width	Use as reference	Reference compound
Int_Std	380.20	1.94	10.00	0.40	Yes	
Drug_A	371.20	1.95	10.00	0.40	No	Int_Std

Method name:	Drug_A_Drug_A		Page number:	Page 2 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

Compound Calibration:

Compound	Response	Calibration	Curve type	Weighting	Origin	Units	ISTD Name	ISTD Units
Drug_A	Area	Internal	Linear	Equal	Ignore	ng/mL	Int_Std	ng/mL

Method name:	Drug_A_Drug_A		Page number:	Page 3 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

QAQC Limits:

Compound	LOD	LOQ	Cutoff	ULOL	Carryover
Drug_A	1.500	1.500	15.000	1000.000	1000.000

Method name:	Drug_A_Drug_A		Page number:	Page 4 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

Groups:

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 5 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

Report options:

Quan report options

Report concentration:	Always
Decimal places to be reported:	3
Show chromatogram on Quantitation report:	True
Display valid compounds only	False

Qual options

Sort Qual results by:	Search Index
Enable limiting peaks:	False
Limit Peaks to :	

User interface options

Shade row when sample is outside of evaluation criteria:	False
Separate ion overlay display :	True
Use alternative calibration report format:	False
Display quan flags and legend	True

ToxLab Forms settings

Quan flags

Flag values below LOD:	True
Flag values below LOQ:	True
Flag values above Cutoff:	True
Flag values above ULOL:	True
Flag values above Carryover:	True
Flag values between LOD and LOQ:	True

Calculated amount option

Calculate concentration as:	Truncated

Tune time tracking options

Enable tune time tracking:	False
Tune file lifetime (hrs):	N/A

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 6 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

QAQC Calibration:

Compound	Max RSD (%)	Min RF	R^2 threshold	Max amt diff (%)
Drug_A	20.00	0.00	0.990	20.000

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 7 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

QAQC QC Check:

Compound	Max RF diff (%)	Min RF
Drug_A	20.00	0.000

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 8 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

QAQC Negative:

Compound	Criterion	Max value
Drug_A	% of LOD	1.500

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 9 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

QAQC ISTD:

Compound	Min recovery (%)	Max recovery (%)	Min RT (-min)	Max RT (+min)
Int_Std	50.00	150.00	0.25	0.25

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 10 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

QAQC Solvent Blank:

Compound	Method	Upper Limit %
Int_Std	None	
Drug_A	Quan Ion RT	0

Method Report

Method name:	Drug_A_Drug_A		Page number:	Page 11 of 11
Master method name:	Drug_A			
Current calibration file:	Drug_A.calx			
Assay type:	Drug_A	Ion range calc method:	Average	
Inj vol:	1.000			
Instrument method:	20x			

QAQC Hydrolysis:

CompoundName	EvaluationMethod	LowerLimit	UpperLimit
Drug_A	Range	15.000	23.000

Method Validation Report

Lab name:	Thermo Fisher Laboratory
Instrument:	Thermo Scientific Instrument
User:	AMER\jamie.humphries
Batch:	Preview2

Page 1 of 3

Method:	Preview2_EPA536-Triazines
	EPA536-Triazines
Cali File:	Preview2.calx

Method Validation Summary

Compound	Avg Conc	Theo Conc	% Diff	Min Conc	Max Conc	% RSD	Max % RSD	
DIA D-5	295652					0.00		IS
DIA	0.358	0.500	-28.34	0.250	0.750	0.00	20.00	
DEA D-7	1778658					0.00		IS
DEA	0.602	0.500	20.45	0.250	0.750	0.00	20.00	
Cyanazine D-5	2224244					0.00		IS
Cyanazine	0.565	0.500	12.90	0.250	0.750	0.00	20.00	
Simazine D-10	505462					0.00		IS
Simazine	0.607	0.500	21.49	0.250	0.750	0.00	20.00	
Atrazine D-5	2334865					0.00		IS
Atrazine	0.512	0.500	2.46	0.250	0.750	0.00	20.00	
Propazine	0.757	0.500	51.41	0.250	0.750	0.00	20.00 <<<	
Propazine D-14	272050					0.00		IS

Manually integrated [　　　　]   **<<< = Failure**

Method Validation Report

Lab name:	Thermo Fisher Laboratory
Instrument:	Thermo Scientific Instrument
User:	AMER\jamie.humphries
Batch:	Preview2

Method:	Preview2_EPA536-Triazines
	EPA536-Triazines
Cali File:	Preview2.calx

Method Validation Report Data

Compound	1
DIA D-5	295652
DIA	0.358
DEA D-7	1778658
DEA	0.602
Cyanazine D-5	2224244
Cyanazine	0.565
Simazine D-10	505462
Simazine	0.607
Atrazine D-5	2334865
Atrazine	0.512
Propazine	0.757
Propazine D-14	272050

Manually integrated ▭

<<< = Failure

Method Validation Report

Lab name:	Thermo Fisher Laboratory			
				Page 3 of 3

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

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

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

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

Quantitation Report

Lab Name: Thermo Lab
Instrument: TQU00637
User: TQU0637RPC
Batch: 011HPLR1

Quantitation Report

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	

C:\Thermo\TraceFinder\1.1\Projects\Default\Default\011HPLR1\Data\L32XLOQ_HP031711.raw
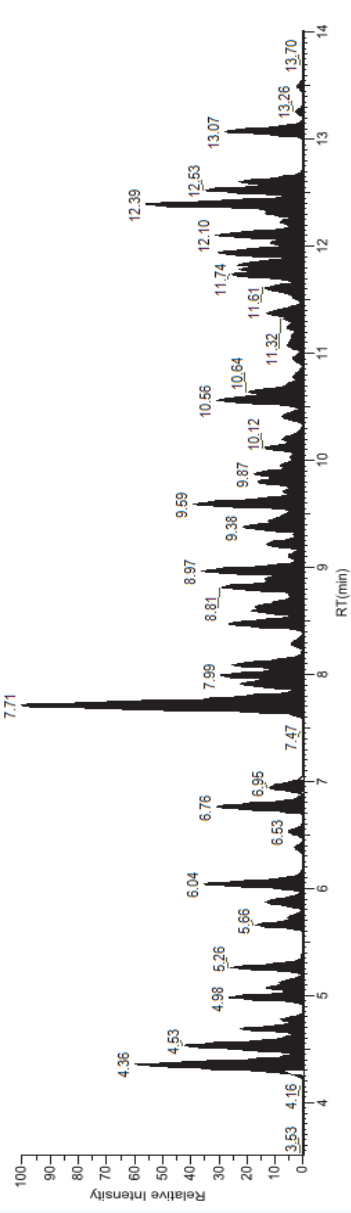
Surrogates

	RT	Qlon	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units	Flags
Propoxur_(S)	7.70	111.10	138563122	Quadratic	0.00	640.78	PPB	640.78	PPB	

Target Compounds

	RT	Qlon	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units	Flags
Oxamyl_Oxime	4.32	72.10	115624994	Quadratic	0.00	1280.93	PPB	1280.93	PPB	
Omethoate	4.34	183.04	47692071	Quadratic	0.00	158.19	PPB	158.19	PPB	
Formetanate	4.36	165.10	418192129	Quadratic	0.00	642.46	PPB	642.46	PPB	
Dinotefuran	4.52	129.14	41994838	Quadratic	0.00	642.34	PPB	642.34	PPB	
Aldicarb_SO	4.52	132.05	46055255	Quadratic	0.00	641.29	PPB	641.29	PPB	
Propamocarb	4.53	102.00	233040768	Quadratic	0.00	638.19	PPB	638.19	PPB	
Pymetrozine	4.57	105.10	19185279	Quadratic	0.00	160.15	PPB	160.15	PPB	
Aldicarb_SO2	4.69	148.04	73839209	Quadratic	0.00	643.38	PPB	643.38	PPB	
Oxamyl	4.78	90.00	36777897	Quadratic	0.00	640.38	PPB	640.38	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

Manually Integrated

Quantitation Report - 2

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:	TQU00637rRPC
Instr:	TQU00637
Response Via:	011HPLR1.calx

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\L32XL OQ_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   PDP_040511

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	

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6/2/2011 11:40:51AM

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

PDP_040511

Manually integrated

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 [ ]

Surrogate Recovery Report

Page 1 of 1

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	

Compound	Conc Added	Conc Recovered	% Recovered	Limits	
Propoxur_(S)	40.00	640.78	1601.95	83.00 - 121.00	**R**

Manually Integrated [   ]   R=Recovery limits exceeded

TIC Report

Page 1 of 1

Lab Name:	Default Laboratory			
Instrument:	Thermo Scientific Instrument	**Method:**	jbe_test_5_jbe_test_q2_c1	
User:	MS110434\ITQ		jbe_test_q2_c1	
Batch:	jbe_test_5	**Cali File:**	jbe_test_5.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
4	6	spl07	N/A		3/15/2011 3:24:54 PM	L135 20 ppm

Peak:	Retention Time	Area	Height	Inj Estimate	In-sample Est	Flag
m-Methoxybenzoic acid, hexadecyl	13.93	224271083	65488496	0.000	0.000	

Compound	CAS Number	Library	Entry	Match Prob	Search Index	Rev Search Index	Formula	Weight
m-Methoxybenzoic acid, hexadecyl	111722113	mainlib	113559	9	565	984	C24H40O3	376
4-Methoxyphenyl octadecyl ether	0	mainlib	88087	7	562	981	C25H44O2	376
1,3-Benzenediol, o-(2-furoyl)-o'-(2-t	0	mainlib	128603	6	556	975	C19H11F3O5	376
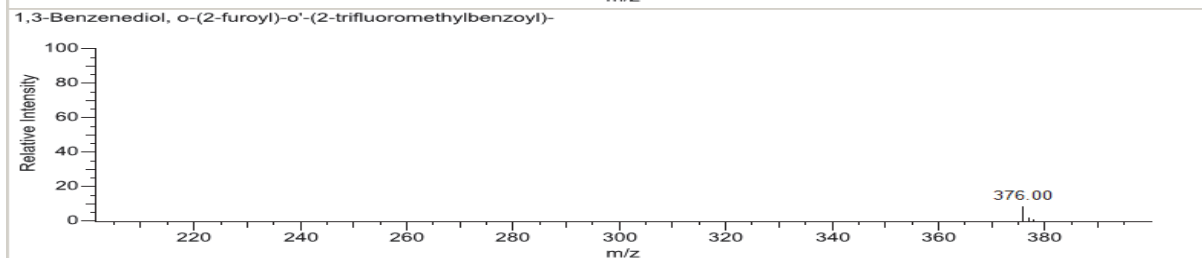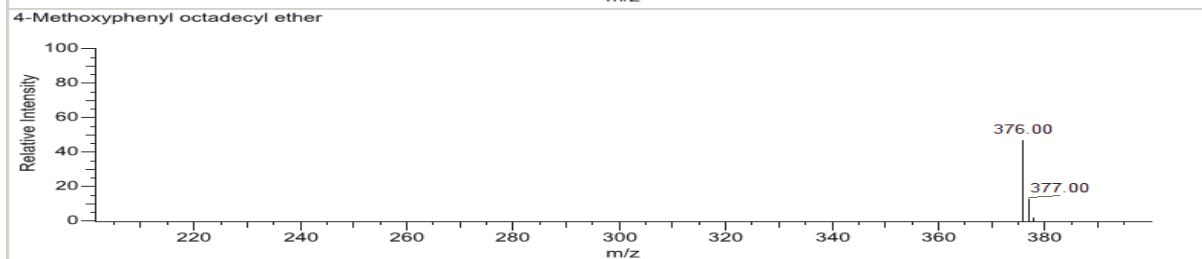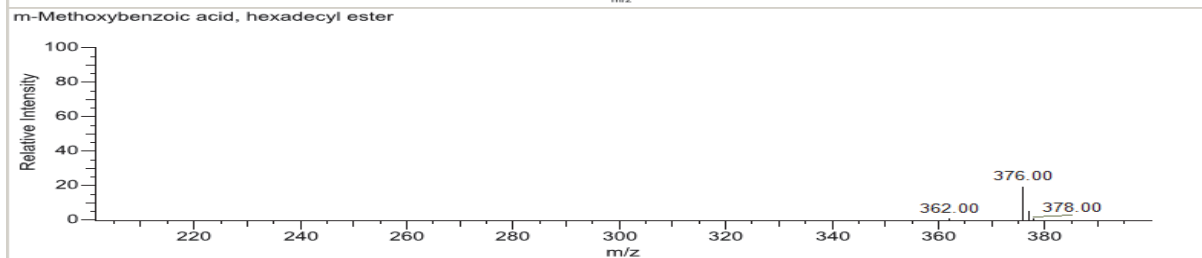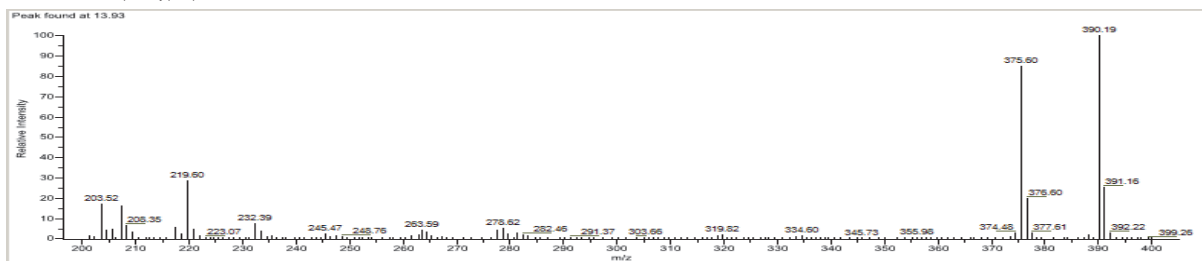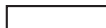
Manually integrated ☐   Flag legend: P = Library entry selected manually

TIC Summary Report

Lab Name:	Default Laboratory			
Instrument:	Thermo Scientific Instrument	Method:	jbe_test_5_jbe_test_q2_c1	
User:	MS110434\ITQ		jbe_test_q2_c1	
Batch:	jbe_test_5	Cali File:	jbe_test_5.calx	

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
4	6	spl07	N/A		3/15/2011 3:24:54 PM	L135 20 ppm

Internal Standards

				Injected		Sample	
Internal Standard	ISTD#	RT	Response	Conc	Units	Conc	Units

Qualitatively-identified Compounds

				Injected		Sample		
Compound	Uses ISTD#	RT	Response	Conc	Units	Conc	Units	Flag
8-Chloro-5-quinolinecarboxylic acid		2.78	566067	0.000		0.000		
8-Chloro-5-quinolinecarboxylic acid		2.90	164769	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		3.07	2136999	0.000		0.000		
Cyclotetrasiloxane, octamethyl-		4.46	1139812	0.000		0.000		
Benzaldehyde, 2,5-bis[(trimethylsilyl)oxy]-		5.44	10912	0.000		0.000		
Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester		5.80	87135	0.000		0.000		
Silicic acid, diethyl bis(trimethylsilyl) ester		7.18	14550	0.000		0.000		
Quinoline, 2-chloro-6-methoxy-4-methyl-		7.74	10864	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		8.43	10854	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		9.40	10900	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		11.02	200098	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		11.02	27413	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		11.08	69527	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		11.13	313964	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		11.33	35676	0.000		0.000		
Padimate O		11.44	843015	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		11.52	13886	0.000		0.000		
Cyclohexa-2,5-diene-1,4-dione, 2-methyl-5-(4-morpholinyl)-		11.91	413305	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		11.96	523374	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		12.07	206827	0.000		0.000		
5-Acetamido-4,7-dioxo-4,7-dihydrobenzofurazan		12.11	91980	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		12.13	43177	0.000		0.000		
5-Acetamido-4,7-dioxo-4,7-dihydrobenzofurazan		12.33	15408	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		12.48	15166	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		12.51	16599	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		12.58	12284	0.000		0.000		
5-Acetamido-4,7-dioxo-4,7-dihydrobenzofurazan		12.81	16241	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		12.84	11652	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		12.86	12466	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		12.90	57442	0.000		0.000		
1,1,1,3,5,5,5-Heptamethyltrisiloxane		12.97	44518	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		12.98	15734	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		13.02	35927	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		13.04	45368	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		13.10	33807	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		13.12	67005	0.000		0.000		
Cyclotrisiloxane, hexamethyl-		13.16	30617	0.000		0.000		

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.
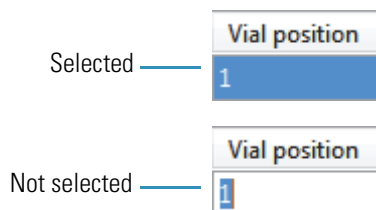
2. Right-click and choose **Copy Down** from the shortcut menu.

   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 |
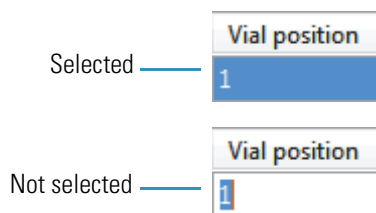
3. Right-click and choose **Fill Down** from the shortcut menu.

   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.
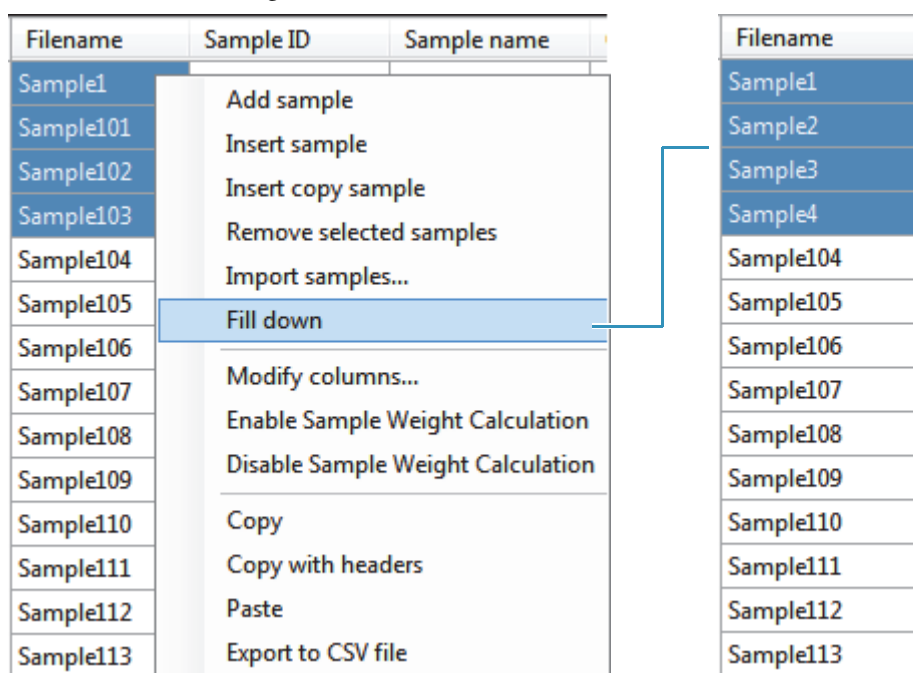
Using Filter Criteria

The filter criteria tool is available from the compound datastore in the Configuration mode and the acquisition list in the Method Development mode.

❖ **To filter the compound list**

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

   For each column, a list of filterable criteria is displayed. In all columns, your filter choices are All, Blanks, and NonBlanks. Other filter criteria are specific to the individual columns.

2. To create a custom filter based on compound values in a specific column, choose **Custom** from the column list.

   The Enter Filter Criteria dialog box opens. See " Enter Filter Criteria dialog box" on page 482.

3. From the Operator list, select an operator.

4. From the Operand list, select an operand.

5. When all conditions are defined, click **OK**.

   The complete filter string is displayed at the bottom of the dialog box, for example, chemical formula = Blanks.

> **Note** The Enter Filter Criteria dialog box is specifically named for the column on which you are filtering. In this example, the selected column is the Compound Name column.

Figure 112. Enter Filter Criteria dialog box
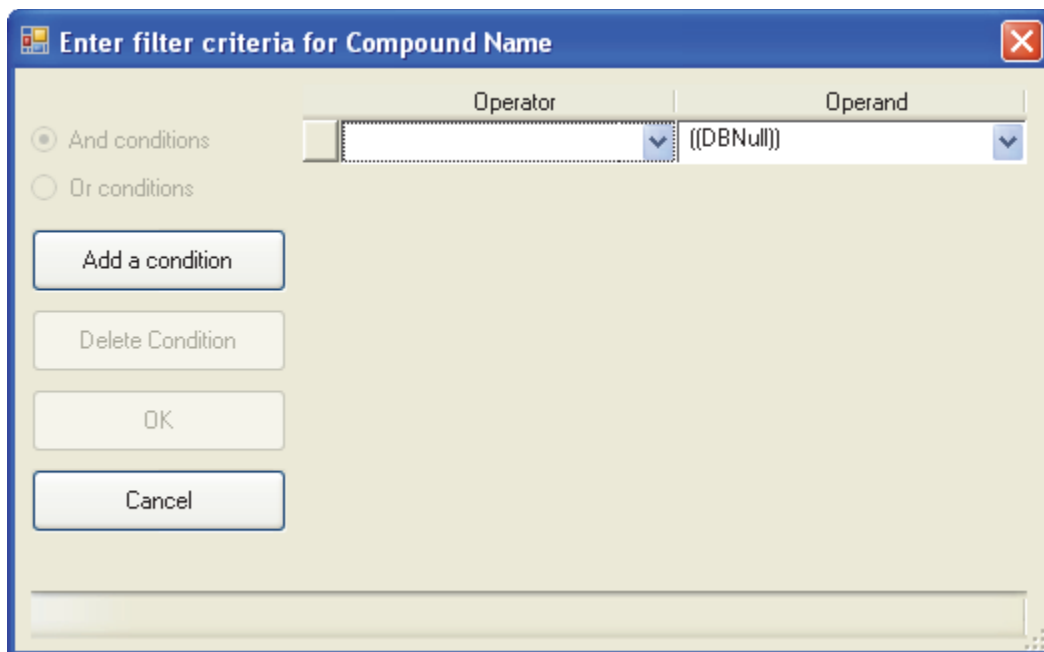
Table 102. Enter Filter Criteria dialog box parameters

Parameter	Description
And Conditions	Requires meeting all filter criteria.
Or Conditions	Requires meeting any of the specified filter criteria.
Add a Condition	Adds a new, empty condition to the filter criteria.
Delete Condition	Deletes the selected condition. Click the box at the left of the row to select the condition.
Operator	The mathematical function applied to the operand.
Operand	The arguments to which the operator is applied.

Index

Symbols

A

B

Q

R