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Preface

The TraceFinder 2.0 application is the newest application in the series of Thermo Scientific GC/MS and LC/MS analytical software.

Contents
- Related Documentation
- Special Notices
- System Requirements
- System Activation
- Contacting Us

❖ To suggest changes to documentation or to Help
Complete a brief survey about this document by clicking the link below. Thank you in advance for your help.

Related Documentation

TraceFinder documentation includes the TraceFinder User Guide and four quick reference guides as PDF files that you can access from the Windows™ Start menu or from within the TraceFinder application.

❖ To view TraceFinder documents using the Start menu
Go to Start > All Programs > Thermo TraceFinder > Manuals and choose one of the following documents:
- 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 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.

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

<table>
<thead>
<tr>
<th>System</th>
<th>Requirements</th>
</tr>
</thead>
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<tr>
<td>Computer</td>
<td>• 2.33 GHz processor dual core with 2 GB RAM</td>
</tr>
<tr>
<td></td>
<td>• CD/R-ROM drive</td>
</tr>
<tr>
<td></td>
<td>• Video card and monitor capable of 1280 × 1024 resolution (XGA)</td>
</tr>
<tr>
<td></td>
<td>• 75 GB available on the C: drive</td>
</tr>
<tr>
<td></td>
<td>• NTFS format</td>
</tr>
<tr>
<td>Instruments</td>
<td>Autosamplers:</td>
</tr>
<tr>
<td>(supported or required)</td>
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</tr>
<tr>
<td></td>
<td>• AS3000</td>
</tr>
<tr>
<td>GC Devices</td>
<td>• FOCUS™ GC</td>
</tr>
<tr>
<td></td>
<td>• Trace GC Ultra™</td>
</tr>
<tr>
<td>GC/MS mass spectrometers</td>
<td>• Microsoft™ Windows XP Professional SP3 or Windows 7 Professional</td>
</tr>
<tr>
<td>Software</td>
<td>• Microsoft Office 2007 SP2 or Microsoft Excel™ 2007 SP2</td>
</tr>
<tr>
<td></td>
<td>• Microsoft .NET Framework 3.5 SP 1</td>
</tr>
<tr>
<td></td>
<td>• Thermo Foundation™ 2.0 SP1</td>
</tr>
<tr>
<td></td>
<td>• Thermo Xcalibur™ 2.2 SP1</td>
</tr>
<tr>
<td></td>
<td>• Adobe™ Reader™ 10.1</td>
</tr>
<tr>
<td></td>
<td>• NIST™ 2008</td>
</tr>
</tbody>
</table>
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.

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

**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.
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.

   **User Info:**
   
   | Name:     | User     | Street Name: | 123 Main Street |
   | Company:  | Thermo Fisher Scientific | City:       | San Jose |
   | E-Mail:   | user@thermofisher.com   | Zip Code:   | 95123   |
   | Telephone:|           | County:      |          |

   **Feature Info:**
   
   | Barcode: |

   **License Text:**
   
   ```xml
   <LicenseRequest version="1.1"><UserInfos><UserInfo name="Name">User</UserInfo><UserInfo name="Company">Thermo Fisher Scientific</UserInfo><UserInfo name="Email">user@thermofisher.com</UserInfo><UserInfo name="Telephone"></UserInfo><UserInfo name="Street">123 Main Street</UserInfo><UserInfo name="City">San Jose</UserInfo><UserInfo name="Zip Code">95123</UserInfo><UserInfo name="County"></UserInfo><UserInfo name="TraceFinder Base"></UserInfo><Feature name="TraceFinder General"></Feature><Feature name="HostID"></Feature><HostID>0026b9800783 00101853d009</HostID></Feature><LicenseTerm>FEATURE TraceFinder General THERMO 1.1.23-apr-2011 uncounted TS_OK HOSTID='0026b9800783 00101853d009' SIGN='</LicenseTerm><LicenseRequest>
   ```

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

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/POQM6P62.
- 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
- TraceFinder Summary of Features
- TraceFinder Workflow
- Reporting Features

About the TraceFinder Application

The TraceFinder application targets the clinical research market, creating the workflows that laboratories use. It supports a focused workflow for specific non-bioanalytical 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 229.

- Processing (.pmd) and instrument (.meth) method files from the Xcalibur data system
  
  See “Working with Master Methods” on page 94 or “Working with Instrument Methods” on page 201.

- Compounds from files that use the datastore (.xml) format
  
  See “Adding Compounds, Quantitation Peaks, and Confirming Ions to a Datastore” on page 59.
• Batches, methods, or templates from the following applications:
  – TraceFinder 1.0
  – TraceFinder 1.1
  – EnviroLab Forms/QuanLab Forms/ToxLab Forms 2.5
  – EnviroLab Forms/QuanLab Forms/ToxLab 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\2.0\ClinTox 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

```
C:\Thermo\TraceFinder\2.0\ClinTox\Projects\ProjectA\SubProjectA1\Batch5135

- Data
- Methods
- Reports
- Batch5135.btx
- Batch5135.btx.key
```
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 clinical research applications. The application has a fully automated acquisition mode and a manual data review 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
- Acquisition mode that acts as a wizard to guide you in creating batches and running samples
- 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, QuanLab Forms, and ToxLab 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 383. Examples of standard reports (as PDF files) are also located in the C:\Thermo\TraceFinder\2.0\ClinTox\ExampleReports folder.

Standard Report Types

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

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

Target Screening Report Types

Target Screening 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 85.

- 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 the TraceFinder 2.0 button, 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.

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

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

6. Click the ToxID 2.1.2 button, and follow the instructions to install the ToxID software.
7. Click the **NIST Library** button, 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**.

8. 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 the **Example Data** button, 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 Clinical Research**.
     
     By default, user security is not enabled and the application does not require a password. To enable user security, see “User Security” on page 85.

- **To log in to the TraceFinder application (when user security is enabled)**
  1. Enter your assigned user name.
     
     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:

     ![Login Error](image)

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

  3. Click **Login**.

     The TraceFinder dashboard opens. See “TraceFinder Dashboard” on page 33.

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

Installing the TraceFinder Application

Figure 2. TraceFinder login screen

Table 1. Login screen parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Username</td>
<td>The user’s assigned user name.</td>
</tr>
<tr>
<td>Password</td>
<td>The assigned password for the user name.</td>
</tr>
<tr>
<td>Login</td>
<td>Verifies the user name and password, and displays the dashboard.</td>
</tr>
<tr>
<td>Exit TraceFinder</td>
<td>Closes the TraceFinder application without logging in.</td>
</tr>
</tbody>
</table>
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 the TraceFinder Power Modules button, 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 87.
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. Launch the XInstall executable file.
2. Click the **NIST** button.
   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, `Xcalibur.png`
   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.

   ![Image showing the Method Template Editor with QED NIST Library selected]
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 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 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 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 TraceFinder, EnviroLab Forms, QuanLab Forms, or ToxLab Forms source versions to compatible TraceFinder 2.0 target versions.

Table 2. Version compatibility

<table>
<thead>
<tr>
<th>Source</th>
<th>TraceFinder 2.0 target</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>General</td>
</tr>
<tr>
<td>TraceFinder 2.0 General</td>
<td>✓</td>
</tr>
<tr>
<td>TraceFinder 1.1 EFS</td>
<td>✓</td>
</tr>
<tr>
<td>TraceFinder 1.1 General</td>
<td>✓</td>
</tr>
<tr>
<td>TraceFinder 1.0.1</td>
<td>✓</td>
</tr>
<tr>
<td>EnviroLab Forms 3.1</td>
<td>✓</td>
</tr>
<tr>
<td>QuanLab Forms 3.1</td>
<td>✓</td>
</tr>
<tr>
<td>ToxLab Forms 3.1</td>
<td>✓</td>
</tr>
<tr>
<td>EnviroLab Forms 2.5.2</td>
<td>✓</td>
</tr>
<tr>
<td>QuanLab Forms 2.5.2</td>
<td>✓</td>
</tr>
<tr>
<td>ToxLab Forms 2.5.2</td>
<td>✓</td>
</tr>
</tbody>
</table>

To open the TraceFinder Legacy Data Converter

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

The TraceFinder Legacy Data Converter window opens.

Follow these procedures:

- To convert a method
- To convert a batch
- To convert a method template
- To convert a batch template
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 you will convert.

The Methods to be Converted list 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 list.

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 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 list, the application checks each method to see if a method with this name exists in the target folder.

- If it exists, the default new name is the old name with “_1” appended.
- If it does not exist, the default new name is blank and the converted method keeps the original 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 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 Notepad text editor window.

**Figure 3.** Sample log file for converting a method

```
====== Start Converting Method from TraceFinder 1.1 EFS to TraceFinder 2.0 EFS ========
- Converting master method from
  'C:\Thermo\TraceFinder\1.1\Methods\Sulphonamide Method\Sulphonamide Method.mmx'
- Creating master method
- Importing properties of object 'MethodData' from XML file
  'C:\Thermo\TraceFinder\1.1\Methods\Sulphonamide Method\Sulphonamide Method.mmx'
- Saving master method
- Copying instrument method
- Successfully converted master method from
  'C:\Thermo\TraceFinder\1.1\Methods\Sulphonamide Method\Sulphonamide Method.mmx'
  to 'C:\Thermo\TraceFinder\2.0\EFS\Methods\Sulphonamide Method_1\Sulphonamide Method_1.mmx'
```
2 Getting Started
Converting Legacy Data

To convert a batch

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

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

   ![TraceFinder Legacy Data Converter interface](image)

   - **Data type**: Batch
   - **Source version**: TraceFinder 1.1 General
   - **Target version**: TraceFinder 2.0 General
   - **Target drive**: C

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

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

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

   ![Batches to be Converted list](image)

   - **Convert**: 1
   - **Name**: BatchA
   - **Source Folder**: C:\Thermo\TraceFinder\1.1\Projects\Project1\SubProject1\BatchA

   IMPORTANT A valid batch file (.btx) must be inside a folder with the same name. For example:

   ```
   C:\Thermo\TraceFinder\1.1\Projects\Project1\SubProject1\BatchA
   ├── Data
   │   └── Methods
   ├── Reports
   └── BatchA.btx
   └── BatchA.btx.key
   ```

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.

   ![Source Folder icon](image)

   - **Data type**: Batch
   - **Source version**: TraceFinder 1.1 General

   ![Browse button](image)

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

<table>
<thead>
<tr>
<th>Batches to be converted</th>
<th>Target default project</th>
<th>Source Folder</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>✓</td>
<td>batch_steroids5</td>
</tr>
<tr>
<td>2</td>
<td>✓</td>
<td>batch_steroids4</td>
</tr>
<tr>
<td>3</td>
<td>✓</td>
<td>Batch_steroid...</td>
</tr>
</tbody>
</table>

4. In the Target Version list, select the version 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 list, the application checks each batch to see if a batch with this name exists in the target folder.

- If it exists, the default new name is the old name with “_1” appended.
- If it does not exist, the default new name is blank and the converted batch keeps the original 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 you will convert, and click 

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

   When the conversion process begins, the application displays a status bar and a Cancel button. You can cancel pending conversions, but not the batch that is currently converting.
When the Status column reports that a batch is successfully converted, the application writes the converted batch to the C:\Thermo\TargetVersion\Projects folder using either the original project and subproject names or the new names 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

```plaintext
== Start Converting Batch from TraceFinder 1.1 General to TraceFinder 2.0 General ==
-- Converting batch from 'C:\Thermo\TraceFinder\1.1\Projects\Default\Default\batch_steroids5\batch_steroids5.XML' to 'C:\Thermo\TraceFinder\2.0\Projects\Default\Default\batch_steroids5\batch_steroids5.xml'
-- Importing properties of object 'BatchData' from XML file
-- Importing properties of object 'SampleData' from XML file
-- Saving sample data
-- Copying raw file from 'C:\Thermo\TraceFinder\1.1\Projects\Default\Default\batch_steroids5\Data\steroids01_110504155226_rss' to 'C:\Thermo\TraceFinder\2.0\Projects\Default\Default\batch_steroids5\Data\steroids01_110504155226.rss'
-- Importing local method for 'batch_steroids5'
-- Importing properties of object 'MethodData' from XML file
-- Saving local method data for 'batch_steroids5\Method\method_steroids\batch_steroids5'
-- Copying instrument method
-- Saving batch data for 'batch_steroids5'
-- Successfully converted batch from 'C:\Thermo\TraceFinder\1.1\Projects\Default\Default\batch_steroids5\batch_steroids5.XML' to 'C:\Thermo\TraceFinder\2.0\Projects\Default\Default\batch_steroids5\batch_steroids5.xml'
```
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 you will convert.

The Method Templates to be Converted list 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 list.

      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 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 list, the application checks each method template to see if a method template with this name exists in the target folder.

• If it exists, the default new name is the old name with “_1” appended.
• If it does not exist, the default new name is blank and the converted method template keeps the original 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 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 2.0 General to TraceFinder 2.0 EFS ======
  Converting method template from 'C:\Thermo\TraceFinder\2.0\General\Templates\Methods\MethodTemplate'
  Importing properties of object 'ProcMethodTemplateData' from XML file
    'C:\Thermo\TraceFinder\2.0\General\Templates\Methods\MethodTemplate4962.pmtx'
  Saving the method template
  Successfully converted method template from 'C:\Thermo\TraceFinder\2.0\General\Templates\Methods\MethodTemplate4962.pmtx'
```
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 you will convert.

   The Batch Templates to be Converted list displays the batch templates in the Templates folder for the selected source version.

3. To convert a batch template that is not in the default list, do the following:
   a. Click the **Source Folder** icon,  

      The application adds a Source Folder box to the window.

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

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

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

      The application displays the selected folder in the Batch Templates to be Converted list.
When you select a folder that contains multiple batch template folders, the application displays all the batch templates.

<table>
<thead>
<tr>
<th>Convert</th>
<th>Name</th>
<th>Source Folder</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Batch_Template_B</td>
<td>C:\Thermo\TraceFinder\2.0\General\Templates\Batches</td>
</tr>
<tr>
<td>2</td>
<td>Batch_Template_A</td>
<td>C:\Thermo\TraceFinder\2.0\General\Templates\Batches</td>
</tr>
<tr>
<td>3</td>
<td>Batch_template_4962B</td>
<td>C:\Thermo\TraceFinder\2.0\General\Templates\Batches</td>
</tr>
</tbody>
</table>

4. In the Target Version list, select the version 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 list, the application checks each batch template to see if a batch template with this name exists in the target folder.

- If it exists, the default new name is the old name with “_1” appended.
- If it does not exist, the default new name is blank and the converted batch template keeps the original 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 you will convert, and click ![Start Converting](StartConverting.png).

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 2.0 General to TraceFinder 2.0 EFS ======
  -- Converting batch template from 'C:\Thermo\TraceFinder\2.0\General\Projects\ProjectA\SubProjectA1\Batch5247\Batch5247.btx'
  -- Importing properties of object 'BatchData' from XML file
    'C:\Thermo\TraceFinder\2.0\General\Projects\ProjectA\SubProjectA1\Batch5247\Batch5247.btx'
  -- Importing properties of object 'SampleData' from XML file
    'C:\Thermo\TraceFinder\2.0\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\2.0\General\Projects\ProjectA\SubProjectA1\Batch5247\Methods\Method2\Batch'
  -- Saving local method data for 'Batch5247_Method2'
  Successfully converted batch template from
    'C:\Thermo\TraceFinder\2.0\General\Projects\ProjectA\SubProjectA1\Batch5247\Batch5247.btx'
  to 'C:\Thermo\TraceFinder\2.0\EFS\Templates\Batches\Batch5247\Batch5247.btx'
```
Choosing a Mode

When user security is enabled, the dashboard provides the current user with options applicable to the role assigned to that user. The following table shows the available modes for each user role.

Table 3. User roles and mode access

<table>
<thead>
<tr>
<th>User role</th>
<th>Method Development</th>
<th>Acquisition</th>
<th>Analysis</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>LabDirector</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>ITAdmin</td>
<td></td>
<td></td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>Supervisor</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Technician</td>
<td></td>
<td></td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>QAQC</td>
<td></td>
<td></td>
<td></td>
<td>✓</td>
</tr>
</tbody>
</table>

**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 33.

2. To change modes from within any of the TraceFinder application modes, click a mode button in the navigation pane.
 Responsibilities of the quality management system:

- The quality management system is designed to ensure the quality of the final product.
- The system includes procedures for the control of raw materials, processes, and finished products.
- Audits are conducted to verify the effectiveness of the system.
- Corrective actions are taken in response to non-conformities.
- Records are maintained to document the quality control activities.

Process control:

- The process control system is designed to ensure that the processes are operated under controlled conditions.
- The system includes procedures for the control of equipment, software, and personnel.
- Regular reviews are conducted to verify the effectiveness of the process control system.
- Corrective actions are taken in response to process deviations.
- Records are maintained to document the process control activities.

Training:

- The training system is designed to ensure that personnel are competent to perform their assigned tasks.
- The system includes procedures for the identification of training needs, the design and delivery of training programs, and the evaluation of training effectiveness.
- Regular reviews are conducted to verify the effectiveness of the training system.
- Corrective actions are taken in response to training deficiencies.
- Records are maintained to document the training activities.

Supplier management:

- The supplier management system is designed to ensure that the quality of the purchased products and services meets the requirements.
- The system includes procedures for the selection, evaluation, and management of suppliers.
- Regular reviews are conducted to verify the effectiveness of the supplier management system.
- Corrective actions are taken in response to supplier deficiencies.
- Records are maintained to document the supplier management activities.
To watch the real-time display from the dashboard

Click **Real Time Status**.

![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 253.
TraceFinder Dashboard

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

![TraceFinder Dashboard Image]

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Real Time Status</td>
<td>Opens the real-time display for the current acquisition. The acquisition progress is displayed within the current mode window.</td>
</tr>
<tr>
<td>Help</td>
<td>Opens the TraceFinder Help.</td>
</tr>
<tr>
<td>Log Off</td>
<td>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 85.</td>
</tr>
<tr>
<td>Acquisition</td>
<td>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 87.</td>
</tr>
<tr>
<td>Analysis</td>
<td>Opens the Analysis mode where you can review batches, batch data, reports, and local methods. See Chapter 6, “Using the Analysis Mode.”</td>
</tr>
</tbody>
</table>
Choosing a Mode

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method Development</td>
<td>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.”</td>
</tr>
<tr>
<td>Configuration</td>
<td>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.”</td>
</tr>
</tbody>
</table>
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.

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.
3 Using the Configuration Mode

Figure 7. Configuration mode navigation pane

Available only to users in the LabDirector or ITAdmin role.

Table 5. Configuration mode navigation pane functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>User Administration</td>
<td>Opens the User Administration view where you can add, remove, or edit user accounts and permissions. See “User Administration” on page 37.</td>
</tr>
<tr>
<td></td>
<td>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 64.</td>
</tr>
<tr>
<td>Project Administration</td>
<td>Opens the Project Administration view where you can create and manage projects and subprojects. See “Project Administration” on page 46.</td>
</tr>
<tr>
<td>Compound Datastore</td>
<td>Opens the Compound Datastore view where you can manage the definition of compounds in the current datastore. See “Compound Datastore” on page 52.</td>
</tr>
<tr>
<td></td>
<td>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 64.</td>
</tr>
<tr>
<td>Application Configuration</td>
<td>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 64.</td>
</tr>
</tbody>
</table>
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 43.

❖ To open the User Administration view

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

   ![Configuration](Configuration.png)

   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 85.

2. Click the User Administration task pane.

   ![User Administration](UserAdministration.png)

   The User Administration view opens. See “User Administration view” on page 41.

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, ![Add User](AddUser.png).

   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 43.

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 38.

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.

   ![User Listing Table]

   **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.

![User Configuration](image)

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, .

   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 "**To edit user information**" on page 38.
Figure 8. User Administration view

Table 6. User Administration view parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Security Groups</strong></td>
<td>All permission levels defined in the TraceFinder application. For detailed descriptions of user permissions, see “Choosing User Roles” on page 43.</td>
</tr>
<tr>
<td><strong>User Listing</strong></td>
<td></td>
</tr>
<tr>
<td>Username</td>
<td>User login names.</td>
</tr>
<tr>
<td>Role</td>
<td>Security group that defines user permissions.</td>
</tr>
<tr>
<td>Account Number</td>
<td>User account numbers.</td>
</tr>
<tr>
<td>Phone Number</td>
<td>User telephone numbers.</td>
</tr>
<tr>
<td>Email Address</td>
<td>User e-mail addresses.</td>
</tr>
<tr>
<td>Enabled</td>
<td>Available or unavailable status for the user account.</td>
</tr>
<tr>
<td><strong>User</strong></td>
<td></td>
</tr>
<tr>
<td>Username</td>
<td>Login name for the current user.</td>
</tr>
<tr>
<td>Role</td>
<td>Security group that defines the current user’s permissions.</td>
</tr>
<tr>
<td>Password</td>
<td>Login password for the current user.</td>
</tr>
<tr>
<td>Full Name</td>
<td>The current user’s actual name.</td>
</tr>
<tr>
<td>Account Number</td>
<td>Optional account number for the current user.</td>
</tr>
<tr>
<td>Phone Number</td>
<td>Optional telephone number for the current user.</td>
</tr>
</tbody>
</table>
### Table 6. User Administration view parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Email Address</td>
<td>E-mail address for the current user. Used to notify user of a randomly generated password.</td>
</tr>
<tr>
<td>Enabled</td>
<td>Allows or disallows access for this user. When this user is currently logged in, disallowing takes effect after the user logs off.</td>
</tr>
<tr>
<td>Reset Password</td>
<td>Makes the password visible as a string of asterisks that you can select and change.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Icon</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Add User" /></td>
<td>Enables the fields in the User area where you can enter information for a new user.</td>
</tr>
<tr>
<td><img src="image" alt="Remove User" /></td>
<td>Deletes all information for the selected user.</td>
</tr>
<tr>
<td><img src="image" alt="Edit User" /></td>
<td>Enables the User area where you can edit any of the parameters for the selected user.</td>
</tr>
<tr>
<td><img src="image" alt="Save Changes" /></td>
<td>Adds the new parameter values to the User Listing table and disables the parameters in the User area.</td>
</tr>
<tr>
<td><img src="image" alt="Cancel Changes" /></td>
<td>Discards all new or edited information.</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>User role</th>
<th>Method</th>
<th>Development</th>
<th>Acquisition</th>
<th>Analysis</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>LabDirector</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
</tr>
<tr>
<td>ITAdmin</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Supervisor</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Technician</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td></td>
<td></td>
</tr>
<tr>
<td>QAQC</td>
<td>✔️</td>
<td>✔️</td>
<td>✔️</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**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.

   ![Configuration](image)

   The Configuration navigation pane opens. See “Configuration mode navigation pane” on page 36.

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

   ![Project Administration](image)

   The Project Administration view opens.

   | Available Drive | Drive Type | Volume Label | Free Capacity | Projects
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C:</td>
<td>Fixed</td>
<td>None</td>
<td>365.6 GB</td>
<td>Project1</td>
</tr>
<tr>
<td>T:</td>
<td>Network</td>
<td>Data Drive 0</td>
<td>914.3 GB</td>
<td>Project2</td>
</tr>
<tr>
<td>X:</td>
<td>Network</td>
<td>Storage</td>
<td>0 GB</td>
<td>Project3</td>
</tr>
</tbody>
</table>

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

   C:\Thermo\TraceFinder\2.0\ClinTox\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 display**
- **To refresh the drives 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:

   ![The selected drive (X) does not have a Projects directory.]

   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 49.

**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 display**
  
  Clear the check box in the Show column.
  
  The application does not list the hidden drive in drive lists. You cannot hide the default drive.

- **To refresh the drives 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 have 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\2.0\ClinTox\Projects folder.

If you installed the TraceFinder example data, the main Projects folder includes an Examples 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.

   ![Projects]

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 you want to delete.

![Project tree]

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.

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.

![Copy hierarchy dialog]

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, Quantitation Peaks, and Confirming Ions to a Datastore
- Choosing Experiment Types

For a description of all the parameters in the Compound Datastore view, see “Compound Datastore view” on page 56.
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 84.

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 36.

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 56.
Using the Configuration Mode

Compound Datastore

To open a compound datastore

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

   The Open Compound Datastore dialog box opens.

   ![Open Compound Datastore dialog box](image)

2. Double-click the name of the datastore you want to open.

   The selected datastore opens in the Compound Datastore view. See “Compound Datastore view” on page 56.

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 (following the instructions, To import compounds), or you can manually add compounds one at a time (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\2.0\ClinTox\Databases\filename.xml

   If the datastore contains any compounds that do not have associated quantitation peaks, the Invalid Compound Datastore Not Saved dialog box opens, listing the compounds.

   ![Invalid Compound Datastore not saved](image)
2. To add a quantitation peak row to the listed compounds, click **Continue**. The application returns you to the Compound Datastore view.

3. Add quantitation peaks to the incomplete compounds before you save the datastore. See “To add a quantitation peak to a compound” on page 61.

* 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 **Save**. The application stores the database as

   …\Thermo\TraceFinder\2.0\ClinTox\Databases\filename.xml

**Figure 9.** Save Compound Datastore dialog box

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compound Datastore Name</td>
<td>Lists the file name for the new datastore.</td>
</tr>
<tr>
<td>Overwrite</td>
<td>Overwrites the selected datastore.</td>
</tr>
<tr>
<td>OK</td>
<td>Writes the new datastore to the Databases folder.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Closes the dialog box and makes no changes to the datastore.</td>
</tr>
</tbody>
</table>
3 Using the Configuration Mode

Compound Datastore

Figure 10. Compound Datastore view

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function icons</strong></td>
<td></td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Adds a new compound row.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Removes the selected row and all quantitation peak and confirming ion rows within it.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Adds a new quantitation peak row to the compound. Each compound requires at least one quantitation peak.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Removes the selected row and all confirming ion rows within it.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Adds a new confirming ion row to the quantitation peak.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Removes the selected confirming ion row.</td>
</tr>
<tr>
<td><strong>Select Experiment Types To Display</strong></td>
<td>Specifies one of these experiment types that each use a different structure for the mass filter. See “Choosing Experiment Types” on page 63.</td>
</tr>
<tr>
<td>• SRM: Selected Reaction Monitoring</td>
<td></td>
</tr>
<tr>
<td>• XIC: Extracted Ion Chromatogram</td>
<td></td>
</tr>
<tr>
<td>• SIM: Single Ion Monitoring</td>
<td></td>
</tr>
<tr>
<td><strong>Compound parameters</strong></td>
<td></td>
</tr>
<tr>
<td>Compound Name</td>
<td>Alphanumeric name assigned to the compound.</td>
</tr>
<tr>
<td>Experiment Type</td>
<td>Experiment type: SRM, XIC, or SIM.</td>
</tr>
<tr>
<td>Category</td>
<td>(Optional) Alphanumeric identifier.</td>
</tr>
<tr>
<td>Ionization</td>
<td>(Optional) Alphanumeric identifier. Valid values: None, ESI, APCI, EI, CI, APPI Default: None</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>(Optional) Alphanumeric chemical identifier.</td>
</tr>
</tbody>
</table>
### Table 9. Compound Datastore view parameters (Sheet 2 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Precursor Mass</strong></td>
<td>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. In confirming ion rows, the precursor mass is a noneditable copy of the quantitation peak precursor mass. Available only for SRM experiments. Default: 0.0 Range: 10.000 to 2999.999</td>
</tr>
<tr>
<td><strong>Product Mass</strong></td>
<td>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</td>
</tr>
<tr>
<td><strong>Mass</strong></td>
<td>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</td>
</tr>
<tr>
<td><strong>Collision Energy</strong></td>
<td>The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: (-250.00) to (250.00)</td>
</tr>
<tr>
<td><strong>RT (min)</strong></td>
<td>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</td>
</tr>
<tr>
<td><strong>Window (sec)</strong></td>
<td>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</td>
</tr>
<tr>
<td><strong>Polarity</strong></td>
<td>(+) (positive) or (–) (negative)</td>
</tr>
<tr>
<td><strong>Lens</strong></td>
<td>(Optional) Range: (-400) to (400)</td>
</tr>
<tr>
<td><strong>Energy Ramp</strong></td>
<td>(Optional) Available only for SRM experiments. Range: 0.00 to 200.00</td>
</tr>
</tbody>
</table>
### Table 9. Compound Datastore view parameters  (Sheet 3 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Confirming ion parameters</strong></td>
<td></td>
</tr>
<tr>
<td>Precursor Mass</td>
<td>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 noneditable field only for SRM experiments. Default: 0.0 Range: 10.000 to 2999.999</td>
</tr>
<tr>
<td>Product Mass</td>
<td>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</td>
</tr>
<tr>
<td>Mass</td>
<td>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</td>
</tr>
<tr>
<td>Collision Energy</td>
<td>The energy used when ions collide with the collision gas. Available only for SRM experiments. Range: –250.00 to 250.00</td>
</tr>
</tbody>
</table>

Adding Compounds, Quantitation 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 quantitation peaks and confirming ions to a compound, or remove quantitation 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 quantitation peak to a compound
- To remove a quantitation peak
- To add a confirming ion to a quantitation 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 quantitation peaks and confirming ions, it lists all the peaks under a single compound name, as in this example for Monuron:

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Experiment Type</th>
<th>Category</th>
<th>Ionization</th>
<th>Chr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monuron</td>
<td>SRM</td>
<td>Class 1</td>
<td>ESI</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Precursor Mass</th>
<th>Product Mass</th>
<th>Collision Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monuron</td>
<td>199.09</td>
<td>46.182</td>
<td>16.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Precursor Mass</th>
<th>Product Mass</th>
<th>Collision Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monuron</td>
<td>199.09</td>
<td>72.105</td>
<td>16.00</td>
</tr>
<tr>
<td>Monuron</td>
<td>199.09</td>
<td>74.104</td>
<td>16.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Precursor Mass</th>
<th>Product Mass</th>
<th>Collision Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monuron</td>
<td>200.09</td>
<td>46.182</td>
<td>16.00</td>
</tr>
<tr>
<td>Monuron</td>
<td>200.09</td>
<td>72.105</td>
<td>16.00</td>
</tr>
<tr>
<td>Monuron</td>
<td>200.09</td>
<td>74.112</td>
<td>16.00</td>
</tr>
</tbody>
</table>
3 Using the Configuration Mode
Compound Datastore

To add a compound to the datastore

1. Click the Add Compound button, or right-click the compounds list and choose Add Compound from the shortcut menu.

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

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Experiment Type</th>
<th>Category</th>
<th>Ionization</th>
<th>Chemical Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>SRM</td>
<td></td>
<td></td>
<td>None</td>
<td></td>
</tr>
</tbody>
</table>

2. Click the first table cell, and enter 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 63.

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

To remove a compound

1. Select the compound row you want to delete.

2. Click the Remove Compound button, 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 quantitation 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 quantitation peak to a compound

1. Select the compound.

2. Click the Add Quan Peak button, or right-click and choose Add Quan Peak from the shortcut menu.

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

3. Enter all required parameters.

For a list of required and optional parameters, see the list of “Compound Datastore view parameters” on page 56.

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

To remove a quantitation peak

1. Select the row of the quantitation peak you want to delete.

2. Click the Remove Quan Peak button, 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 quantitation 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 quantitation peak rows.
To add a confirming ion to a quantitation peak

1. Click the **Add Confirming Ion** icon, or right-click the quantitation peak row and choose **Add Confirming Ion** from the shortcut menu.

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

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Experiment Type</th>
<th>Category</th>
</tr>
</thead>
<tbody>
<tr>
<td>NewCompound1</td>
<td>IM</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Mass</th>
<th>RT (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NewCompound1</td>
<td>111.00</td>
<td>1.100</td>
</tr>
</tbody>
</table>

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 63.

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

To remove a confirming ion

1. Select the confirming ion row 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 36.

2. Click Application Configuration.

The Application Configuration view opens.

<table>
<thead>
<tr>
<th>Page</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reports</td>
<td>See “Specifying the Reports Configuration” on page 65.</td>
</tr>
<tr>
<td>Defaults</td>
<td>See “Specifying Configuration Defaults” on page 70.</td>
</tr>
<tr>
<td>Detection</td>
<td>See “Specifying Detection Parameters” on page 72.</td>
</tr>
<tr>
<td>Optional Features</td>
<td>See “Enabling Optional Features” on page 84.</td>
</tr>
</tbody>
</table>

3. In the Application Configuration list, click the type of information 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 PDFs of report formats are located in the following folder:

C:\Thermo\TraceFinder\2.0\ClinTox\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 66.

❖ 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 separate reports 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 .xltem 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. For
descriptions of the parameters on the Reports page, see “Reports page parameters” on page 69.
Figure 11. Reports page showing standard reports

<table>
<thead>
<tr>
<th>Installed Reports</th>
<th>Type</th>
<th>Displayed Reports</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Batch Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Batch Summary Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Calibration Curve Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Calibration Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Chromatogram Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Compound Calibration Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Compound Calibration Report - Alternate</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Confirmation Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Calibration Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Internal Standard Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Internal Standard Report ...</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Sample Report 1</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Sample Report 1 Long</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Sample Report 2</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Sample Report 2 Long</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Sample Report 3</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>High Density Sample Report 3 Long</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Internal Standard Summary Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Ion Ratio Failure Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Manual Integration Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Method Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Negative Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Qualitative Peak Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Qualitative Summary Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Quality Control Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Quantitation Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Quantitation Report - 2</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Sample Report</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Sample Report Long</td>
<td>Standard</td>
<td></td>
</tr>
<tr>
<td>Solvent Blank Report</td>
<td>Standard</td>
<td></td>
</tr>
</tbody>
</table>

[Diagram showing installed reports with icons for adding, removing, and applying changes]
### Figure 12. Reports page showing custom reports

<table>
<thead>
<tr>
<th>Installed Reports</th>
<th>Displayed Reports</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Type</td>
</tr>
<tr>
<td>AllCalibrationReport</td>
<td>Custom</td>
</tr>
<tr>
<td>Alternate BatchReport</td>
<td>Custom</td>
</tr>
<tr>
<td>Alternate CalibrationReport</td>
<td>Custom</td>
</tr>
<tr>
<td>Alternate ConfirmationReport</td>
<td>Custom</td>
</tr>
<tr>
<td>Alternate MatrixSpikeReport</td>
<td>Custom</td>
</tr>
<tr>
<td>Alternate SampleReport</td>
<td>Custom</td>
</tr>
<tr>
<td>Alternate SummaryReport</td>
<td>Custom</td>
</tr>
<tr>
<td>BatchReport</td>
<td>Custom</td>
</tr>
<tr>
<td>BlankReport</td>
<td>Custom</td>
</tr>
<tr>
<td>CalibrationDensityReport</td>
<td>Custom</td>
</tr>
<tr>
<td>CalibrationReport</td>
<td>Custom</td>
</tr>
<tr>
<td>Check:StandardReport</td>
<td>Custom</td>
</tr>
<tr>
<td>CompoundCalibrationReport</td>
<td>Custom</td>
</tr>
<tr>
<td>ConfirmationReport</td>
<td>Custom</td>
</tr>
<tr>
<td>ConfirmationReport2</td>
<td>Custom</td>
</tr>
<tr>
<td>HighDensitySampleReport1Long</td>
<td>Custom</td>
</tr>
<tr>
<td>HighDensitySampleReport2Long</td>
<td>Custom</td>
</tr>
<tr>
<td>HighDensitySampleReport3Long</td>
<td>Custom</td>
</tr>
<tr>
<td>HighDensitySampleReport4</td>
<td>Custom</td>
</tr>
<tr>
<td>HighDensitySampleReport5</td>
<td>Custom</td>
</tr>
<tr>
<td>QuantiitationReport</td>
<td>Custom</td>
</tr>
<tr>
<td>SteroidAnalysisReport</td>
<td>Custom</td>
</tr>
</tbody>
</table>

### Figure 13. Reports page showing target screening reports

<table>
<thead>
<tr>
<th>Installed Reports</th>
<th>Displayed Reports</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Type</td>
</tr>
<tr>
<td>Target Screening Long Report</td>
<td>TargetScreening</td>
</tr>
<tr>
<td>Target Screening Summary Report</td>
<td>TargetScreening</td>
</tr>
</tbody>
</table>

**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 84.
### Table 11. Reports page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Installed Reports</td>
<td>All reports listed in this pane are potentially available but are not selected for use in the application.</td>
</tr>
<tr>
<td>Displayed Reports</td>
<td>All reports listed in this pane are selected for use in the application.</td>
</tr>
<tr>
<td>&gt;&gt;</td>
<td>Moves all reports from the Installed Reports list to the Displayed Reports list.</td>
</tr>
<tr>
<td>&gt;</td>
<td>Moves the selected reports from the Installed Reports list to the Displayed Reports list.</td>
</tr>
<tr>
<td>&lt;</td>
<td>Moves the selected reports from the Displayed Reports list to the Installed Reports list.</td>
</tr>
<tr>
<td>&lt;&lt;</td>
<td>Moves all reports from the Displayed Reports list to the Installed Reports list.</td>
</tr>
<tr>
<td>Import</td>
<td>Opens a browser where you can select a report file to add to the Installed Reports list.</td>
</tr>
<tr>
<td>Undo Changes</td>
<td>Returns the report selections to their original state (when you first opened this page).</td>
</tr>
<tr>
<td>Apply</td>
<td>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.</td>
</tr>
</tbody>
</table>
Specifying Configuration Defaults

Use the Application Configuration view of the Configuration mode to specify the default laboratory and instrument names, the 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 0 to 5, inclusive.
   The default mass precision is 2. The TraceFinder application uses this mass precision value 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

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” on page 73.

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 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.
### Table 12. Common peak detection parameters

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

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

Figure 15. Genesis peak detection page

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>Specifies the Genesis peak detection algorithm.</td>
</tr>
<tr>
<td>Detection Method</td>
<td>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.</td>
</tr>
<tr>
<td>Smoothing</td>
<td>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</td>
</tr>
<tr>
<td>Parameter</td>
<td>Description</td>
</tr>
<tr>
<td>----------------------------</td>
<td>--------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>S/N threshold</td>
<td>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</td>
</tr>
<tr>
<td>Enable Valley Detection</td>
<td>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.</td>
</tr>
<tr>
<td>Expected Width (sec)</td>
<td>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 ( \frac{\text{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</td>
</tr>
<tr>
<td>Constrain Peak Width</td>
<td>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.</td>
</tr>
<tr>
<td>Peak Height (%)</td>
<td>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%</td>
</tr>
<tr>
<td>Tailing Factor</td>
<td>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</td>
</tr>
<tr>
<td>Min Peak Height (S/N)</td>
<td>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</td>
</tr>
</tbody>
</table>
### Table 13. Genesis peak detection page parameters  (Sheet 3 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak S/N Cutoff</td>
<td>The peak edge is set to values below this signal-to-noise ratio. This test assumes it has found an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio. When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the TraceFinder application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 10000.0</td>
</tr>
<tr>
<td>Valley Rise (%)</td>
<td>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</td>
</tr>
<tr>
<td>Valley S/N</td>
<td>Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher. Range: 1.0 to 100.0 Default: 2.0</td>
</tr>
<tr>
<td># Background Scans</td>
<td>Number of background scans performed by the TraceFinder application.</td>
</tr>
<tr>
<td>Report Noise As</td>
<td>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.</td>
</tr>
</tbody>
</table>
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 16. ICIS peak detection page

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>Specifies the ICIS peak detection algorithm.</td>
</tr>
<tr>
<td>Detection Method</td>
<td>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.</td>
</tr>
<tr>
<td>Smoothing</td>
<td>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</td>
</tr>
</tbody>
</table>
Table 14. ICIS peak detection page parameters (Sheet 2 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Range:</th>
<th>Default:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area Noise Factor</td>
<td>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.</td>
<td>1 through 500</td>
<td>5</td>
</tr>
<tr>
<td>Peak Noise Factor</td>
<td>The noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value.</td>
<td>1 through 1000</td>
<td>10</td>
</tr>
<tr>
<td>Baseline Window</td>
<td>The TraceFinder application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value.</td>
<td>1 through 500</td>
<td>40</td>
</tr>
<tr>
<td>Constrain Peak Width</td>
<td>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.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Peak Height (%)</td>
<td>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.</td>
<td>0.0 to 100.0 %</td>
<td></td>
</tr>
<tr>
<td>Tailing Factor</td>
<td>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. The text box is active only when you select the Constrain the Peak Width check box.</td>
<td>0.5 through 9.0</td>
<td></td>
</tr>
<tr>
<td>Min Peak Height (S/n)</td>
<td>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.</td>
<td>0.0 (all peaks) through 999.0</td>
<td></td>
</tr>
<tr>
<td>Noise Method</td>
<td>The options are INCOS or Repetitive.</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>INCOS: Uses a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value.</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>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.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Table 14. ICIS peak detection page parameters (Sheet 3 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min Peak Width</td>
<td>The minimum number of scans required in a peak. The ICIS peak detection algorithm uses this value.</td>
</tr>
<tr>
<td></td>
<td>Range: 0 to 100 scans</td>
</tr>
<tr>
<td></td>
<td>Default: 3</td>
</tr>
<tr>
<td>Multiplet Resolution</td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>Range: 1 to 500 scans</td>
</tr>
<tr>
<td></td>
<td>Default: 10</td>
</tr>
<tr>
<td>Area Tail Extension</td>
<td>The number of scans past the peak endpoint to use in averaging the intensity. The ICIS peak detection algorithm uses this value.</td>
</tr>
<tr>
<td></td>
<td>Range: 0 to 100 scans</td>
</tr>
<tr>
<td></td>
<td>Default: 5</td>
</tr>
<tr>
<td>Area Scan Window</td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>Range: 0 to 100 scans</td>
</tr>
<tr>
<td></td>
<td>Default: 0</td>
</tr>
<tr>
<td>RMS</td>
<td>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.</td>
</tr>
</tbody>
</table>
Avalon Detection Method

The Avalon peak detection algorithm is designed for UV data. The Avalon peak detection algorithm also supports negative peaks.

**Figure 17.** Avalon peak detection page

```
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>Specifies the Avalon peak detection algorithm.</td>
</tr>
<tr>
<td>Detection Method</td>
<td>Highest peak: Uses the highest peak in the chromatogram for component identification.</td>
</tr>
<tr>
<td></td>
<td>Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.</td>
</tr>
<tr>
<td>Smoothing</td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>Range: Any odd integer from 1 through 15 points</td>
</tr>
<tr>
<td></td>
<td>Default: 1</td>
</tr>
<tr>
<td>Time/Event/Value</td>
<td>Displays the events specified in the Avalon Event List dialog box. Initially displays only the default events that cannot be edited or deleted.</td>
</tr>
<tr>
<td>Edit</td>
<td>Opens the Avalon Event List dialog box where you can edit the Time/Event/Value parameters. See &quot;Avalon Event List&quot; on page 81.</td>
</tr>
</tbody>
</table>

```

**Table 15.** Avalon peak detection page parameters

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Start Threshold</td>
<td>100000.000</td>
<td></td>
</tr>
<tr>
<td>Initial End Threshold</td>
<td>100000.000</td>
<td></td>
</tr>
<tr>
<td>Initial Area Threshold</td>
<td>100000.000</td>
<td></td>
</tr>
<tr>
<td>Initial P-P Threshold</td>
<td>1.000</td>
<td></td>
</tr>
<tr>
<td>Initial Bunch Factor</td>
<td>1.000</td>
<td></td>
</tr>
<tr>
<td>Initial Negative Peaks</td>
<td>Off</td>
<td></td>
</tr>
<tr>
<td>Initial Tension</td>
<td>1.000</td>
<td></td>
</tr>
</tbody>
</table>
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” on page 82.

Figure 18. Avalon Event List dialog box

Table 16. Avalon Event List dialog box parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (Min)</td>
<td>Specifies the start time of the event.</td>
</tr>
<tr>
<td>Event</td>
<td>Specifies the type of event. For a detailed list of events and value ranges, see “Event types” on page 82.</td>
</tr>
<tr>
<td>Value</td>
<td>Specifies the value of the event.</td>
</tr>
<tr>
<td>Add</td>
<td>Adds a new event to the list with the current Time/Event/Value parameters.</td>
</tr>
<tr>
<td>Delete</td>
<td>Removes the selected Time/Event/Value parameter from the event list.</td>
</tr>
<tr>
<td>Change</td>
<td>Applies the current parameter values.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Closes the dialog box without making any changes. Any additions, deletions, or changes revert to their original state.</td>
</tr>
<tr>
<td>Apply</td>
<td>Closes the dialog box.</td>
</tr>
</tbody>
</table>
Figure 19. Event types

Table 17. Event type definitions (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start Threshold</td>
<td>Specifies the threshold at the start of a peak. The Start Threshold is</td>
</tr>
<tr>
<td></td>
<td>directly related to the RMS noise in the chromatogram. Range: 0 to 999999999</td>
</tr>
<tr>
<td>End Threshold</td>
<td>Specifies the threshold at the end of a peak. The End Threshold is</td>
</tr>
<tr>
<td></td>
<td>directly related to the RMS noise in the chromatogram. Range: 0 to 999999999</td>
</tr>
<tr>
<td>Area Threshold</td>
<td>Controls the area cutoff. Any peaks with a final area less than the area</td>
</tr>
<tr>
<td></td>
<td>threshold will not be detected. This control is in units of area for the</td>
</tr>
<tr>
<td></td>
<td>data. Range: 0 to 999999999</td>
</tr>
<tr>
<td>P-P Threshold</td>
<td>The peak-to-peak resolution threshold controls how much peak overlap must</td>
</tr>
<tr>
<td></td>
<td>be present before two or more adjacent peaks create a peak cluster. Peak</td>
</tr>
<tr>
<td></td>
<td>clusters have a baseline drop instead of valley-to-valley baselines.</td>
</tr>
<tr>
<td></td>
<td>Specified as a percent of peak height overlap. Specified as a percent of</td>
</tr>
<tr>
<td></td>
<td>peak height overlap. Range: 0.1 to 99.99</td>
</tr>
<tr>
<td>Negative Peaks</td>
<td>Permits detection of a negative going peak. Automatically resets after</td>
</tr>
<tr>
<td></td>
<td>finding a negative peak. Valid values: On or Off</td>
</tr>
<tr>
<td>Bunch Factor</td>
<td>Specifies the number of points grouped together during peak detection.</td>
</tr>
<tr>
<td></td>
<td>This event controls the bunching of chromatographic points during</td>
</tr>
<tr>
<td></td>
<td>integration and does not affect the final area calculation of the peak.</td>
</tr>
<tr>
<td></td>
<td>A high bunch factor groups peaks into clusters. Range: 0 to 999</td>
</tr>
</tbody>
</table>
### Table 17. Event type definitions (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tension</td>
<td>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</td>
</tr>
<tr>
<td>Tangent Skim</td>
<td>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</td>
</tr>
<tr>
<td>Shoulders On</td>
<td>Allows peak shoulders to be detected (peaks which are separated by an inflection rather than a valley) Sets a threshold for the derivative.</td>
</tr>
<tr>
<td>Shoulders Off</td>
<td>Disables peak shoulder detection. Range: 0 to 50</td>
</tr>
<tr>
<td>Force Cluster On</td>
<td>Force the following peaks to be treated as a cluster (single peak).</td>
</tr>
<tr>
<td>Force Cluster Off</td>
<td>End the forced clustering of peaks.</td>
</tr>
<tr>
<td>Disable Cluster On</td>
<td>Prevent any peaks from being clustered.</td>
</tr>
<tr>
<td>Disable Cluster Off</td>
<td>Permit clusters to occur again.</td>
</tr>
</tbody>
</table>
Enabling Optional Features

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

- User Security
- Target Screening
- Quick Acquisition
- Compound Datastore
- Delay Calibration Calculation
- Batch Wizard Style
- Multiplexing
- 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 43.

❖ 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 43. 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 66.
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 87.

- **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 94.

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 120.
- Displays the Compound Datastore task pane on the Configuration mode navigation pane. See “Compound Datastore” on page 52.
- Enables the Export SRM Data command in the Method Development mode. See “Exporting SRM Data” on page 200.

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 294.

   **Note** The Batch Template Wizard feature is not available when you enable multiplexing. See “Multiplexing” on page 87.

2. Click **Apply**.

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

3. Click **Yes**.

**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.
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 229) or monitor an acquisition (see “Devices Page” on page 256).

**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 87.
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 roles 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 a detailed description of all the features on the Method Development navigation pane, see “Method Development navigation pane” on page 92.
Figure 20. Method Development navigation pane

Table 18. Method Development navigation pane functions (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method View</td>
<td>See “Working with Master Methods” on page 94.</td>
</tr>
<tr>
<td>Create Method</td>
<td>Opens the Create Master Method dialog box where you can choose the process you want to use to begin your master method.</td>
</tr>
<tr>
<td>Open Method</td>
<td>Opens the Open Master Method dialog box where you can choose a master method to open.</td>
</tr>
</tbody>
</table>
Table 18. Method Development navigation pane functions (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Import Published Method</td>
<td>Opens the Import Published Method dialog box where you can select a published method to import.</td>
</tr>
</tbody>
</table>
| Export SRM Data        | Writes the selected reaction monitoring (SRM) table to the following file: \...\Thermo\TraceFinder\2.0\ClinTox\Methods\methodname.xml  
You can use the data in this file 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 86.  
The compounds in the Acquisition List must contain at least one SRM experiment type. |
| Recent Files           | Displays recently saved master methods.                                                                                                                                                                                           |
| New Instrument Method  | Opens the Instrument View where you can specify instrument settings for your configured instruments.  
If the instrument 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 208.                                                                                                                                                                               |
| 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 you can begin 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 begin 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 21.* Create Master Method dialog box

![Create Master Method dialog box](image-url)

There are multiple ways to create a master method.

**Select the technique you want to use.**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Use Method Forge</td>
<td>Performs peak detection against a raw data file. Performs library lookup if requested.</td>
</tr>
<tr>
<td>Import Xcalibur Processing Method</td>
<td>Imports a previously created processing method, finding configured compounds and reference spectra.</td>
</tr>
<tr>
<td>Associate a raw data file</td>
<td>Creates a blank master method and associates a raw data file, allowing manual peak selection.</td>
</tr>
<tr>
<td>Select compounds from CDS</td>
<td>Creates a blank master method and displays the configured compound datastore, allowing compound selection.</td>
</tr>
</tbody>
</table>

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 a detailed description of all the Method Forge parameters, see “Method Forge dialog box parameters” on page 102.

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.

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 95.

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

The Method Forge dialog box opens. For a detailed description of all the features on the Method Forge dialog box, see “Method Forge dialog box” on page 101.

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 189.

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:

<table>
<thead>
<tr>
<th>steroids03</th>
<th>RT (min)</th>
<th>Compound Name</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total Progress</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Detecting Peaks</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Analyzing Spectrum</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.99</td>
<td>Peak@1.99 + c Full ms2 303.30@cid40...</td>
</tr>
<tr>
<td></td>
<td>3.18</td>
<td>Peak@3.18 + c Full ms2 315.30@cid40.00[100...</td>
</tr>
<tr>
<td></td>
<td>1.39</td>
<td>Peak@1.39 + c Full ms2 331.30@cid40.00[100...</td>
</tr>
<tr>
<td></td>
<td>0.67</td>
<td>Peak@0.67 + c Full ms2 363.30@cid40.00[150...</td>
</tr>
</tbody>
</table>

The Method Forge process searches the NIST library and displays the identified compound names instead of peak times.

When the acquisition completes, Method Forge performs peak detection, datastore searching, and characteristic ion and reference spectrum identification. 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 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 the **Add to CDS** button 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 a detailed description of all the features on the General page, see “General page” on page 117.

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 110.

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

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

   ![Method View](Image)

   The Create Master Method dialog box opens. See “Create Master Method dialog box” on page 95.

2. In the Create Master Method dialog box, select the **Use Method Forge** option and click **OK**.

   ![Use Method Forge](Image)

   The Method Forge dialog box opens. For a detailed description of all the features on the Method Forge dialog box, see “Importing an Xcalibur Master Method” on page 103.

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 about creating a custom method template, see “Creating a Method Template” on page 189.
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.

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 a detailed description of all the features on the General page, see “General page” on page 117.

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 110.

**Figure 22.** Method Forge dialog box
### Table 19. Method Forge dialog box parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Method template selection</strong></td>
<td></td>
</tr>
<tr>
<td>Use the Default Template</td>
<td>Creates a new method with the default template.</td>
</tr>
<tr>
<td>Select a Custom Template</td>
<td>Lists all the available method templates. For detailed instructions about creating a custom method template, see “Creating a Method Template” on page 189.</td>
</tr>
<tr>
<td>Name the Master Method</td>
<td>The name for the new master method.</td>
</tr>
<tr>
<td>Automatically Create the Master Method</td>
<td>When the acquisition completes, Method Forge performs peak detection, library searching, and characteristic ion and reference spectrum identification. This information is loaded into a new master method. This process occurs immediately when you specify an existing raw data file.</td>
</tr>
<tr>
<td><strong>Raw file selection</strong></td>
<td></td>
</tr>
<tr>
<td>Use an Existing Raw Data File</td>
<td>Enables the Raw Filename box where you can select a raw data file used in creating the master method.</td>
</tr>
<tr>
<td>Acquire a New Raw Data File</td>
<td>Enables functions to acquire data to create a raw data file used in creating the master method.</td>
</tr>
<tr>
<td>Instrument Method</td>
<td>The saved method (.meth) file used for acquiring the data.</td>
</tr>
<tr>
<td>Raw Filename</td>
<td>The file name where the TraceFinder application writes the raw data.</td>
</tr>
<tr>
<td>Path</td>
<td>The location where the TraceFinder application saves the raw data file.</td>
</tr>
<tr>
<td>Sample Comment (Optional)</td>
<td>(Optional) Comment about the acquired sample or the data file.</td>
</tr>
<tr>
<td>Manual Injection</td>
<td>Performs a manual acquisition.</td>
</tr>
<tr>
<td>Use Autosampler</td>
<td>Performs an autosampler acquisition.</td>
</tr>
<tr>
<td>Vial Position</td>
<td>The tray vial number used for the autosampler acquisition.</td>
</tr>
<tr>
<td>Injection Amount</td>
<td>The volume (in milliliters) injected by the autosampler acquisition.</td>
</tr>
<tr>
<td><strong>Function button</strong></td>
<td></td>
</tr>
<tr>
<td>Overwrite</td>
<td>Overwrites the specified master method name. This function is enabled only when the specified master method name already exists.</td>
</tr>
<tr>
<td>OK</td>
<td>Creates a master method using the data and parameters you specified.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Closes Method Forge and does not create a master method.</td>
</tr>
</tbody>
</table>
**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**.

     ![Create Method](method-view.png)

     The Create Master Method dialog box opens. See “Create Master Method dialog box” on page 95.

  2. In the Create Master Method dialog box, select the **Import Xcalibur Processing Method** option and click **OK**.

     ![Import Xcalibur Processing Method](import-xcalibur.png)

     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 the raw data file, and open the file.

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

     You can set the mass precision decimal places to any integer between 0 and 5, inclusive.

     **Note** When you associate a raw data file, the application reads the mass precision from the file and this parameter is unavailable.
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 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 the Add to CDS button 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 a detailed description of all the features on the General page, see “General page” on page 117.


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 110.
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 95.

2. In the Create Master Method dialog box, select the Associate a Raw Data File option and click OK.

The Associate a Raw Data File dialog box opens.

3. Click the browse button and locate a raw data file to associate with the method.

4. To set a reference spectrum, select the Yes option.

The TraceFinder application adds all compounds found in the raw data file to your method and displays the General page of the Master Method View. For a detailed description of all the features on the General page, see “General page” on page 117.
5. From the Instrument Method list on the General page, select an instrument method.

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

   If the compounds in the associated raw data file are not found in the Compound Datastore, you cannot save the method. Follow the instructions “To add compounds to the method” on page 106.

   For a detailed description of how to modify a master method, see “Editing a Master Method” on page 110.

   ◇ To add compounds to the method

1. Click the **Compounds** tab.

   The Detection page is selected by default.

   ![Compounds page](image)

   **Note** When the Compound Datastore is enabled, the Compounds page includes an Acquisition List tab. See “Enabling Optional Features” on page 84.

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

   ![Detection page](image)

2. Select a filter from the Filter list.

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

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

   ![Filter menu](image)
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 quan peak, and the second and third largest ions as the confirming ions.

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

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

c. Click **OK**.

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

For a detailed description of all the features on the Detection page, see “Editing the Compounds Page” on page 120.

For a detailed description of how to modify a master method, see “Editing a Master Method” on page 110.

**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 86.

❖ **To select compounds from the datastore**

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

The Create Master Method dialog box opens.

2. In the Create Master Method dialog box, select the **Select Compounds from CDS** option and click **OK**.

   ![Select Compounds from CDS](image)

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 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

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Select All</td>
<td>Selects all compounds in the compound datastore.</td>
</tr>
<tr>
<td>Deselect All</td>
<td>Clears all compounds in the compound datastore.</td>
</tr>
<tr>
<td>Copy Down</td>
<td>Copies the state (checked or cleared) of the currently selected compound to all compounds below it in the compound list.</td>
</tr>
</tbody>
</table>

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 120.

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” on page 110.
**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 legacy TraceFinder, EnviroLab Forms, QuanLab Forms, or ToxLab Forms applications. To convert legacy methods, see “Converting Legacy Data” on page 19.

ullet To open a saved master method

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

   ![Method Development](image)

   The Method Development navigation pane opens.

   ![Method View](image)

   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.

The Open Master Method dialog box displays 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 a detailed description of all the features on the General page, see “General page” on page 117.
Editing the General Page

The General page defines basic information about the master method. For a detailed description of all the features on the General page, see “General page” on page 117.

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 120.

   ![Ion range calc method and Use level](image)

5. From the Qualitative Peak Processing Template box, select a template for performing peak detection on quantitative samples following target compound analysis.
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 instrument setup shows multiple configured instruments.

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

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

   The TraceFinder application returns you to the General page.
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.

![Update Instrument Method dialog box](image)

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 you want to use to perform peak detection on quantitative samples following compound analysis.

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

C:\Thermo\TraceFinder\2.0\ClinTox\Templates\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 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.

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 specified to subtract scans from both sides of the peak, 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 specified to subtract 3 scans before the peak 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, Select Reference sample:]

2. Click **Select**.

The Open Chromatograph Reference Sample dialog box opens.

![Open Chromatograph Reference Sample]

**Note** If you are creating a new method, you will not see any reference samples here. You must create and save a batch using this 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, it 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 you want to use.
  2. Specify the number of millimass units or parts per million to use as the $m/z \pm$ tolerance value.

The application applies this mass tolerance to the extracted chromatograms.
Figure 23. General page

![Master Method View - Method](image)

**Table 21. General page parameters (Sheet 1 of 3)**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lab Name</td>
<td>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 70.</td>
</tr>
<tr>
<td>Assay Type</td>
<td>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).</td>
</tr>
</tbody>
</table>
Table 21. General page parameters (Sheet 2 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection Volume</td>
<td>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</td>
</tr>
<tr>
<td>Ion Range Calc Method</td>
<td>The TraceFinder application uses the selected ion range calc method to calculate the ion ratio range windows: Manual (default), Average, Level, or Weighted average. When you select Level, an additional list is displayed where you can select a calibration level amount. To define these calibration levels on the Compounds page, see “Editing the Compounds Page” on page 120.</td>
</tr>
<tr>
<td>Instrument Method</td>
<td>Instrument method used for acquiring samples.</td>
</tr>
<tr>
<td>Edit</td>
<td>Opens the Thermo Xcalibur Instrument Setup dialog box where you can edit the instrument method.</td>
</tr>
<tr>
<td>Update</td>
<td>Choose one of the following:</td>
</tr>
<tr>
<td></td>
<td>• <strong>Send to Xcalibur Method</strong>: Overwrites the Xcalibur method with the current instrument method.</td>
</tr>
<tr>
<td></td>
<td>• <strong>Get From Xcalibur Method</strong>: Overwrites the current instrument method with the Xcalibur method.</td>
</tr>
<tr>
<td>Qualitative Peak Processing Template</td>
<td>The TraceFinder application uses the qualitative peak processing template to perform peak detection on quantitative samples following compound analysis.</td>
</tr>
<tr>
<td>Background Subtraction Range Option</td>
<td>Valid values: None, Before Peak, After Peak, Both Sides of Peak Default: None</td>
</tr>
<tr>
<td>Number of Scans to Subtract</td>
<td>Valid values: Even numbered integers Default: 0</td>
</tr>
<tr>
<td>Stepoff Value</td>
<td>Offset from the selected peak to the first subtracted peak.</td>
</tr>
<tr>
<td>Set Chromatogram Reference Sample</td>
<td>Valid values: None, External Default: None</td>
</tr>
<tr>
<td>Set Reference Sample</td>
<td>This parameter is enabled only when Set Chromatogram Reference Sample is set to External. Click the Select button to choose a reference sample from the project folders.</td>
</tr>
</tbody>
</table>
Table 21. General page parameters  (Sheet 3 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Tolerance</td>
<td>Upper limit of MMU or PPM.</td>
</tr>
<tr>
<td></td>
<td>Default: 500</td>
</tr>
<tr>
<td></td>
<td>Range: 0.1 through 50 000</td>
</tr>
<tr>
<td></td>
<td>• (Default) MMU (millimass units): MMU is a static calculation to the extracted mass.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td>Notes</td>
<td>Notes you add about the method.</td>
</tr>
</tbody>
</table>
Editing the Compounds Page

Use the Compounds page to set all parameters for the identification, detection, and quantification for the target compound list.

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

- Acquisition List
- Identification
- Detection
- Calibration
- Calibration Levels
- QC Levels
- Real Time Viewer

Each page on the Compounds page (except the Acquisition List page) uses a right-click shortcut menu. See “Using the Shortcut Menu Commands” on page 162.

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 a detailed description of all the features on the Acquisition List page, see “Acquisition List page” on page 122.

The Acquisition List page is displayed only when you enable the Compound Datastore option in the Configuration mode. See “Compound Datastore” on page 86.

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, \( \text{ fishermen } \), 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, 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, 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 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>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Select All</td>
<td>Selects all compounds in the compound datastore.</td>
</tr>
<tr>
<td>Deselect All</td>
<td>Clears all compounds in the compound datastore.</td>
</tr>
<tr>
<td>Copy Down</td>
<td>Copies the state (checked or cleared) of the currently selected compound to all compounds below it in the compound list.</td>
</tr>
</tbody>
</table>

4. Click Apply.

The TraceFinder application adds the compounds to the Acquisition List and Compounds pages of the Master Method View.
Figure 24. Acquisition List page

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function Icons</strong></td>
<td></td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Opens the Select Compounds to Add dialog box that lists all the compounds defined in the compound datastore.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>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.</td>
</tr>
<tr>
<td><strong>Compound parameters</strong></td>
<td></td>
</tr>
<tr>
<td>Compound Name</td>
<td>Alphanumeric name assigned to the compound.</td>
</tr>
<tr>
<td>Experiment Type</td>
<td>Experiment type: SRM, XIC, or SIM.</td>
</tr>
<tr>
<td>Category</td>
<td>(Optional) Alphanumeric identifier.</td>
</tr>
<tr>
<td>Ionization</td>
<td>(Optional) Alphanumeric identifier. Valid values: ESI, APCI, EI, CI, APPI</td>
</tr>
<tr>
<td>Chemical Formula</td>
<td>(Optional) Alphanumeric chemical identifier.</td>
</tr>
<tr>
<td><strong>Quantitation peak parameters</strong></td>
<td></td>
</tr>
<tr>
<td>Precursor Mass</td>
<td>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</td>
</tr>
<tr>
<td>Product Mass</td>
<td>The mass-to-charge ratio of the quan 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</td>
</tr>
<tr>
<td>Mass</td>
<td>The mass-to-charge ratio of the quan 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</td>
</tr>
</tbody>
</table>
### Table 23. Acquisition List page parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
</table>
| 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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
</table>
| 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 quan 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 quan 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 a description of all values on the Identification page, see “Identification page” on page 125.

❖ To filter the displayed compounds

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

<table>
<thead>
<tr>
<th>Compound type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quan Compounds</td>
<td>Displays only quan compounds, such as target compounds, internal standards, and surrogates.</td>
</tr>
<tr>
<td>Target Compounds</td>
<td>Displays only target compounds.</td>
</tr>
<tr>
<td>Internal Standards</td>
<td>Displays only internal standard compounds.</td>
</tr>
</tbody>
</table>
Figure 25. Identification page

Table 24. Identification page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>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&lt;br&gt;Start time = RT – (Window/2)&lt;br&gt;Stop time = RT + (Window/2)&lt;br&gt;Start and stop range: 0.00 to 999.00</td>
</tr>
<tr>
<td>Compound</td>
<td>A list of compounds that have been identified. To customize the compound names, click the cell and type a new name. To display a filtered list of compounds, use the Show list.</td>
</tr>
<tr>
<td>Compound Type</td>
<td>Compound types are Target Compound and Internal Standard. The TraceFinder application uses target compounds and internal standards in quantitative analysis.</td>
</tr>
<tr>
<td>Active</td>
<td>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 to the Batch View and Data Review view in the Analysis mode.</td>
</tr>
<tr>
<td>CAS No</td>
<td>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.</td>
</tr>
<tr>
<td>Use as RT Reference</td>
<td>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.</td>
</tr>
<tr>
<td>Reference Compound</td>
<td>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.</td>
</tr>
</tbody>
</table>
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
- Signal
- Detect
- Spectrum
- Ratios

On the Detection page (see “Detection page” on page 134), 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 quantification peak, mass range, or confirming ion. The TraceFinder application automatically uses the first match it finds as the compound name, the base peak of the mass spectrum as the quan peak, and the second and third largest ions as the confirming ions.

Follow these procedures:

- To filter the displayed compounds
- To add compounds to the method
- To change the compound reference spectrum
- To replace a quan mass
- To add a mass to the existing quan mass ranges
- To add a quan peak
- To add a mass as a new compound
- To replace a confirming ion
- To add a mass as a new confirming ion
- To save the new method
To filter the displayed compounds

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

- Quan Compounds: Displays only quan compounds, such as target compounds, internal standards, and surrogates.
- Target Compounds: Displays only target compounds.
- Internal Standards: Displays only internal standard compounds.

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.

2. Browse to a raw data file to associate with the method and open the file.

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 112.

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 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 quan peak, and the second and third largest ions as the confirming ions.

If the name of the first match is already in the library, the Add New Compound dialog box opens.
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 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 quan peak pane with this spectrum.

To replace a quan mass

1. Click the pane for the quan 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 Mass as Quan Mass 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 ions. See “Ratios” on page 154.

To add a mass to the existing quan 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 Mass to Existing Quan Mass 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 quan 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 ions. See “Ratios” on page 154.
To add a quan 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 Mass as New Quan Peak from the shortcut menu.
   The application adds a new quan peak to the compound.

To add a mass 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 Mass 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 quan peak, and the second and third largest ions as the confirming ions.
   If the name of the first match is already in the library, the Add New Compound dialog
   box opens with the matching compound selected.
3. (Optional) In the Add New Compound dialog box, 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 confirming ion

1. Click the pane for the confirming ion 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 Mass as Confirming Ion from the shortcut menu. The TraceFinder application replaces the confirming ion with the selected mass.

To add a mass as a new confirming ion

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 Mass as New Confirming Ion from the shortcut menu. The TraceFinder application adds the confirming ion to the quan peak.

You can use the shortcut menu on the spectrum pane for this new confirming ion to perform any of the tasks you could perform on the original confirming ions.

To save the new method

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:

```plaintext
...\Thermo\TraceFinder\2.0\ClinTox\Methods
```
4 Using the Method Development Mode

Working with Master Methods

Figure 28. Detection page

- Compound list:
  1. 1,3-Dichlorobenzene
  2. 1,4-Dichlorobenzene
  3. 1,4-Dichlorobenzene
  4. 1,2-Dichlorobenzene
  5. Hexachloroethane
  6. Nitrobenzene-d5
  7. 1,2,4-Trichlorobenzene
  8. Naphthalene-d8
  9. Hexachloropropene
  10. Hexachlorobutadiene
  11. Pentachloroethane
  12. 1,2,4,5-Tetrachlorobenzene
  13. Hexachlorocyclopentene
  14. 2-Fluorobiphenyl
  15. 2-Chloronaphthalene
  16. Acenaphthene-d10
  17. Hydrogen bromide
  18. Hexachlorobenzene
  19. Phenanthrene-d10
  20. p-Terphenyl-d14
  21. Chrysene-d12

- QuanPeak1
  - Quan peak
  - Confirming peak 1

- Times
- Signal
- Detect

- Expected RT (min): 5.14
- Window (sec): 30.00
- View width (min): 0.75

- Signal
- Detect
- Ratios

- Detector: MS
- Filter: 
- Trace: Mass range
- m/z: 128.00

- Filter: 10441216 BP: 149.9

RT: 4.435, 32791478.0 | C:\xcalibur\data|
### Table 25. Detection page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compound List</td>
<td>Lists all compounds in the master method.</td>
</tr>
<tr>
<td>Quan Peak</td>
<td>Displays a chromatogram for the quan peak and its confirming ions. The quan peak and confirming ion panes include additional pages for retention time, signal, detection, spectrum, and ratio parameters.</td>
</tr>
<tr>
<td>Filter</td>
<td>Displays the filter used for the raw data file.</td>
</tr>
<tr>
<td>Reference Chromatogram and Spectra</td>
<td>Displays a reference chromatogram and spectra for the raw data file.</td>
</tr>
</tbody>
</table>

**Additional pages**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Times</td>
<td>Defines the retention time and window for a quan peak. See “Times” on page 136.</td>
</tr>
<tr>
<td>Signal</td>
<td>Defines the detector and its parameters used to display each chromatogram trace. See “Signal” on page 137.</td>
</tr>
<tr>
<td>Detect</td>
<td>Defines the peak detection algorithm and its options. See “Detect” on page 140.</td>
</tr>
<tr>
<td>Spectrum</td>
<td>Defines a reference mass spectrum for a quan peak or compound. See “Spectrum” on page 149.</td>
</tr>
<tr>
<td>Ratios</td>
<td>Defines the criteria for evaluating, confirming, or qualifying ions. See “Ratios” on page 154.</td>
</tr>
</tbody>
</table>
Times

Use the Times page to define the retention time and window for a quan peak.

**Figure 29.** Times page

![Times page](image)

**Table 26.** Times page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expected RT (min)</td>
<td>Expected retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Window (sec)</td>
<td>Width of the window (in seconds) to indicate how far around the expected retention time the system looks for a peak apex.</td>
</tr>
<tr>
<td>View Width (min)</td>
<td>Viewable size 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.</td>
</tr>
</tbody>
</table>
Signal

Use the Signal page to define the detector and its parameters as you display each chromatogram trace. For a detailed description of all the features on the Signal page, see “Signal page parameters” on page 138.

❖ To specify ranges of ions for detection and integration

1. In the Ranges area, click Edit.

The Edit Mass Ranges dialog box opens where you can enter rows using a center of mass or a range.

**Figure 30.** Edit Mass Ranges dialog box

![Edit Mass Ranges dialog box](image)

2. Enter a value in the Center Mass box and click Add.

The application adds a row with this value to the ranges grid. Center mass values are listed in the Start m/z column. The application uses a range of one amu centered on this value.

3. 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.

4. 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.

5. Click Apply.

When you are editing a master method, the application applies the entries to the list of ranges.
Figure 31. Signal page

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Detector</td>
<td>MS: Mass spectrometers. Analog: Supplemental detectors (for example, FID, ECD). AD 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.</td>
</tr>
<tr>
<td>Filter</td>
<td>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.</td>
</tr>
<tr>
<td>Trace</td>
<td>Represents a specific range of the data. In conjunction with the filter, the TraceFinder application uses the trace to identify the characteristic ions for a compound. The options are: Mass Range, TIC, or Base Peak.</td>
</tr>
</tbody>
</table>
Table 27. Signal page parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ranges</strong></td>
<td></td>
</tr>
<tr>
<td>Edit</td>
<td>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 137.</td>
</tr>
<tr>
<td>Start m/z</td>
<td>Specifies ranges of ions for detection and integration. The application sums the multiple ions specified by these ranges.</td>
</tr>
<tr>
<td>End m/z</td>
<td>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.</td>
</tr>
</tbody>
</table>
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.

For a detailed description of all the features on the Detect page for Genesis sensitivity, see “Detect page parameters for Genesis” on page 142.

For a detailed description of all the features on the Detect page for ICIS sensitivity, see “Detect page parameters for ICIS” on page 145.

For a detailed description of all the features on the Detect page for Avalon sensitivity, see “Detect page parameters for Avalon” on page 147.

❖ To apply current peak detection settings to all peaks

1. Edit the parameters for either the Quan peak or a Confirming peak.

2. Right-click the Detect page and choose Apply to All Peaks in Method from the shortcut menu.

   The application updates all compounds in the method with the current settings on the Detect page. These updates apply to both quan and confirming ions.

❖ To apply current peak detection settings to all peaks that use the same detection mode

1. Edit the parameters for either the Quan peak or a Confirming peak.

2. Right-click the Detect page and choose Apply to All Peaks with Like Sensitivity Setting from the shortcut menu.

   The application uses the current settings on the Detect page to update all compounds in the method that use the same sensitivity mode (Genesis, ICIS, or Avalon). These updates apply to both quan and confirming ions that use the same sensitivity mode.
Figure 32. Detect page for Genesis
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>Specifies the Genesis peak detection algorithm.</td>
</tr>
<tr>
<td>Detection Method</td>
<td>Highest peak: Uses the highest peak in the chromatogram for component identification.</td>
</tr>
<tr>
<td></td>
<td>Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.</td>
</tr>
<tr>
<td>Smoothing</td>
<td>Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration.</td>
</tr>
<tr>
<td></td>
<td>Range: Any odd integer from 1 through 15 points. Default: 1</td>
</tr>
<tr>
<td>S/N Threshold</td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>Range: 0.0 to 999.0</td>
</tr>
<tr>
<td>Enable Valley Detection</td>
<td>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.</td>
</tr>
<tr>
<td>Expected Width (sec)</td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>Range: 0.0 to 999.0</td>
</tr>
<tr>
<td>Constrain Peak Width</td>
<td>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.</td>
</tr>
<tr>
<td>Peak Height (%)</td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>Range: 0.0 to 100.0 %</td>
</tr>
</tbody>
</table>
### 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

### Peak S/N Cutoff
The peak edge is set to values below this signal-to-noise ratio. This test identifies an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio.

When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the TraceFinder application defines the right and left edges of the peak when the S/N reaches a value less than 200.

Range: 50.0 to 10000.0

### Valley Rise (%)
The peak trace can rise above the baseline by this percentage after passing through a minimum (before or after the peak).

This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.

When the trace exceeds rise percentage, the TraceFinder application applies valley detection peak integration criteria.

The TraceFinder application applies this test to both the left and right edges of the peak.

The rise percentage criteria is useful for integrating peaks with long tails.

Range: 0.1 to 500.0

### Valley S/N
Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher.

Range: 1.0 to 100.0
Default: 2.0

### # 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.

---

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tailing Factor</td>
<td>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.</td>
</tr>
<tr>
<td>Min Peak Height (S/N)</td>
<td>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.</td>
</tr>
<tr>
<td>Peak S/N Cutoff</td>
<td>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.</td>
</tr>
<tr>
<td>Valley Rise (%)</td>
<td>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.</td>
</tr>
<tr>
<td>Valley S/N</td>
<td>Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher.</td>
</tr>
<tr>
<td># Background Scans</td>
<td>Number of background scans performed by the TraceFinder application.</td>
</tr>
<tr>
<td>Report Noise As</td>
<td>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.</td>
</tr>
</tbody>
</table>
Figure 33. Detect page for ICIS
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>Specifies the ICIS peak detection algorithm.</td>
</tr>
<tr>
<td>Detection Method</td>
<td>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.</td>
</tr>
<tr>
<td>Smoothing</td>
<td>Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. Range: Any odd integer from 1 through 15 points Default: 1</td>
</tr>
<tr>
<td>Area Noise Factor</td>
<td>The noise level multiplier used to determine the peak edge after the location of the possible peak. Range: 1 through 500 Default: 5</td>
</tr>
<tr>
<td>Peak Noise Factor</td>
<td>The noise level multiplier used to determine the potential peak signal threshold. Range: 1 through 1000 Default: 10</td>
</tr>
<tr>
<td>Baseline Window</td>
<td>The TraceFinder application looks for a local minima over this number of scans. Range: 1 through 500 Default: 40</td>
</tr>
<tr>
<td>Constrain Peak Width</td>
<td>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.</td>
</tr>
<tr>
<td>Peak Height (%)</td>
<td>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%</td>
</tr>
<tr>
<td>Tailing Factor</td>
<td>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</td>
</tr>
</tbody>
</table>
Table 29. Detect page parameters for ICIS  (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min Peak Height (S/N)</td>
<td>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</td>
</tr>
<tr>
<td>Noise Method</td>
<td>The options are INCOS or Repetitive.</td>
</tr>
<tr>
<td></td>
<td>INCOS: Uses a single pass algorithm to determine the noise level.</td>
</tr>
<tr>
<td></td>
<td>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.</td>
</tr>
<tr>
<td>Min Peak Width</td>
<td>The minimum number of scans required in a peak.</td>
</tr>
<tr>
<td></td>
<td>Range: 0 to 100 scans</td>
</tr>
<tr>
<td></td>
<td>Default: 3</td>
</tr>
<tr>
<td>Multiplet Resolution</td>
<td>The minimum separation in scans between the apexes of two potential peaks. This is a criterion to determine if two peaks are resolved.</td>
</tr>
<tr>
<td></td>
<td>Range: 1 to 500 scans</td>
</tr>
<tr>
<td></td>
<td>Default: 10</td>
</tr>
<tr>
<td>Area Tail Extension</td>
<td>The number of scans past the peak endpoint to use in averaging the intensity.</td>
</tr>
<tr>
<td></td>
<td>Range: 0 to 100 scans</td>
</tr>
<tr>
<td></td>
<td>Default: 5</td>
</tr>
<tr>
<td>Area Scan Window</td>
<td>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.</td>
</tr>
<tr>
<td></td>
<td>Range: 0 to 100 scans</td>
</tr>
<tr>
<td></td>
<td>Default: 0</td>
</tr>
<tr>
<td>RMS</td>
<td>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.</td>
</tr>
</tbody>
</table>
Table 30. Detect page parameters for Avalon (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>Specifies the Avalon peak detection algorithm.</td>
</tr>
<tr>
<td>Detection Method</td>
<td>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.</td>
</tr>
</tbody>
</table>
### Table 30. Detect page parameters for Avalon (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Smoothing</td>
<td>Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration.</td>
</tr>
<tr>
<td></td>
<td>Range: Any odd integer from 1 through 15 points</td>
</tr>
<tr>
<td></td>
<td>Default: 1</td>
</tr>
<tr>
<td>Autocalc Initial Events</td>
<td>Automatically calculates the events in the Event list.</td>
</tr>
<tr>
<td>Edit</td>
<td>Opens the Avalon Event List dialog box. See “Avalon Event List” on page 81.</td>
</tr>
</tbody>
</table>
Spectrum

Use the Spectrum page to store a reference mass spectrum for a quan peak or compound.

For a detailed description of all the shortcut menu commands on the Spectrum page, see “Spectrum shortcut menu functions” on page 153.

Follow these procedures:

• To update confirming ion ratios
• To change the quantitation mass used for a quan peak
• To add ions together to get an accumulated signal
• To add a quan 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 quan 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 quan 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 $m/z$ 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 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 quan peak and a quan peak with an updated quan mass.
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Figure 35. Original quan peak mass example

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

Figure 36. Updated quan 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 quan peak signal.

❖ **To add a quan 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 quan peak.
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 \textbf{Add This Mass as New Confirming Ion} from the shortcut menu.

The TraceFinder application adds the selected mass as a confirming peak for this quan 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 \textbf{Reset Scaling} from the shortcut menu.
### Table 31. Spectrum shortcut menu functions (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Functions</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Update Confirming Ion Ratios With This Spectrum</td>
<td>Updates the confirming ion ratios using the selected peak.</td>
</tr>
<tr>
<td>Set This Mass as Quan Mass</td>
<td>Adds the quan mass of the selected ion to the quantitation mass used for the quan peak. You can choose to update the ion ratios or not update the ion ratios using this reference spectrum.</td>
</tr>
<tr>
<td>Add This Mass to Existing Quan Mass Range</td>
<td>Adds the selected mass to your existing quan mass range. You can choose to update the ion ratios to adjust the confirming ion comparisons to the new summed quan peak signal.</td>
</tr>
<tr>
<td>Set This Mass as New Quan Peak</td>
<td>Adds a new quan peak to an existing compound.</td>
</tr>
</tbody>
</table>
### Ratios

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

For a detailed description of all the features on the Ratios page, see “Ratios page parameters” on page 155.

#### 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:

![Ratios page screenshot]

- The target ratio is expected to be 61.02% and the window is Absolute 20%, so the acceptable window for this confirming ion is 41.02 to 81.02%.

- If, instead, 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 is 48.82 to 73.22%.

### Table 31. Spectrum shortcut menu functions (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Functions</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Add This Mass as New Confirming Ion</td>
<td>Adds one or more confirming ions to an existing compound.</td>
</tr>
<tr>
<td>Reset Scaling</td>
<td>Returns the chromatogram or spectrum display to its original size.</td>
</tr>
</tbody>
</table>
Figure 38. Ratios page

Table 32. Ratios page parameters

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

Figure 39. Calibration page

<table>
<thead>
<tr>
<th>RT</th>
<th>Compound</th>
<th>Compound type</th>
<th>Standard type</th>
<th>Response via</th>
<th>Curve type</th>
<th>Origin</th>
<th>Weighting</th>
<th>Units</th>
<th>ISTD</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.82</td>
<td>Propane, 1-chlor</td>
<td>Target Compound</td>
<td>Internal</td>
<td>Area</td>
<td>Linear</td>
<td>Ignore</td>
<td>Equal</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8.03</td>
<td>Acetamiprid</td>
<td>Target Compound</td>
<td>Internal</td>
<td>Area</td>
<td>Linear</td>
<td>Ignore</td>
<td>Equal</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.62</td>
<td>1-Methyl2-butox</td>
<td>Target Compound</td>
<td>Internal</td>
<td>Area</td>
<td>Linear</td>
<td>Ignore</td>
<td>Equal</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.59</td>
<td>Aldochlor</td>
<td>Target Compound</td>
<td>Internal</td>
<td>Area</td>
<td>Linear</td>
<td>Ignore</td>
<td>Equal</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.75</td>
<td>Acephate</td>
<td>Target Compound</td>
<td>Internal</td>
<td>Area</td>
<td>Linear</td>
<td>Ignore</td>
<td>Equal</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12.40</td>
<td>Carbon dioxide</td>
<td>Target Compound</td>
<td>Internal</td>
<td>Area</td>
<td>Linear</td>
<td>Ignore</td>
<td>Equal</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 33. Calibration page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>Compound Type</td>
<td>Displays the compound type as a Target Compound or Internal Standard.</td>
</tr>
<tr>
<td>Standard Type</td>
<td>Specifies Internal or External standards.</td>
</tr>
<tr>
<td>Response Via</td>
<td>The use of area or height.</td>
</tr>
<tr>
<td>Curve Type</td>
<td>Specifies Linear, Quadratic, or AverageRF curve types.</td>
</tr>
<tr>
<td>Origin</td>
<td>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.</td>
</tr>
<tr>
<td>Weighting</td>
<td>Specifies the weighting as Equal, 1/X, 1/X^2, 1/Y, or 1/Y^2.</td>
</tr>
<tr>
<td>Units</td>
<td>The units to be displayed with the calculated values.</td>
</tr>
<tr>
<td>ISTD</td>
<td>The internal standard (ISTD) for a target compound or surrogate if the standard type is set to Internal. If you set the standard type to External, this field is inactive.</td>
</tr>
<tr>
<td>Amount</td>
<td>The amount of the internal standard for ISTD compounds.</td>
</tr>
</tbody>
</table>
**Calibration Levels**

On the Calibration levels page for a master method, you can define the standards for calibration. You can edit calibration levels and concentrations for master methods only. The contents of this page are read-only when you are editing a local method.

❖ **To specify calibration levels and concentrations**

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

<table>
<thead>
<tr>
<th>RT</th>
<th>Compound</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.00... Acetanipid</td>
</tr>
<tr>
<td>2</td>
<td>7.62 1-Methyldecylamine</td>
</tr>
</tbody>
</table>

2. In the Manage Calibration Levels area, type a value for the first calibration level.

The TraceFinder 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 level for each compound.

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 you want to copy, right-click, and choose **Copy Down** from the shortcut menu.
Using the Method Development Mode

Working with Master Methods

Figure 40. Calibration Levels page

<table>
<thead>
<tr>
<th>RT</th>
<th>Compound</th>
<th>cal1</th>
<th>cal2</th>
<th>cal3</th>
<th>cal4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Acetaminiprid</td>
<td>10.000</td>
<td>25.000</td>
<td>50.000</td>
<td>75.000</td>
</tr>
<tr>
<td>2</td>
<td>1-Methyldecylamine</td>
<td>10.000</td>
<td>25.000</td>
<td>50.000</td>
<td>75.000</td>
</tr>
<tr>
<td>3</td>
<td>Allidochlor</td>
<td>10.000</td>
<td>25.000</td>
<td>50.000</td>
<td>75.000</td>
</tr>
<tr>
<td>4</td>
<td>Acetate</td>
<td>10.000</td>
<td>25.000</td>
<td>50.000</td>
<td>75.000</td>
</tr>
<tr>
<td>5</td>
<td>Carbon dioxide</td>
<td>10.000</td>
<td>25.000</td>
<td>50.000</td>
<td>75.000</td>
</tr>
</tbody>
</table>

Table 34. Calibration levels page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>Cal1-Caln</td>
<td>User-defined calibration levels for the compound.</td>
</tr>
<tr>
<td>Manage Calibration Levels</td>
<td>Defines values for each of the calibration level values for the selected compound.</td>
</tr>
</tbody>
</table>
QC Levels

Use the 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 a detailed description of all the features on the QC Levels page, see “QC levels page parameters” on page 160.

- To specify QC levels and concentrations

1. Select the compound whose QC levels, percentage test values, and concentrations you want to define.

<table>
<thead>
<tr>
<th>RT</th>
<th>Compound</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.00... Acetaminipid</td>
</tr>
<tr>
<td>2</td>
<td>7.62</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>QC levels</th>
<th></th>
<th>% Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>QC1</td>
<td>.00</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>NA</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>QC levels</th>
<th></th>
<th>% Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>QC1</td>
<td>5.00</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>.00</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>QC levels</th>
<th></th>
<th>% Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>QC1</td>
<td>5.00</td>
</tr>
<tr>
<td>2</td>
<td>QC2</td>
<td>5.00</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>.00</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Acquisition List</th>
<th>Identification</th>
<th>Detection</th>
<th>Calibration</th>
<th>Calibration levels</th>
<th>QC levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Compound</td>
<td></td>
<td></td>
<td>QC1</td>
<td>QC2</td>
</tr>
<tr>
<td>1 6.00,6.00,6.00...</td>
<td>Acetamiprid</td>
<td></td>
<td></td>
<td>10.000</td>
<td>15.000</td>
</tr>
<tr>
<td>2 7.52</td>
<td>1-Methyldodecyamine</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

7. To specify the same concentration values for all compounds, select the value 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**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>QC1-QCn</td>
<td>User-defined quality control levels for the compound.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>QC levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Level</td>
</tr>
<tr>
<td>1 QC1</td>
</tr>
<tr>
<td>2 QC2</td>
</tr>
<tr>
<td>3 QC3</td>
</tr>
</tbody>
</table>
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 253.

Figure 42. Real Time Viewer page

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Show Quan Peaks Only</td>
<td>Displays only quan peaks in the compounds list. Quan peaks are indicated with a dot in the Quan Peak column.</td>
</tr>
</tbody>
</table>

**Displayable Traces**

- **Quan Peak**: Checks indicate quan peak traces. Unchecked traces indicate confirming ions.
- **Compound Name**: Names of all compounds in the method.
- **Trace**: Lists the simple mass or precursor mass for all traces—both quan peak and confirming ion—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.
Using the Method Development Mode

Working with Master Methods

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;&lt;</td>
<td>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.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Traces to Display in Real Time Viewer (0/25)</th>
<th>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.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Move to Top</td>
<td>Moves the selected trace to the top of the Traces to Display... list and the second position in the real-time display.</td>
</tr>
<tr>
<td>Move Up</td>
<td>Moves the selected trace up one position in the list.</td>
</tr>
<tr>
<td>Move Down</td>
<td>Moves the selected trace down one position in the list.</td>
</tr>
<tr>
<td>Move to Bottom</td>
<td>Moves the selected trace to the bottom of the list.</td>
</tr>
</tbody>
</table>

Using the Shortcut Menu Commands

Each page on the Compounds page (except the Acquisition List page) 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 (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copy Down</td>
<td>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.”</td>
</tr>
<tr>
<td>Display Retention Time Column</td>
<td>Displays or hides the RT column in the compound list.</td>
</tr>
<tr>
<td>Delete Compound From Method</td>
<td>Removes the selected compound from the current master method.</td>
</tr>
</tbody>
</table>
### Table 37. Compounds page shortcut menu (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copy</td>
<td>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.</td>
</tr>
<tr>
<td>Copy With Headers</td>
<td>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.</td>
</tr>
<tr>
<td>Paste</td>
<td>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.</td>
</tr>
<tr>
<td>Undo Last Paste</td>
<td>Removes the last pasted item in the method development compound list.</td>
</tr>
<tr>
<td>Export to CSV File</td>
<td>Opens the Save As dialog box where you can save the current compound list to a .csv file.</td>
</tr>
</tbody>
</table>
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
- QC Check
- Negative
- ISTD
- Solvent Blank
- Hydrolysis
Limits

Use the Limits page to define levels of review for quantified results. Quantified results appear on printed and electronic reports. You can also define when a quantified value is reported instead of reporting less than a particular limit.

Figure 43. Limits page

![Limits page](image)

Figure 44. Limits page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>LOD (Detection Limit)</td>
<td>Limit of detection. The lowest amount that can be detected. Usually derived from a method detection limit (mdl) study.</td>
</tr>
<tr>
<td>LOQ (Quantitation Limit)</td>
<td>Limit of quantitation. The lowest amount that can be confidently and accurately quantitated. This is usually the lowest calibration amount.</td>
</tr>
<tr>
<td>Cutoff</td>
<td>Also called limit of reporting (LOR) in some industries. This is the lowest amount that can be reported, as determined by each laboratory's standard operating practices.</td>
</tr>
<tr>
<td>ULOL (Linearity Limit)</td>
<td>Upper limit of linearity. This is usually the highest calibrator amount.</td>
</tr>
<tr>
<td>Carryover Limit</td>
<td>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.</td>
</tr>
</tbody>
</table>
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 45. Calibration page

Table 38. Calibration page parameters

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

Use the QC Check 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 Quality Control report, the TraceFinder application flags the calculated values for internal standard compounds that exceed these limits.

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

**Figure 46.** QC Check page

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>Max RF Diff (%)</td>
<td>The maximum deviation between the response factor (RF) of the QC sample and the average response factor from the calibration (when in average RF mode).</td>
</tr>
<tr>
<td>Min RF</td>
<td>The minimum response factor for the QC sample (when in average RF mode).</td>
</tr>
</tbody>
</table>
Negative

Use the Negative 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.

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

❖ To specify the maximum concentration as a percentage

1. From the Method column list, select one of the following methods:
   - % of LOD
   - % of LOQ
   - % of LOR

2. In the Percentage column, type a percentage value.

❖ To specify the maximum concentration

1. From the Method column list, select Concentration.

2. In the Max Conc column, type an absolute value.

Figure 47. Negative page

Table 40. Negative page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>Method</td>
<td>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.</td>
</tr>
<tr>
<td>Percentage</td>
<td>The percentage of the LOR, LOD, or LOQ if you are using the percentage approach.</td>
</tr>
<tr>
<td>Max Conc</td>
<td>The maximum concentration if you are using an absolute value.</td>
</tr>
</tbody>
</table>
ISTD

Use the ISTD page to review the response and retention time of internal standards (if 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 you have not identified any compounds as internal standards, this page does not show any values.

Figure 48. ISTD page

Table 41. ISTD page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>Min Recovery (%)</td>
<td>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.</td>
</tr>
<tr>
<td>Max Recovery (%)</td>
<td>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.</td>
</tr>
<tr>
<td>Min RT (–min)</td>
<td>The 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.</td>
</tr>
</tbody>
</table>
**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

![Solvent Blank page](image)

**Table 42.** Solvent Blank page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>Method</td>
<td>The evaluation process to use as a response for the quan ion only (Quan Ion RT) or a summed response for the quan ion and any confirming ions (All Ion RT). To deactivate the solvent blank test for a specific compound, select <strong>None</strong>.</td>
</tr>
<tr>
<td>Upper Limit</td>
<td>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.</td>
</tr>
</tbody>
</table>
Hydrolysis

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

Figure 50. Hydrolysis page

Table 43. Hydrolysis page parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Compound</td>
<td>The compound name.</td>
</tr>
<tr>
<td>Method</td>
<td>The evaluation process to use, specified as either a lower threshold or a range. To deactivate the hydrolysis test for a specific compound, select None.</td>
</tr>
<tr>
<td>Threshold/Lower Limit</td>
<td>For compounds using the Threshold method, this specifies the threshold value for the hydrolysis test. Values below this threshold are flagged in the Hydrolysis report. For compounds using the Range method, this specifies the lower limit of the range.</td>
</tr>
<tr>
<td>Upper Limit</td>
<td>For compounds using the Range method, this parameter specifies the upper limit of the range.</td>
</tr>
</tbody>
</table>

Shortcut menu

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copy Down</td>
<td>Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, “Using Copy Down and Fill Down.”</td>
</tr>
<tr>
<td>Display Retention Time Column</td>
<td>Displays or hides the RT column in the compound list.</td>
</tr>
<tr>
<td>Delete Compound From Method</td>
<td>Removes the selected compound from the current master method.</td>
</tr>
<tr>
<td>Copy</td>
<td>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.</td>
</tr>
<tr>
<td>Copy With Headers</td>
<td>Copies the data in the selected rows or columns and the associated column headers to the Clipboard. Use this command to copy compound information to another application, such as an Excel spreadsheet.</td>
</tr>
</tbody>
</table>
Table 43. Hydrolysis page parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paste</td>
<td>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.</td>
</tr>
<tr>
<td>Undo Last Paste</td>
<td>Removes the last pasted item in the method development compound list.</td>
</tr>
<tr>
<td>Export to CSV File</td>
<td>Opens the Save As dialog box where you can save the current compound list to a .csv file.</td>
</tr>
</tbody>
</table>
Editing the Groups Page

Use the Groups page of the Master Method View to organize compounds into functional or logical groups. You can use these groups for creating a subset of target compounds. For a detailed description of all the features on the Groups page, see “Groups page parameters” on page 174.

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 you want to view.

   ![Show List]

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.

   ![Groups 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 51. Groups page

Table 44. Groups page parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compounds</td>
<td>Lists all available compounds.</td>
</tr>
<tr>
<td>Groups</td>
<td>Lists all available groups.</td>
</tr>
<tr>
<td>Add Group</td>
<td>Opens the Add a New Group dialog box where you can create a new group.</td>
</tr>
</tbody>
</table>

Shortcut menu

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empty Group</td>
<td>Removes all compounds from the selected group.</td>
</tr>
<tr>
<td>Rename Group</td>
<td>Changes the name of the selected group.</td>
</tr>
<tr>
<td>Delete Group</td>
<td>Removes the selected group and all the compounds in it.</td>
</tr>
<tr>
<td>Remove From Group</td>
<td>Removes the selected compound from its group.</td>
</tr>
</tbody>
</table>
Editing the Reports Page

Use the Reports page to specify how you want to save or print your reports. For a detailed description of the features on the Reports page, see “Reports page parameters” on page 176.

For the Quantitation Report type, you can modify quan report, user interface, quan flag, and surrogate correction options in the Report Options pane.

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 65.
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 52.** Reports page

**Table 45.** Reports page parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Example</td>
<td>Opens a PDF that displays an example of the report type.</td>
</tr>
<tr>
<td>Report Name</td>
<td>The name of a report.</td>
</tr>
<tr>
<td>Report Description</td>
<td>The user-defined description to be used on a report.</td>
</tr>
<tr>
<td>Report Type</td>
<td>The type of report: Standard, Custom, or Target Screening.</td>
</tr>
<tr>
<td>Print</td>
<td>Sends reports to the printer.</td>
</tr>
<tr>
<td>Create PDF</td>
<td>Saves reports as PDF files.</td>
</tr>
<tr>
<td></td>
<td>Available only for standard and target screening reports.</td>
</tr>
<tr>
<td>Create XML</td>
<td>Exports reports in XML format.</td>
</tr>
<tr>
<td></td>
<td>Available only for standard reports.</td>
</tr>
</tbody>
</table>
### Table 45. Reports page parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Create XLSM</td>
<td>Exports reports in Excel Macro-Enabled Workbook (.xlsx) format. Available only for custom reports.</td>
</tr>
<tr>
<td>Batch Level</td>
<td>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 <strong>B</strong> 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 65.</td>
</tr>
</tbody>
</table>
**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 specify the concentration calculation method**
- **To track the use of the tune file**

**To specify quantitation limits**

1. To report the calculated concentration at all times or only when the quantified value exceeds LOD, LOQ, or LOR, choose the appropriate value from the Report Concentration list.
   
   For a description of concentration limits, see “Editing the QAQC Page” on page 164.

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

- **Shade row when sample is outside of evaluation criteria**
- **Separate ion overlay display**
- **Use alternate calibration report format**
- **Display Quan flags and legend**

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 7 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

- **Flag values below LOD**
- **Flag values below LOQ**
- **Flag values above LDR**
- **Flag values above ULOD**
- **Flag values above Carryover**
- **Flag values between LOD and LOQ**

Select the values 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 the “**Quan Report Settings page parameters**” on page 181.
To specify the concentration calculation method

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

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

See “To specify quantitation limits” on page 178.

To track the use of the tune file

1. Select the **Enable Tune Time Tracking** check box.
   
   This option tracks the number of hours between the last instrument tune and each sample acquisition.

2. In the Tune File Lifetime box, enter the number of hours 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 53. Quan Report Settings page

Table 46. Quan Report Settings page parameters  (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Quan Limits Flags</strong></td>
<td></td>
</tr>
<tr>
<td>Report Concentration</td>
<td>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, &gt;LOD, &gt;LOQ, or &gt;LOR.</td>
</tr>
<tr>
<td>Decimal Places to Be Reported</td>
<td>Number of decimal places to be included in the report. Maximum value is 6.</td>
</tr>
<tr>
<td>Show Chromatogram on Quantitation Report</td>
<td>Displays a chromatogram (TIC trace) of the sample on the quantitation report.</td>
</tr>
<tr>
<td>Display Compounds Above Set Limit</td>
<td>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.</td>
</tr>
<tr>
<td><strong>User Interface Options</strong></td>
<td></td>
</tr>
<tr>
<td>Shade Row When Sample is Outside of Evaluation Criteria</td>
<td>Shades a compound row on any of the reports if a value fails one of the criteria used for evaluation.</td>
</tr>
<tr>
<td>Separate Ion Overlay Display</td>
<td>Separates the ion overlay pane from the confirming ion plots in data review.</td>
</tr>
<tr>
<td>Use Alternate Calibration Report Format</td>
<td>Uses an alternate format for the Calibration Report that is designed to print more concisely (this report is limited to a maximum of 7 calibration standards).</td>
</tr>
<tr>
<td>Display Quan Flags and Legend</td>
<td>Displays manual flags, confirming manual flags, quan flags, and a legend on high density reports.</td>
</tr>
</tbody>
</table>
Table 46. Quan Report Settings page parameters  (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Quan Flag Options</strong></td>
<td>Values that are above or below limits defined on the Limits page. These flags appear on a variety of reports.</td>
</tr>
<tr>
<td>Flag Values Below LOD</td>
<td>Flags values below the limit of detection (LOD).</td>
</tr>
<tr>
<td>Flag Values Below LOQ</td>
<td>Flags values below the limit of quantitation (LOQ).</td>
</tr>
<tr>
<td>Flag Values Above LOR</td>
<td>Flags values above the limit of reporting (LOR).</td>
</tr>
<tr>
<td>Flag Values Above ULOL</td>
<td>Flags values above the upper limit of linearity (ULOL).</td>
</tr>
<tr>
<td>Flag Values Above Carryover</td>
<td>Flags values above the carryover limit.</td>
</tr>
<tr>
<td>Flag Values Between LOD and LOQ</td>
<td>Flags values between the limit of detection and the limit of quantitation known as the J flag.</td>
</tr>
<tr>
<td><strong>Calculated Amount Option</strong></td>
<td></td>
</tr>
<tr>
<td>Calculate Concentration As</td>
<td>Specifies the Rounded or Truncated method for reporting concentration amounts.</td>
</tr>
<tr>
<td><strong>Tune Time Tracking Options</strong></td>
<td></td>
</tr>
<tr>
<td>Enable Tune Time Tracking</td>
<td>Tracks the number of hours between the last instrument tune and each sample acquisition.</td>
</tr>
<tr>
<td>Tune File Lifetime</td>
<td>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.</td>
</tr>
</tbody>
</table>
Specifying Target Screening Settings

Use the options on the Target Screening Settings page to set the parameters required to produce Target Screening reports. For a detailed description of the features on the Target Screening Settings page, see “Target Screening Settings page parameters” on page 186.

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 188.

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 MS³ 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

<table>
<thead>
<tr>
<th>Semi Quantitative:</th>
<th>Measurement Unit (e.g. ng/ml): ng/ml</th>
</tr>
</thead>
<tbody>
<tr>
<td>Report Semi-Quantitative Result</td>
<td>Scan Intensity</td>
</tr>
<tr>
<td>Calculation based on:</td>
<td>⚫</td>
</tr>
</tbody>
</table>

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

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 quan ion.
   
   For example, when the Ion Ratio Window is 20% and the quan 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

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

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 54.** Target Screening Settings page

**Table 47.** Target Screening Settings page parameters  (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Processing Configuration File</td>
<td>Specifies a configuration file (.csv).</td>
</tr>
<tr>
<td>Screening Method</td>
<td>Specifies one of the following screening methods:</td>
</tr>
<tr>
<td></td>
<td>• (Default) Auto Detect</td>
</tr>
<tr>
<td></td>
<td>• Based on Full MS2 scans</td>
</tr>
<tr>
<td></td>
<td>• Based on SRM and MS2 scans</td>
</tr>
<tr>
<td></td>
<td>• Based on MS2 and MS3 scans</td>
</tr>
<tr>
<td></td>
<td>• Based on MS3 scans</td>
</tr>
<tr>
<td></td>
<td>• Based on accurate mass scans</td>
</tr>
<tr>
<td></td>
<td>• Based on SRM scans</td>
</tr>
<tr>
<td></td>
<td>• Based on Exactive screening method</td>
</tr>
<tr>
<td><strong>Note</strong></td>
<td>Using the Auto Detect method, the ToxID application can identify the screening experiment implemented in the acquired data file.</td>
</tr>
<tr>
<td>Company Name</td>
<td>Specifies the name of the company to print on the report.</td>
</tr>
<tr>
<td>Laboratory Name</td>
<td>Specifies the name of the laboratory to print on the report.</td>
</tr>
<tr>
<td>Company Logo</td>
<td>Specifies a graphic file (.jpg, .gif, or .bmp) to print on the report.</td>
</tr>
<tr>
<td>m/z Window (mu)</td>
<td>Specifies a value for the window above and below the m/z value for the compounds.</td>
</tr>
</tbody>
</table>
Table 47. Target Screening Settings page parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT Window (min)</td>
<td>Specifies a value for the window above and below the retention time value for the compounds.</td>
</tr>
<tr>
<td>MS2 Search Library</td>
<td>Specifies the names of as many as three search libraries for searching MS/MS spectra.</td>
</tr>
<tr>
<td>MS3 Search Library</td>
<td>Specifies the names of as many as three search libraries for searching MS3 spectra.</td>
</tr>
<tr>
<td>Use Full MS Scan to Confirm</td>
<td>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.</td>
</tr>
<tr>
<td>Semi Quantitative</td>
<td></td>
</tr>
<tr>
<td>Report Semi-Quantitative Result</td>
<td></td>
</tr>
<tr>
<td>Measurement Unit</td>
<td></td>
</tr>
<tr>
<td>Calculation Based On</td>
<td>Specifies one of the following calculation methods:</td>
</tr>
<tr>
<td></td>
<td>• Scan Intensity: Specifies that the application measures the intensity of the MS/MS peak without performing background subtraction.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td>Ion Ratio Calculation Method (In SRM Experiment)</td>
<td></td>
</tr>
<tr>
<td>Use Scan at Peak Apex</td>
<td>Specifies that the application calculates the ion ratio based on the peak apex scan spectrum.</td>
</tr>
<tr>
<td>Use Average Scan</td>
<td>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.</td>
</tr>
<tr>
<td>Ion Ratio Window(%)</td>
<td></td>
</tr>
<tr>
<td>Exact Mass Experiment</td>
<td></td>
</tr>
<tr>
<td>Exact Mass Window</td>
<td>Specifies a value in parts per million for the accurate mass experiment.</td>
</tr>
<tr>
<td>Exactive</td>
<td></td>
</tr>
<tr>
<td>Adduct 1–n</td>
<td>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+</td>
</tr>
<tr>
<td>No Specified Retention Time</td>
<td>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.</td>
</tr>
<tr>
<td>Report All Compounds Listed in Configuration File</td>
<td>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.</td>
</tr>
</tbody>
</table>
Figure 55. 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
Acquisition 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 1

Peak 2

Peak 3

Peak 4

Peak 5

Peak 6

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-Acetylcodine | 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.

   ![Method Development](image)

   The Method Development navigation pane opens.

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

   ![Method View](image)

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 195.
To specify peak criteria

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 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 quan mass and two confirming ions.

   The system selects the most intense ion to use as the quantitation mass and uses this mass for the mathematical operations.
2. To define the criteria for evaluating confirming or qualifying ions, select the **Specify Default Ion Ratio Ranges** check box and set the following values:

   a. To specify the maximum difference in retention time between a confirming ion peak and the quantification ion peak, set a value in the Ion Coelution (min) box.

   b. To specify an absolute or relative calculation approach for determining the acceptable ion ratio range, select **Absolute** or **Relative** from the Window Type list.

   c. To specify the acceptable ion ratio range, set a value in the Window (+/- %) box.

3. To include the peak spectrum in the processing method, select the **Include Compound Peak Spectrum as Reference Spectrum** check box.

   ✤ **To calibrate the compounds**

   ![Calibrate the compounds](image)

   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 you specify. For additional information about the Genesis algorithm, see “Genesis Detection Method” on page 74.

2. Select or clear the **Exclude Matching Quan Peaks** check box and specify a value for the exclusion window.

   The application excludes quan peaks in a range plus/minus the value 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\2.0\ClinTox\Templates\Methods
Figure 56. Method Template Editor dialog box
Table 48. Method Template Editor dialog box parameters (Sheet 1 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Find the peaks</strong></td>
<td><strong>Description</strong></td>
</tr>
<tr>
<td>Sensitivity</td>
<td>Defines how extensively the peak detector algorithm searches for low-level peaks.</td>
</tr>
<tr>
<td>Limit the Retention Time Range</td>
<td>Min RT specifies the beginning of the range. Max RT specifies the end of the range.</td>
</tr>
<tr>
<td>Enable Peak Threshold</td>
<td>Specifies whether to select peaks by relative height or area and the percentage of the highest peak that results in compound selection.</td>
</tr>
<tr>
<td>Only Select Top Peaks</td>
<td>Displays a specific number of the largest peaks by height or area.</td>
</tr>
<tr>
<td><strong>Identify the peaks</strong></td>
<td><strong>Description</strong></td>
</tr>
<tr>
<td>Use These Libraries</td>
<td>Lists the libraries you can search.</td>
</tr>
<tr>
<td>Limit Library Hits</td>
<td>Specifies the number of hits returned when the system searches a spectrum against the selected libraries.</td>
</tr>
<tr>
<td>Best Match Method</td>
<td>Specifies how to sort the library searches. Valid values: Search Index, Reverse Search Index, Match Probability</td>
</tr>
<tr>
<td><strong>Handle confirming ions</strong></td>
<td><strong>Description</strong></td>
</tr>
<tr>
<td>Include Confirming Ions/Number Of Confirming Ions</td>
<td>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 quant mass and two confirming ions.</td>
</tr>
<tr>
<td>Specify Default Ion Ratio Ranges</td>
<td>Enables the ion ratio range features.</td>
</tr>
<tr>
<td></td>
<td>Ion Coelution specifies the maximum difference in retention time between a confirming ion peak and the quantification ion peak.</td>
</tr>
<tr>
<td></td>
<td>Window Type specifies an Absolute or Relative calculation approach for determining the acceptable ion ratio range.</td>
</tr>
<tr>
<td></td>
<td>Window (+/-%) specifies the acceptable ion ratio range.</td>
</tr>
<tr>
<td>Include Compound Peak Spectrum as Reference Spectrum</td>
<td>Includes the peak spectrum in the processing method. Use this setting to perform a spectra comparison in Data Review.</td>
</tr>
<tr>
<td><strong>Calibrate the compounds</strong></td>
<td><strong>Description</strong></td>
</tr>
<tr>
<td>Calibration Method</td>
<td>Specifies an internal or external calibration method.</td>
</tr>
<tr>
<td>Curve Type</td>
<td>Specifies a linear, quadratic, or average RF curve type.</td>
</tr>
</tbody>
</table>
Table 48. Method Template Editor dialog box parameters (Sheet 2 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin</td>
<td>Specifies that the origin is ignored, forced, or included in the generated calibration curve.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td></td>
<td>• Force: Specifies that the calibration curve passes through the origin of the data point plot when the calibration curve is generated.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td>Weighting</td>
<td>Specifies the weighting for the calibration data points.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td></td>
<td>• 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).</td>
</tr>
<tr>
<td></td>
<td>• 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).</td>
</tr>
<tr>
<td>Response Via</td>
<td>Specifies if the TraceFinder application uses area or height in response calculations.</td>
</tr>
<tr>
<td></td>
<td>• Area: Specifies that the application use this peak area value in response calculations.</td>
</tr>
<tr>
<td></td>
<td>• Height: Specifies that the application use this peak height value in response calculations.</td>
</tr>
<tr>
<td>Qualitative Peak Processing</td>
<td>The application uses the Genesis algorithm to match internal standards.</td>
</tr>
<tr>
<td>Use Genesis Algorithm For Qual Processing</td>
<td></td>
</tr>
<tr>
<td>ISTD Matching</td>
<td>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.</td>
</tr>
</tbody>
</table>
Table 48. Method Template Editor dialog box parameters  (Sheet 3 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exclude Matching Quan Peaks</td>
<td>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.</td>
</tr>
<tr>
<td>Exclusion Window</td>
<td>Defines a range plus/minus the Exclusion Window value you specify.</td>
</tr>
<tr>
<td>Use Data Dependent Scans</td>
<td>Constrains the Qual Mode view in the Data Review to only data-dependent scan spectra. See “Qual Mode” on page 313. In addition to the peak information, the TIC Report and TIC Summary report display information about the data-dependent filtered data.</td>
</tr>
</tbody>
</table>
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\2.0\ClinTox\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.

   ![Import Published Method dialog box]

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\2.0\ClinTox\Methods

   You can use any of the Open Method commands to open this method just as you would a method 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 86.

To export SRM data to an XML file

1. Open the master method whose SRM data 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\2.0\ClinTox\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 57. SRM TSQ Quantum™ example

```xml
<xml version="1.0" encoding="UTF-8"
TSQMassList
  TSQListItem
    ParentMass
    ProductMass
    CollisionEnergy
    StartTime
    StopTime
    Polarity
    Name
  TSQListItem
    ParentMass
    ProductMass
    CollisionEnergy
    StartTime
    StopTime
    Polarity
    Name
```
**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.

   - New instrument method
   - Open instrument method
   - Import published method
To create a new instrument method


   The Thermo Xcalibur Instrument Setup window opens.

   **Figure 58.** Example instrument setup showing multiple configured instruments

2. Click the icon for the instrument 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.

![File Summary Information dialog box](image)

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:

```plaintext
...\Xcalibur\methods
```
To create a new multiplexing instrument method


   The Thermo Xcalibur Instrument Setup window opens.

**Figure 59.** Example instrument setup showing a configured multiplexed instrument

2. Click the icon for the instrument 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 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.

![File Summary Information dialog box](image)

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


2. In the browser, select an instrument method from the list and open the file. 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 to another name.

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

**Figure 60.** 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.

![Import Published Method dialog box]

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

   For instructions for importing the master methods, see “Importing Published Master Methods” on page 199.

3. Click Import.

   The Save Instrument Method dialog box opens.

![Save Instrument Method dialog box]

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](image)

   The Method Development navigation pane opens.

2. In the Method Development navigation pane, click **Development Batch**.

   ![Development Batch](image)

   The Development Batch view opens a new, empty batch.

<table>
<thead>
<tr>
<th>Development Batch - [C:\Thermo\TraceFinder\2.0\ClinTox\Temp]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filename</td>
</tr>
<tr>
<td>----------</td>
</tr>
<tr>
<td>1</td>
</tr>
</tbody>
</table>

**Note** The Channel column is available only when you have enabled multiplexing in the Configuration mode. See “Multiplexing” on page 87.
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\2.0\ClinTox\Temp

2. In the browser, do one of the following:

   Locate the folder 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 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.”

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 87.

Figure 61. Completed Development Batch

<table>
<thead>
<tr>
<th>Development Batch</th>
<th>Filename</th>
<th>Sample ID</th>
<th>Sample name</th>
<th>Vial position</th>
<th>Injection volume</th>
<th>Instrument Method</th>
<th>Channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>File1</td>
<td>1</td>
<td></td>
<td>1</td>
<td>100</td>
<td>Anabolic Steroids</td>
<td>Channel 1</td>
</tr>
<tr>
<td>2</td>
<td>File2</td>
<td>2</td>
<td></td>
<td>2</td>
<td>100</td>
<td>Anabolic Steroids</td>
<td>Channel 2</td>
</tr>
</tbody>
</table>
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 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 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\2.0\ClinTox\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

In 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 84.

✦ **To run a quick acquisition**

1. Choose Go > Quick Acquire Sample from the main menu.

   The Quick Acquisition dialog box opens.

   ![Quick Acquisition dialog box]

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 254.
   - 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 \( \mu L \); the maximum injection volume allowed is 5000 \( \mu L \).

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 254.
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 87.

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 251.
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 62.** Task pane when you enter the Acquisition mode

![Task pane](image)

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 63. Example task pane when you have completed the Acquisition mode.

Categories in the Sample Definition list:
- QC Samples: QC
- Calibration Samples: Calibrator
- Blank Samples: Negative
- 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**

To create an original batch, start with the instructions “To start a new batch” on page 224.

❖ **To acquire a previously saved (.tbr) batch**

To acquire a previously saved batch, start with the instructions “To select a ready-to-acquire batch” on page 226.
To edit and process a previously acquired batch

To process a previously acquired batch, start with the instructions “To select a previously acquired batch” on page 227.

To create a batch template

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 228 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.

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 229.
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.

   ![New Batch Table](image)

   **New batch**

<table>
<thead>
<tr>
<th>Project:</th>
<th>Ready to acquire</th>
<th>Acquired batches</th>
<th>Template</th>
</tr>
</thead>
<tbody>
<tr>
<td>Project1</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

   **Available Templates**

<table>
<thead>
<tr>
<th>Template name</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Batch_Template4600</td>
<td>Method1</td>
</tr>
</tbody>
</table>

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 229.
5 Using the Acquisition Mode

Working with Batches

❖ 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\2.0\ClinTox\Projects\projectname\subprojectname

2. Select the batch you want to acquire.

   ![Batch List Table]

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 samples 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 242.

   –Or–

   To edit the samples list, click **Previous**.
   
   For detailed instructions, see “Defining the Sample List” on page 229.

   –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\2.0\ClinTox\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 229.

   - 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.
5 Using the Acquisition Mode

Working with Batches

❖ 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” on page 229.
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. See “Sample Definition view” on page 236.

As you enter sample values, you can use the Copy Down and Fill Down commands to 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 238.
- When you are editing a previously acquired batch or a .tbr batch, the Finish Selection view opens. See “Submitting the Batch” on page 242.

**To add samples to the list**

1. Select the number of sample rows to add and click Add.

2. Type a file name in the Filename column for each sample. Each file name must be unique.

3. Select a sample type from the Sample Type list for each sample.

<table>
<thead>
<tr>
<th>Available sample types</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specimen</td>
</tr>
<tr>
<td>Specimen/Qual</td>
</tr>
<tr>
<td>QC</td>
</tr>
<tr>
<td>Solvent</td>
</tr>
<tr>
<td>Calibrator</td>
</tr>
<tr>
<td>Hydrolysis</td>
</tr>
<tr>
<td>Unextracted</td>
</tr>
<tr>
<td>Negative</td>
</tr>
</tbody>
</table>

For a detailed description of each sample type, see “Sample Types” on page 266.
4. For each Calibrator or QC sample, select a level from the Level list.

   The sample levels are defined in the master method. If there 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 samples 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, specimen samples.

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

   2. Select the number of samples to insert and click **Insert**.

      The application inserts the Specimen samples above the selected sample.

<table>
<thead>
<tr>
<th>Status</th>
<th>Filename</th>
<th>Sample Type</th>
<th>Level</th>
<th>Sample ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cal_5</td>
<td>Calibrator</td>
<td>10</td>
<td>cal = 5 ng/μL</td>
</tr>
<tr>
<td>2</td>
<td>Unknown2</td>
<td>Specimen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Unknown1</td>
<td>Specimen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>cal_10</td>
<td>Calibrator</td>
<td>10</td>
<td>cal = 10 ng/μL</td>
</tr>
</tbody>
</table>
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 266.

<table>
<thead>
<tr>
<th>Available sample types</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specimen</td>
</tr>
<tr>
<td>Solvent</td>
</tr>
<tr>
<td>Unextracted</td>
</tr>
</tbody>
</table>

5. For each Calibrator or QC sample, click the Level cell and select a level from the list.
   The sample levels are defined in the master method. If there are no levels to select from the Level list, ask a user with 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 samples 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**.

   The Sample Import Tool dialog box opens.

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 Samples list.

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

<table>
<thead>
<tr>
<th>Xcalibur column</th>
<th>TraceFinder column</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position</td>
<td>Vial position</td>
</tr>
<tr>
<td>Inj Vol</td>
<td>Injection volume</td>
</tr>
<tr>
<td>Dil Factor</td>
<td>Conversion Factor</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Xcalibur sample type</th>
<th>TraceFinder sample type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blank</td>
<td>Negative</td>
</tr>
<tr>
<td>Std Bracket</td>
<td>Calibrator</td>
</tr>
</tbody>
</table>

5. For each Calibrator or QC sample, click the Level cell and select a level from the list.

   The sample levels are defined in the master method. If there are no levels to select from the Level list, ask a user with 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 samples 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).

<table>
<thead>
<tr>
<th>Sample Name</th>
<th>Type</th>
<th>Channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>cal_50_INJ001</td>
<td>Calibrator</td>
<td>10</td>
</tr>
<tr>
<td>cal_50_INJ002</td>
<td>Calibrator</td>
<td>10</td>
</tr>
<tr>
<td>cal_50</td>
<td>Calibrator</td>
<td>10</td>
</tr>
<tr>
<td>cal_10_INJ001</td>
<td>Calibrator</td>
<td>10</td>
</tr>
<tr>
<td>cal_10</td>
<td>Calibrator</td>
<td>10</td>
</tr>
</tbody>
</table>

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 87.

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 84.

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 (the rightmost column in the sample list).

<table>
<thead>
<tr>
<th>Channel</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Auto</td>
<td></td>
</tr>
<tr>
<td>Channel 1</td>
<td></td>
</tr>
<tr>
<td>Channel 2</td>
<td></td>
</tr>
<tr>
<td>Channel 3</td>
<td></td>
</tr>
<tr>
<td>Channel 4</td>
<td></td>
</tr>
</tbody>
</table>

   Note: The Channel column is available only when you have enabled multiplexing in the Configuration mode. See “Multiplexing” on page 87.

   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.
5 Using the Acquisition Mode
Working with Batches

Figure 64. Sample Definition view

Table 49. Sample Definition view parameters  (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Sample Controls</strong></td>
<td></td>
</tr>
<tr>
<td>Add</td>
<td>Adds the specified number of empty rows to the sample grid.</td>
</tr>
<tr>
<td>Insert</td>
<td>Inserts the specified number of empty rows above the selected row.</td>
</tr>
<tr>
<td>Import</td>
<td>Opens the Sample Import Tool where you can import samples defined in a .csv file or an .xml file.</td>
</tr>
<tr>
<td>Multiplexing Channels</td>
<td>These features are available only when you have enabled multiplexing in the Configuration mode. See “Multiplexing” on page 87.</td>
</tr>
<tr>
<td>All Channels</td>
<td>Uses all configured channels to acquire this batch.</td>
</tr>
<tr>
<td>Channel 1-n</td>
<td>Uses only the selected channels to acquire this batch.</td>
</tr>
<tr>
<td>Previous</td>
<td>Returns you to the previous Acquisition mode view.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Confirms that you want to exit the Acquisition mode. When you cancel out of the Acquisition mode, your edits are not saved.</td>
</tr>
<tr>
<td>Save</td>
<td>Saves this batch as a to-be-run (.tbr) batch.</td>
</tr>
<tr>
<td>Next</td>
<td>Takes you to the next Acquisition mode view.</td>
</tr>
<tr>
<td><strong>Shortcut menu</strong></td>
<td></td>
</tr>
<tr>
<td>Add Sample</td>
<td>Adds a single empty row to the sample grid.</td>
</tr>
<tr>
<td>Insert Sample</td>
<td>Inserts a single empty row to the sample grid above the selected row.</td>
</tr>
<tr>
<td>Insert Copy Sample</td>
<td>Copies the currently selected row and inserts a copy above the row.</td>
</tr>
<tr>
<td>Reinject Selected Samples</td>
<td>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.</td>
</tr>
<tr>
<td>Remove Selected Samples</td>
<td>Removes selected samples from the sample grid.</td>
</tr>
<tr>
<td>Import Samples</td>
<td>Opens the Sample Import Tool. See “To import samples into the list” on page 232.</td>
</tr>
</tbody>
</table>
### Table 49. Sample Definition view parameters  (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copy Down</td>
<td>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.”</td>
</tr>
<tr>
<td>Fill Down</td>
<td>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.”</td>
</tr>
<tr>
<td>Modify Columns</td>
<td>Opens the Modify Columns dialog box. See “Column Display” on page 286.</td>
</tr>
<tr>
<td>Copy</td>
<td>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.</td>
</tr>
<tr>
<td>Copy With Headers</td>
<td>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 Acquisition mode sample list.</td>
</tr>
<tr>
<td>Paste</td>
<td>Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column.</td>
</tr>
<tr>
<td>Undo Last Paste</td>
<td>Removes the last pasted item in the Acquisition mode sample list.</td>
</tr>
<tr>
<td>Export to CSV File</td>
<td>Opens the Save As dialog box where you can save the current sample list to a .csv file.</td>
</tr>
<tr>
<td>Status Color Codes</td>
<td>![Sample status icons]</td>
</tr>
<tr>
<td>Sample is not acquired.</td>
<td></td>
</tr>
<tr>
<td>Sample is acquired but not processed.</td>
<td></td>
</tr>
<tr>
<td>Sample is acquired and processed.</td>
<td></td>
</tr>
<tr>
<td>Sample is currently acquiring.</td>
<td></td>
</tr>
</tbody>
</table>
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 240. 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 have finished specifying your report options, click Next to go to the Finish view and submit your batch. See “Submitting the Batch” on page 242.

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

\...\TraceFinder\2.0\ClinTox\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 65.** Report Selection view

---

**Table 50.** Report Selection parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Example</td>
<td>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.</td>
</tr>
<tr>
<td>Report Name</td>
<td>The name of a report.</td>
</tr>
<tr>
<td>Report Description</td>
<td>User-editable description to be used on a report.</td>
</tr>
<tr>
<td>Report Type</td>
<td>The type of report: Standard, Custom, or Target Screening.</td>
</tr>
<tr>
<td>Print</td>
<td>Reports to be sent to the printer.</td>
</tr>
<tr>
<td>Create PDF</td>
<td>Reports to be saved as PDF files. Available only for standard and target screening reports.</td>
</tr>
<tr>
<td>Create XML</td>
<td>Reports to be exported in XML format. Available only for standard reports.</td>
</tr>
<tr>
<td>Create XLSM</td>
<td>Reports to be exported in Excel Macro-Enabled Workbook (.xlsm) format. Available only for custom reports.</td>
</tr>
</tbody>
</table>
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 65.

## Shortcut menu:
- **Copy Down**
  - Copies the selected or cleared state to all subsequent reports in the column.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Batch Level</td>
<td>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 65.</td>
</tr>
</tbody>
</table>
**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 249.

**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.

2. To add calibration data from the current batch to the selected calibration file, select the Extend Calibration option.

Note: You must acquire at least one batch with the current method to create a .calx calibration file.
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 51. Instrument states

<table>
<thead>
<tr>
<th>Instrument state</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turn Device On</td>
<td>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</td>
</tr>
<tr>
<td>Turn Device Standby</td>
<td>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.</td>
</tr>
<tr>
<td>Turn Device Off</td>
<td>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.</td>
</tr>
</tbody>
</table>

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 a detailed description of the parameters, see “Submit Options dialog box” on page 246.

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.

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 66.** Submit Options dialog box

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>User Name</td>
<td>Name of the current user.</td>
</tr>
<tr>
<td>Acquire Data</td>
<td>(Default) Submits the current batch to acquisition.</td>
</tr>
<tr>
<td>Process Data</td>
<td>(Default) Processes the data for the current batch.</td>
</tr>
</tbody>
</table>
**Table 52.** Submit Options dialog box parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Create Reports</td>
<td>Creates reports for the current batch.</td>
</tr>
<tr>
<td><strong>Acquisition pane</strong></td>
<td></td>
</tr>
<tr>
<td>Device Name</td>
<td>Lists all configured instruments.</td>
</tr>
<tr>
<td></td>
<td>If the instrument you want to use is not configured, close the TraceFinder</td>
</tr>
<tr>
<td></td>
<td>application, configure the instrument, and then reopen the TraceFinder</td>
</tr>
<tr>
<td></td>
<td>application. You cannot configure an instrument while the TraceFinder</td>
</tr>
<tr>
<td></td>
<td>application is running.</td>
</tr>
<tr>
<td>Use</td>
<td>Specifies the instruments used for this acquisition.</td>
</tr>
<tr>
<td>Start Device</td>
<td>Specifies the instrument that initiates the communication with the other</td>
</tr>
<tr>
<td></td>
<td>instruments. This is usually the autosampler.</td>
</tr>
<tr>
<td>Start When Ready</td>
<td>Starts the specified device when all the instruments are ready to acquire</td>
</tr>
<tr>
<td></td>
<td>data. When this is cleared, individual instruments can start at different</td>
</tr>
<tr>
<td></td>
<td>times and then must wait for the last instrument to be ready.</td>
</tr>
<tr>
<td>Priority Sequence</td>
<td>With multiplexing enabled, places the batch immediately after the currently</td>
</tr>
<tr>
<td></td>
<td>acquiring batch.</td>
</tr>
<tr>
<td></td>
<td>Without multiplexing enabled, specifies one of the following priority</td>
</tr>
<tr>
<td></td>
<td>options to place the batch in the queue:</td>
</tr>
<tr>
<td></td>
<td>• <strong>Next Available Batch</strong> places the batch immediately after the currently</td>
</tr>
<tr>
<td></td>
<td>acquiring batch.</td>
</tr>
<tr>
<td></td>
<td>• <strong>Next Available Sample</strong> places the batch immediately after the currently</td>
</tr>
<tr>
<td></td>
<td>acquiring sample.</td>
</tr>
<tr>
<td>Post-run System</td>
<td>Specifies the system state after it acquires the last batch.</td>
</tr>
<tr>
<td>State</td>
<td>On (default), Standby, or Off.</td>
</tr>
<tr>
<td>Hide/Show Details</td>
<td>Collapses or expands the acquisition details of the Submit Options dialog</td>
</tr>
<tr>
<td></td>
<td>box.</td>
</tr>
<tr>
<td>OK</td>
<td>Begins the selected processes.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Closes the Submit Options dialog box without submitting any tasks.</td>
</tr>
</tbody>
</table>
To view the output files

- The TraceFinder application writes saved batches to the subproject folder with the file extension .tbr (to be run):

  …\TraceFinder\2.0\ClinTox\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
Using the Acquisition Mode

Working with Batches

Figure 67. Finish view

Review the batch

System Status

- Devices
  - Accela A5

- Batch Status
  - Project: Default
    - SubProject: Default
    - Name: Batch Sample

- Sequence Status
  - Number of samples: 6
  - Number of unacquired samples: 6

- Reports Status
  - Print: 0
    - PDF: 3
    - XML: 5
    - XLSM: 4

- Method Status
  - Local method: Batch_Sample_Method1A
  - Instrument method: Instrument1
  - Number of compounds: 1

System Startup Method

- AS Method 1

System Shutdown Method

- AS Method 2
  - Auto TSRM Update

Calibration

- Extend calibration
  - Batch.calx

Table 53. Finish view parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>System Status</td>
<td>The System Status pane displays the following:</td>
</tr>
<tr>
<td></td>
<td>• Devices used for the acquisition</td>
</tr>
<tr>
<td></td>
<td>• Project, subproject, and name of the batch</td>
</tr>
<tr>
<td></td>
<td>• Number of samples in the batch</td>
</tr>
<tr>
<td></td>
<td>• Number of standard and custom reports to be printed and saved as PDF, XML, or XLSM files</td>
</tr>
<tr>
<td></td>
<td>• Local method and instrument method used for the batch</td>
</tr>
<tr>
<td></td>
<td>• Number of compounds in the method</td>
</tr>
<tr>
<td>System Startup Method</td>
<td>The instrument method that runs before the batch. No autosampler injection takes place. This feature is not available for all instruments.</td>
</tr>
<tr>
<td>System Shutdown Method</td>
<td>The instrument method that runs after the batch. No autosampler injection takes place. This feature is not available for all instruments.</td>
</tr>
</tbody>
</table>
### Table 53. Finish view parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Auto TSRM Update</td>
<td>Updates the TSQ method with mass transitions, collision energy, and other appropriate data for TSRM functionality.</td>
</tr>
</tbody>
</table>
| 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 84.

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 254.

      - 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 254.
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 68.** 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**, **Pause** buttons to control batches in the Acquisition queue.
Instrument Page

Use the Instrument page to monitor the currently acquiring sample.

<table>
<thead>
<tr>
<th>Acquisition</th>
<th>Instrument</th>
<th>Devices</th>
<th>Queues</th>
</tr>
</thead>
<tbody>
<tr>
<td>Instrument:</td>
<td>Xcalibur Instrument</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Run state:</td>
<td>Acquiring</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Batch:</td>
<td>Batch_2011_9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sample ID:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vis:</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Filename:</td>
<td>Unknown1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inst. method:</td>
<td>C:\Thermo\TraceFinder\2.0...</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Devices:

<table>
<thead>
<tr>
<th>Name</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accela A5</td>
<td>Running</td>
</tr>
</tbody>
</table>
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 access the Aria multiplexing controls
- To control the channels
- To view the pressure trace

**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 access the Aria multiplexing controls**

Click **Direct Control**.

The AriaMuxVi Direct Ctl dialog box opens.

For a detailed description of the features in this dialog box, refer to the *Transcend Systems with Xcalibur Software User Guide*. 
To control the channels

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

Table 54. Autosampler shortcut menu commands

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>On</td>
<td>Turns on a stopped pump and continues acquiring the sample list assigned to that channel.</td>
</tr>
<tr>
<td>Off</td>
<td>After the current sample completes, the application stops acquiring and the pump shuts down.</td>
</tr>
<tr>
<td>Standby</td>
<td>After the current sample completes, the application stops acquiring. The pump continues to run.</td>
</tr>
</tbody>
</table>
| 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 \texttt{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 \texttt{Pres 1} or \texttt{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.
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 261.

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).
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 69.** Queue-level shortcut menu

<table>
<thead>
<tr>
<th>Real time status</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Acquisition</strong></td>
</tr>
<tr>
<td><img src="" alt="Acquisition Queue - 1 batch (Ready)" /></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

**Table 55.** Queue-level shortcut menu commands (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pause Queue</td>
<td>After the current sample completes, the application pauses the specified queue. Only the selected queue is affected.</td>
</tr>
<tr>
<td>Stop Active Batch</td>
<td>Removes all pending samples from the specified queue. The active sample is not affected.</td>
</tr>
</tbody>
</table>
Batch-Level Commands

Use the batch-level commands to pause or remove entire batches or samples within batches from any of the queues on the Queues page. See “Batch-level shortcut menu” on page 263.

Follow these procedures:

• To stop a batch

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

     \[\textbf{Note}\] 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).

     \[\textbf{Note}\] 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.

---

**Table 55. Queue-level shortcut menu commands (Sheet 2 of 2)**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stop All Batches</td>
<td>Removes all pending samples and batches from the specified queue. The active sample is not affected.</td>
</tr>
<tr>
<td>Remove Pending Batches</td>
<td>Removes all pending batches from the specified queue. The active batch is not affected.</td>
</tr>
</tbody>
</table>
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.

![Batch-level shortcut menu](image)

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

**Figure 70**. Batch-level shortcut menu

![Real time status](image)

**Table 56.** Batch-level shortcut menu commands

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stop Batch</td>
<td>After the current sample completes, the application removes all samples in the selected batch.</td>
</tr>
<tr>
<td>Remove Pending Batch</td>
<td>Removes all samples from the selected pending batch.</td>
</tr>
<tr>
<td>Remove Pending Samples</td>
<td>Removes all pending samples from the selected batch.</td>
</tr>
</tbody>
</table>
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 161.

❖ 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 71. 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.”

**Figure 72. Sample type definitions**

<table>
<thead>
<tr>
<th>Sample type</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Negative</td>
<td>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.</td>
</tr>
<tr>
<td>Unextracted</td>
<td>Similar to a Negative sample, but contains target compounds. By analyzing a sample, you can confirm that there are no residual compounds in the solvent system that can cause erroneous results.</td>
</tr>
<tr>
<td>Calibrator</td>
<td>(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.</td>
</tr>
<tr>
<td>QC</td>
<td>(Quality Check) Contains a known amount of one or more specific target compounds. The application places check standard samples in the sequence so that it can test quantitative analysis results for quality assurance purposes. After the application analyzes the QC sample, it compares the measured quantity with the expected value and an acceptability range. The quantitative analysis of a QC sample is classified as passed if the difference between the observed and expected quantities is within the user-defined tolerance. A QC sample is classified as failed if the difference between the observed and expected quantities is outside the user-defined tolerance.</td>
</tr>
<tr>
<td>Solvent</td>
<td>Contains only solvent.</td>
</tr>
<tr>
<td>Specimen</td>
<td>Used for quantitative analysis of samples.</td>
</tr>
<tr>
<td>Specimen/Qual</td>
<td>Used for quantitative and qualitative analysis of samples.</td>
</tr>
<tr>
<td>Hydrolysis</td>
<td>Checks the degradation of compounds dissolved in water.</td>
</tr>
</tbody>
</table>
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

In the Analysis mode, you can

- 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.

![Analysis Navigation Pane](image)
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 84.

**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 254.
   - 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.

![Quick Acquisition dialog box]

  c. In the Injection Volume box, type an injection volume.
  d. Click OK.
  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 254.
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.

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:

- Use the sample list to create a batch. See “Creating a New Batch” on page 275.
- Use the Automated Batch Reports pane to select the type of output formats you want to generate for the reports. See “Editing Report Output Formats” on page 286.
- Use the Compound Active Status pane to make specific compounds active or inactive. See “Setting Compound Active Status” on page 288.

Use the Batch View toolbar or shortcut menu to create the sample list and submit samples for acquisition. See “Batch View Toolbar” on page 273 or “Batch View Shortcut Menu” on page 273.

Tip: To resize the panes, drag the separators that divide the panes.
### Batch View Toolbar

The Batch View includes this toolbar for creating and submitting a batch.

<table>
<thead>
<tr>
<th>Icon</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>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 276.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Inserts a new, empty sample or samples above the selected sample. See the instructions “To insert samples into the list” on page 277.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Removes the selected samples from the samples list. See the instructions “To remove samples from the list” on page 278.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Adds imported samples from a .csv, .xml, or .sld file to the samples list. See the instructions “To import samples into the list” on page 277.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Submits only the selected samples for acquisition, processing, or report generation. See the instructions “To submit selected samples” on page 291.</td>
</tr>
<tr>
<td><img src="image" alt="Icon" /></td>
<td>Submits the batch for acquisition, processing, or report generation. See the instructions “To submit all samples in the batch” on page 290.</td>
</tr>
</tbody>
</table>

### Batch View Shortcut Menu

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

**Table 57. Batch View shortcut menu commands**

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Add Sample</td>
<td>Adds a single empty row to the sample grid.</td>
</tr>
<tr>
<td>Insert Sample</td>
<td>Inserts a single empty row to the sample grid above the selected row.</td>
</tr>
<tr>
<td>Insert Copy Sample</td>
<td>Copies the currently selected row and inserts a copy above the row.</td>
</tr>
<tr>
<td>Reinject Selected Samples</td>
<td>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.</td>
</tr>
<tr>
<td>Remove Selected Samples</td>
<td>Removes selected samples from the sample grid.</td>
</tr>
<tr>
<td>Import Samples</td>
<td>Opens the Sample Import Tool. See “To import samples into the list” on page 277.</td>
</tr>
<tr>
<td>Browse In Raw File</td>
<td>Opens a dialog box where you can select a raw data file to use for the sample row.</td>
</tr>
<tr>
<td>Map Raw Files To Samples</td>
<td>Opens a dialog box where you can select raw data files to use for the sample rows.</td>
</tr>
</tbody>
</table>
Table 57. Batch View shortcut menu commands  (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copy Down</td>
<td>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.</td>
</tr>
<tr>
<td>Fill Down</td>
<td>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.</td>
</tr>
<tr>
<td>Modify Columns</td>
<td>Opens the Modify Columns dialog box. See “Column Display” on page 312.</td>
</tr>
<tr>
<td>Copy</td>
<td>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.</td>
</tr>
<tr>
<td>Copy With Headers</td>
<td>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.</td>
</tr>
</tbody>
</table>

For example:

![Copy With Headers from TraceFinder](image)

<table>
<thead>
<tr>
<th>Paste</th>
<th>Pastes a single column of copied data from another application, such as an Excel spreadsheet, into the selected column.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Undo Last Paste</td>
<td>Removes the last pasted item in the Batch View.</td>
</tr>
<tr>
<td>Export to CSV File</td>
<td>Opens the Save As dialog box where you can save the current sample list to a .csv file.</td>
</tr>
</tbody>
</table>
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.

![Method list](image)

3. Select a drive from the Storage Location list.

![Drive selection](image)

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 47.

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.

![Batch view](image)

**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** button, ![Add Sample button](image).

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

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

- To insert a single sample row, right-click and choose Insert Sample from the shortcut menu.
- To insert multiple sample rows, select the number of rows and then click the Insert Sample button.

The application inserts the Specimen samples above the selected sample.

<table>
<thead>
<tr>
<th>Status</th>
<th>Filename</th>
<th>Sample type</th>
<th>Level</th>
<th>Sample ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cal_5</td>
<td>Calibrator</td>
<td>10</td>
<td>cal = 5 ng/μL</td>
</tr>
<tr>
<td>2</td>
<td>Unknown2</td>
<td>Specimen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Unknown1</td>
<td>Specimen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>cal_10</td>
<td>Calibrator</td>
<td>10</td>
<td>cal = 10 ng/μL</td>
</tr>
</tbody>
</table>

To import samples into the list

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

The Sample Import Tool dialog box opens.

2. Click Browse and select a .csv, .xml, or .sld file that contains the samples you want 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 samples list.

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

<table>
<thead>
<tr>
<th>Xcalibur column</th>
<th>TraceFinder column</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position</td>
<td>Vial Position</td>
</tr>
<tr>
<td>Inj Vol</td>
<td>Injection Volume</td>
</tr>
<tr>
<td>Dil Factor</td>
<td>Conversion Factor</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Xcalibur sample type</th>
<th>TraceFinder sample type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blank</td>
<td>Negative</td>
</tr>
<tr>
<td>Std Bracket</td>
<td>Calibrator</td>
</tr>
</tbody>
</table>

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 87.

❖ **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 copy a sample**

1. Select the sample 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 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.

<table>
<thead>
<tr>
<th>Available sample types</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specimen Specimen/Qual QC</td>
</tr>
<tr>
<td>Solvent Calibrator Hydrolysis</td>
</tr>
<tr>
<td>Unextracted Negative</td>
</tr>
</tbody>
</table>

3. For each Calibrator or QC sample, select a level from the Level list.

   The sample levels are defined in the master method. If there 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.
6 Using the Analysis Mode

Working in the Batch View

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 samples 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.

   ![Modify Columns dialog box](image)

   **Table 58. Modify Columns dialog box buttons**

<table>
<thead>
<tr>
<th>Button</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Move all columns to the Displayed Columns pane." /></td>
<td>Moves all columns to the Displayed Columns pane.</td>
</tr>
<tr>
<td><img src="image" alt="Move the selected column to the Available Columns pane." /></td>
<td>Moves the selected column to the Displayed Columns pane.</td>
</tr>
<tr>
<td><img src="image" alt="Move the selected column to the Available Columns pane. You cannot move the Status, Filename, Sample Type, or Level columns." /></td>
<td>Moves the selected column to the Available Columns pane. You cannot move the Status, Filename, Sample Type, or Level columns.</td>
</tr>
<tr>
<td><img src="image" alt="Move all columns except Status, Filename, Sample Type, or Level to the Available Columns pane." /></td>
<td>Moves all columns except Status, Filename, Sample Type, or Level to the Available Columns pane.</td>
</tr>
<tr>
<td><img src="image" alt="Move 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." /></td>
<td>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.</td>
</tr>
<tr>
<td><img src="image" alt="Move 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." /></td>
<td>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.</td>
</tr>
</tbody>
</table>

2. Use the arrow buttons to move all the columns you want to display 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 the **Up** and **Down** buttons 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; 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.

   ![Sample Table]

   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 samples 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.

![Open Batch Dialog Box]

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.

To edit samples in a batch

Use the commands described in “Working in the Batch View” on page 271.

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 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).

<table>
<thead>
<tr>
<th>Sample</th>
<th>Status</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>cal_50_INJ001</td>
<td>Calibrato</td>
<td>10</td>
</tr>
<tr>
<td>cal_50_INJ002</td>
<td>Calibrato</td>
<td>10</td>
</tr>
<tr>
<td>cal_50</td>
<td>Calibrato</td>
<td>10</td>
</tr>
<tr>
<td>cal_10_INJ001</td>
<td>Calibrato</td>
<td>10</td>
</tr>
<tr>
<td>cal_10</td>
<td>Calibrato</td>
<td>10</td>
</tr>
</tbody>
</table>

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.

   For detailed instructions for specifying which reports and output formats are generated, see “Specifying the Reports Configuration” on page 65.

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 Table]

   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 65.

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 samples 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 settings in the local method. See “Identification” on page 124.

<table>
<thead>
<tr>
<th>Compound Active Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compound</td>
</tr>
<tr>
<td>1 Benzenamine, 2,4-dibromo-</td>
</tr>
<tr>
<td>2 Acetamide, N-{2-hydroxyphenyl}-</td>
</tr>
<tr>
<td>3 2,6-Dichloronitrosobenzene</td>
</tr>
<tr>
<td>4 6-Methyl-3,5-heptadiene-2-one</td>
</tr>
</tbody>
</table>

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:

<table>
<thead>
<tr>
<th>Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,6-Dichloronitrosobenzene</td>
</tr>
<tr>
<td>6-Methyl-3,5-heptadiene-2-one</td>
</tr>
<tr>
<td>Acetamide, N-{2-hydroxyphenyl}-</td>
</tr>
<tr>
<td>Benzenamine, 2,4-dibromo-</td>
</tr>
</tbody>
</table>

For instructions for changing the active/inactive status in the Data Review view, see “Inactive and Excluded Compounds” on page 316.
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 73.** Active and inactive compounds in the Local Method View

![Local Method View - Batch_steroids1_Method_steroids*](image)

<table>
<thead>
<tr>
<th>RT</th>
<th>Compound</th>
<th>Compound type</th>
<th>Active</th>
<th>CAS No</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Benzenamine, 2,4-dibromo-</td>
<td>Target Compound</td>
<td>✓</td>
<td>615576</td>
</tr>
<tr>
<td>2</td>
<td>Acetamide, N-(2-hydroxyphenyl)-</td>
<td>Target Compound</td>
<td></td>
<td>614902</td>
</tr>
</tbody>
</table>

For details about setting the status on the Identification page, see “Identification” on page 124.

**Figure 74.** Active and inactive compounds in the Batch View

![Batch View - Batch_steroids1*](image)

<table>
<thead>
<tr>
<th>Compound</th>
<th>Active</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzenamine, 2,4-dibromo-</td>
<td>✓</td>
</tr>
<tr>
<td>Acetamide, N-(2-hydroxyphenyl)-</td>
<td></td>
</tr>
<tr>
<td>2,6-Dichloronitrosobenzene</td>
<td>✓</td>
</tr>
</tbody>
</table>

For details about setting the status in the Batch View, see “Setting Compound Active Status” on page 288.

**Figure 75.** Active and inactive compounds in the Data Review view

![Data Review - Batch_steroids1*](image)

<table>
<thead>
<tr>
<th>Compound</th>
<th>Active</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,6-Dichloronitrosobenzene</td>
<td>✓</td>
</tr>
<tr>
<td>6-Methyl-3,5-heptadiene-2-one</td>
<td></td>
</tr>
<tr>
<td>Acetamide, N-(2-hydroxyphenyl)-</td>
<td></td>
</tr>
<tr>
<td>Benzenamine, 2,4-dibromo-</td>
<td></td>
</tr>
</tbody>
</table>

For details about setting the status in the Data Review view, see “Inactive and Excluded Compounds” on page 316.
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 292.

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 273.

❖ To submit all samples in the batch

1. Click the Submit Batch button.

   The Submit Options dialog box opens. See “Submit Options dialog box” on page 292.

2. Select the tasks 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 you want to submit.

2. Click the Submit Selected Samples button.

   The Submit Options dialog box opens. See “Submit Options dialog box” on page 292.

3. Select the tasks 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.
6 Using the Analysis Mode

Working in the Batch View

Figure 76. Submit Options dialog box

Table 59. Submit Options dialog box parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>User Name</td>
<td>Name of the current user.</td>
</tr>
<tr>
<td>Samples</td>
<td>Reports the range of samples to be acquired, processed, or reported.</td>
</tr>
<tr>
<td>Acquire Data</td>
<td>(Default) Submits the current batch to acquisition.</td>
</tr>
<tr>
<td>Process Data</td>
<td>(Default) Processes the data for the current batch.</td>
</tr>
<tr>
<td>Create Reports</td>
<td>Creates reports for the current batch.</td>
</tr>
</tbody>
</table>
If the instrument 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.

Use

Specifies the instruments used for this acquisition.

Start Device

Specifies the instrument that will initiate 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.

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.

Post-run System State

Specifies the system state after it acquires the last batch. On (default), Standby, or Off.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Device Name</td>
<td>Lists all configured instruments.</td>
</tr>
<tr>
<td>Use</td>
<td>Specifies the instruments used for this acquisition.</td>
</tr>
<tr>
<td>Start Device</td>
<td>Specifies the instrument that will initiate communication with the other instruments. This is usually the autosampler.</td>
</tr>
<tr>
<td>Start When Ready</td>
<td>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.</td>
</tr>
</tbody>
</table>
| 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. |
| Post-run System State | Specifies the system state after it acquires the last batch. On (default), Standby, or Off. |

<table>
<thead>
<tr>
<th>Buttons</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hide/Show Details</td>
<td>Collapses or expands the acquisition details of the Submit Options dialog box.</td>
</tr>
<tr>
<td>OK</td>
<td>Begins the selected processes.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Closes the Submit Options dialog box without submitting any tasks.</td>
</tr>
</tbody>
</table>
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 95 and “Working in the Batch Template Editor” on page 374.

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 button.

The Batch Template Selection page of the Batch Wizard opens.
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” on page 296.

❖ 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 the layout you want to use.

   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.
6 Using the Analysis Mode
Creating a Batch Using the Batch Wizard

**Figure 77.** Batch Template Selection page

![Batch Wizard window](image)

**Table 60.** Batch Template Selection parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Starting Vial Position</td>
<td>The vial position where you want to begin acquiring samples. Default: 1</td>
</tr>
<tr>
<td>Total Batch Rows</td>
<td>The number of sample rows in the batch template.</td>
</tr>
<tr>
<td>Assay Type</td>
<td>The assay type specified in the master method used to create the batch template.</td>
</tr>
</tbody>
</table>
| 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\2.0\ClinTox\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 60. Batch Template Selection parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Next</td>
<td>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 297.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.</td>
</tr>
</tbody>
</table>

---

### 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 300.

#### To enter a 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, Specimen sample to the end of the sample list.

2. In the Filename column for each sample, type a file name.

3. Select a sample type from the Sample Type list for each sample.

   For a detailed description of sample types, see “Sample Types” on page 266.

4. For each Calibrator or QC sample, select a level from the Level list.

   The sample levels are defined in the master method. If there are no levels to select 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**  This function is not available in Quick Mode.

- **To remove samples from the batch**

  1. Select the samples you want to remove.
  2. Right-click and choose Remove Selected Samples from the shortcut menu, or click the remove samples icon, ![Remove Samples Icon].

     The application removes the selected samples from the sample list.

   **Note**  This function is not available in Quick Mode.

- **To insert samples into the batch**

  1. Select the sample above where you want to insert a new sample.
  2. Right-click and choose Insert Sample from the shortcut menu.

     The application inserts a new, Specimen sample above the selected sample.

   **Note**  This function is not available in Quick Mode.

- **To copy a sample**

  1. Select the sample 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**  This function is not available in Quick Mode.

- **To move a sample up or down in the sample list**

  1. Select the sample 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**  This function is 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** This function is not available in Quick Mode.
### Table 61. Batch Specification parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Batch Template</td>
<td>Displays the path names of the batch template, master method, batch file, and calibration file used to create this batch.</td>
</tr>
<tr>
<td>Master Method</td>
<td></td>
</tr>
<tr>
<td>Batch File</td>
<td></td>
</tr>
<tr>
<td>Calibration File</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Adds a new, Unknown sample to the end of the sample list. This function is not available in Quick Mode.</td>
</tr>
<tr>
<td>Remove Selected Samples</td>
<td></td>
</tr>
<tr>
<td>Quick mode</td>
<td>Limits the columns of information in the Batch Specification page to the following:</td>
</tr>
<tr>
<td></td>
<td>• Sample Type</td>
</tr>
<tr>
<td></td>
<td>• Sample ID</td>
</tr>
<tr>
<td></td>
<td>• Injection Volume</td>
</tr>
<tr>
<td></td>
<td>• Conversion Factor</td>
</tr>
<tr>
<td>Help</td>
<td>Opens the “Creating a Batch Using the Batch Wizard” topic (this topic) in the application Help tool.</td>
</tr>
<tr>
<td>Back</td>
<td>Returns you to the Batch Template Selection page where you can choose a different batch template, master method, or starting vial position.</td>
</tr>
<tr>
<td>Next</td>
<td>Takes you to the Finish page where you can submit the batch for acquisition or processing. See “Submitting the Batch” on page 302.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.</td>
</tr>
</tbody>
</table>

### Shortcut Menu

| Add Sample         | Adds a single empty row to the sample list.                                                           |
| Insert Sample      | Inserts a new, Specimen sample above the selected row.                                                  |
| Insert Copy Sample | Copies the currently selected row and inserts a copy above the row.                                    |
| Remove Selected Samples |                                                                                                        |
| 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” on page 303.

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 290.

❖ 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 304.

❖ 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 304.
### Table 62. Finish parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Modify Calibrations or Active Compounds by Group</td>
<td>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.</td>
</tr>
<tr>
<td>Batch Name</td>
<td>Name of the current batch in the form: \textit{MasterMethodName_MMDDYYYY}</td>
</tr>
<tr>
<td>Help</td>
<td>Opens the “Creating a Batch Using the Batch Wizard” topic (this topic) in the application Help tool.</td>
</tr>
<tr>
<td>Back</td>
<td>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 297.</td>
</tr>
</tbody>
</table>

**Figure 79. Finish page**

The Batch Wizard interface showing the completion of a batch with a checkered flag background.

```
Batch name: Method2067_12212009

Modify Calibrations or Active Compounds by Group

Please make sure the Batch name you want is typed into the box below.

Batch Name: Method2067_12212009

Help < Back Finish Cancel
```
Selecting Calibration Files and Compounds

From the Calibration and Compound Selection page, you can edit the calibration file or edit the list of compounds you want to identify. For descriptions of the parameters on the Calibration and Compound Selection page, see “Calibration and Compound Selection Page” on page 305.

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 302.

❖ To identify specific compounds or groups of compounds
1. In the Compound Groups area, select the groups that include the compounds you want 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 302.

Figure 80. Calibration and Compound Selection Page

Table 63. Calibration and Compound Selection parameters (Sheet 1 of 2) (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibration File</td>
<td>Name of the current batch in the form: MasterMethodName_MMDDYYYY_</td>
</tr>
<tr>
<td>Create New</td>
<td>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.</td>
</tr>
</tbody>
</table>
6 Using the Analysis Mode
Creating a Batch Using the Batch Wizard

Table 63. Calibration and Compound Selection parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extend Calibrations</td>
<td>Adds calibration data from the current batch to the selected calibration file.</td>
</tr>
<tr>
<td>Compound Groups</td>
<td>Displays all available groups defined in the Groups page of the Master Method View. See “Editing the Groups Page” on page 126.</td>
</tr>
<tr>
<td>Included Compounds</td>
<td>Displays all available compounds that you can identify in the samples. Compounds marked as Active are identified in the batch samples.</td>
</tr>
<tr>
<td>Help</td>
<td>Opens the “Creating a Batch Using the Batch Wizard” topic (this topic) in the application Help tool.</td>
</tr>
<tr>
<td>Back</td>
<td>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 297.</td>
</tr>
<tr>
<td>Next</td>
<td>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 302.</td>
</tr>
<tr>
<td>Cancel</td>
<td>Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.</td>
</tr>
</tbody>
</table>
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 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 samples list and one of two modes: Quan Mode or Qual Mode. The Qual Mode is available only for Specimen/Qual sample types. When you view the data for a Specimen/Qual sample type, you can switch between Qual Mode and Quan Mode.

This section includes the following topics:

- Samples List
- Quan Mode
- Qual Mode
Samples List

Use the samples list to select a particular sample. To see the columns in a sample list and view their descriptions, see “Samples list” on page 309.

Status indicators for each sample indicate if the sample is currently acquiring, not acquired, acquired, or processed.

The samples list includes the following features:

- Column Display
- Status Indicators
- Caution Flags
- Compound Flags
- Inactive and Excluded Compounds

The samples 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 samples 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 samples 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 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.

- In Qual Mode, the samples list works with the peaks pane to select a unique sample and peak combination, which then has its textual and graphical values displayed in the Qual Mode pane.
Cells in the samples 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 64.** Samples list columns (Sheet 1 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Status</td>
<td>- Sample is not acquired.</td>
</tr>
<tr>
<td></td>
<td>- Sample is acquired but not processed.</td>
</tr>
<tr>
<td></td>
<td>- Sample is acquired and processed.</td>
</tr>
<tr>
<td></td>
<td>- Sample is currently acquiring.</td>
</tr>
<tr>
<td>Flags</td>
<td>Displayed only when a compound within the sample has an error.</td>
</tr>
<tr>
<td>Filename</td>
<td>Name of the raw data file that contains the sample data.</td>
</tr>
<tr>
<td>Sample Type</td>
<td>Defines how the TraceFinder application processes the sample data. Each sample is classified as one of the following sample types: Specimen, Specimen/Qual, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative</td>
</tr>
</tbody>
</table>
Table 64. Samples list columns (Sheet 2 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Level</td>
<td>The level defined for a calibration sample or quality control sample.</td>
</tr>
<tr>
<td>Sample ID</td>
<td>A user-defined alphanumeric string that identifies a sample.</td>
</tr>
<tr>
<td>Sample Name</td>
<td>A user-defined name that identifies a sample.</td>
</tr>
<tr>
<td>Comment</td>
<td>A user-defined comment for the sample.</td>
</tr>
<tr>
<td>Vial Position</td>
<td>The tray vial number used for the autosampler acquisition.</td>
</tr>
<tr>
<td>Injection Volume</td>
<td>The injection volume in microliters of sample to be injected. 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 range displayed. The Injection Volume value set in the master method overwrites the value in the instrument method. Range: 0.1 through 5000 μL.</td>
</tr>
<tr>
<td>Integration Mode</td>
<td>Indicates whether the peaks have been manually integrated or integrated from the original method.</td>
</tr>
<tr>
<td>Height</td>
<td>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).</td>
</tr>
<tr>
<td>Area</td>
<td>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).</td>
</tr>
<tr>
<td>Actual RT</td>
<td>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.</td>
</tr>
<tr>
<td>Expected RT</td>
<td>Expected retention time for the compound.</td>
</tr>
<tr>
<td>Calc Amt</td>
<td>The amount present in the sample, as determined using the calibration curve and the response ratio.</td>
</tr>
<tr>
<td>Theo Amt</td>
<td>Theoretical amount of the compound expected in the sample.</td>
</tr>
<tr>
<td>Sample Amt</td>
<td>The injected volume multiplied by the correction 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 correction factor is 1000, and your sample amount is 1000.</td>
</tr>
<tr>
<td>Resp Ratio</td>
<td>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.</td>
</tr>
</tbody>
</table>
Table 64. Samples list columns (Sheet 3 of 3)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IS Amt</td>
<td>Amount of internal standard.</td>
</tr>
<tr>
<td>IS Resp</td>
<td>Response of the internal standard.</td>
</tr>
<tr>
<td>Active</td>
<td>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.</td>
</tr>
<tr>
<td>Excluded</td>
<td>Turns a compound on or off in the Calibration curve of the Qualification pane.</td>
</tr>
<tr>
<td>%Diff</td>
<td>The calculated amount minus the expected amount, divided by the expected amount, and then multiplied by 100.</td>
</tr>
<tr>
<td>%RSD</td>
<td>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.</td>
</tr>
<tr>
<td>%CV</td>
<td>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.</td>
</tr>
<tr>
<td>Channel</td>
<td>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 87.</td>
</tr>
</tbody>
</table>
Column Display

The samples list can contain many columns of information. You can scroll to see all the columns of information, and you can customize which columns you want to display and their display order.

Follow these procedures:

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

❖ To scroll the samples list

Use the scroll bar at the bottom of the samples list to view all the information.

When you use the horizontal scroll bar at the bottom of the samples 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” on page 313.

2. Use the arrow buttons to move all the columns you want to display 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 the Up and Down buttons 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; the last column in the list represents the rightmost column in the Batch View sample list.

   **Note** You cannot move the Status, Flags, Filename, and Sample Type columns.

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

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection volume</td>
<td>100</td>
</tr>
<tr>
<td>Vial position</td>
<td>100</td>
</tr>
</tbody>
</table>

   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 82.** Modify Columns dialog box

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>&gt;&gt;</strong></td>
<td>Moves all columns to the Displayed Columns pane.</td>
</tr>
<tr>
<td><strong>&gt;</strong></td>
<td>Moves the selected column to the Displayed Columns pane.</td>
</tr>
<tr>
<td><strong>&lt;</strong></td>
<td>Moves the selected column to the Available Columns pane. You cannot move the Status, Flags, Filename, and Sample Type columns.</td>
</tr>
<tr>
<td><strong>&lt;&lt;</strong></td>
<td>Moves all columns except Status, Flags, Filename, and Sample Type to the Available Columns pane.</td>
</tr>
<tr>
<td><strong>Up</strong></td>
<td>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.</td>
</tr>
<tr>
<td><strong>Down</strong></td>
<td>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.</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Method: Method1</th>
<th>Instrument: Thermo Scientific Instrument</th>
</tr>
</thead>
<tbody>
<tr>
<td>Status</td>
<td>Flags</td>
</tr>
<tr>
<td>1</td>
<td>![status indicator]</td>
</tr>
<tr>
<td>2</td>
<td>![status indicator]</td>
</tr>
</tbody>
</table>

Caution Flags

The Flags column in the samples 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.

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 Specimen sample types.
Compound Flags

<table>
<thead>
<tr>
<th>Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2-Benzenedicarboxylic acid, 4-methyl-</td>
</tr>
<tr>
<td>2-Propyn-1-amine, N-methyl-</td>
</tr>
<tr>
<td>9,10-Anthracenedione</td>
</tr>
</tbody>
</table>

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 164.)
- For compounds that are not found
- For compounds that are not found in Calibrator or QC sample types
- For compounds that are outside the specified ion ratio range

These criteria do not apply to Negative 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.

```
<table>
<thead>
<tr>
<th>Status</th>
<th>Flags</th>
<th>Filename</th>
<th>Sample type</th>
<th>Active</th>
<th>Excluded</th>
<th>Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>Unknown1</td>
<td>Specimen</td>
<td></td>
<td></td>
<td>2,6-Dichloronitrosobenzene</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>Unknown2</td>
<td>Specimen</td>
<td></td>
<td></td>
<td>6-Methyl-3,5-heptadiene-2-one</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>Unknown3</td>
<td>Specimen</td>
<td></td>
<td></td>
<td>Acetamide, N-[2-hydroxyphenyl]</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>Unknown4</td>
<td>Specimen</td>
<td></td>
<td></td>
<td>Benzenamine, 2,4-dibromo-</td>
</tr>
</tbody>
</table>
```

Follow these procedures:

- To make a sample active or inactive
- To exclude a calibration point

**To make a sample active or inactive**

1. Select the sample in the samples 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 samples 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.
To exclude a calibration point

In the samples 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.
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 quantitative peak and confirming ion information for selected compounds that are found in the processed samples.

In addition to the Quan Mode, the Quan Mode view uses the following panes:

- Compounds
- Quantification Peak
- Qualification
Compounds

The Compounds pane works with the samples list pane to display textual and graphical values for a unique file and compound combination.

Follow these procedures:

• To sort the compounds list
• To display peaks for a specific compound
• To display specific problems with a compound
• To display the internal standard for a compound

❖ To sort the compounds list

In the Compounds pane, right-click and choose one of the following sort styles from the shortcut menu:

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sort By Flag And</td>
<td>Sorts the compounds first by flag and then within each flag group, sorts the compounds alphabetically.</td>
</tr>
<tr>
<td>Alphabetical</td>
<td></td>
</tr>
<tr>
<td>Sort By Flag And</td>
<td>Sorts the compounds first by flag and then within each flag group, sorts the compounds by retention time.</td>
</tr>
<tr>
<td>Retention Time</td>
<td></td>
</tr>
<tr>
<td>Sort By Alphabetical</td>
<td>Sorts the compounds alphabetically (1-n followed by a-z).</td>
</tr>
<tr>
<td>Sort By Retention Time</td>
<td>Sorts the compounds from shorter retention time to longer retention time.</td>
</tr>
</tbody>
</table>
To display peaks for a specific compound

1. In the samples list, select the sample.
   The Compounds pane lists all compounds specified in the method.
2. In the Compounds pane, select the compound in the sample.
   The Quantification Peak pane displays the peaks for the selected compound and its internal standard.

To display specific problems with a compound

Hold the cursor over the flag to display the problems with the compound.

Calibration Amount Diff 100% > max calibration amount diff 20%

methyltestosterone
To display the internal standard for a compound

1. Right-click the Quan Peak pane and choose **Show Internal Standard** from the shortcut menu.

![Show Internal Standard](image)

**Note** By default, the application does not display the ISTD pane.

The Quantification Peak pane displays an ISTD pane with the internal standard for the selected sample and compound.

![Quan Peak: 1 + ISTD: 1](image)

2. To hide the ISTD pane, right-click the Quan Peak or ISTD pane and choose **Hide Internal Standard** from the shortcut menu.
Quantification Peak

The Quantification Peak pane displays the compound selected in the samples list and Compound pane. 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 method values were originally calculated based on the processing method parameters. The manual values are a result of what has been edited.

When the sample contains an internal standard, the chromatogram shows both the analyte and the internal standard in side-by-side panes.

Follow these procedures:

- To zoom in on a peak
- To manually integrate a quantification or qualification ion
- 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

For a description of commands on the shortcut menu, see “Quantification Peak Shortcut Menu” on page 326.

❖ To zoom in on a peak

1. In the chromatogram plot, drag your 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 integrate a quantification or qualification ion

1. Place your cursor over one of the two peak delimiter tags in the Quantification 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.

Both the Quantification Peak pane and the Integration mode column in the Quantification Data pane reflect the change between method and manual modes. The generated reports for these data identify the manual modifications.

- **Note** Because a Blank Report displays only the quan mass, when you manually integrate a confirming ion, the manual integration flag in the report is displayed on the quan mass.

To manually add a peak

1. Right-click anywhere in the Quantification 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 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](image)

   Manually added base points

   m/z: 109.00, 279.10, 297.30

To remove a manually created peak

Right-click the chromatogram plot, and choose Remove Peak from the shortcut menu.

The application removes the manually added peak.
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** Because a Blank Report displays only the quan mass, when you manually integrate a confirming ion, the manual integration flag in the report is displayed on the quan mass.

To change the displayed information for detected peaks

1. Right-click the quantification 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 quantification 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.

To modify the peak detection settings

1. Right-click the chromatogram view and choose Peak Detection Settings from the shortcut menu.

The Peak Detection Settings dialog box opens. Use the Peak Detection Settings dialog box to adjust detection settings that were specified in the method.
2. Edit any of the detection settings.
   
   For detailed descriptions of all detection settings, see “Detection” on page 126.

3. To save your changes to this compound in all samples in this batch, click **Apply to ALL**.
Quantification Peak Shortcut Menu

The Quantification Peak shortcut menu includes the following commands:

Table 65. Quantification Peak shortcut menu commands

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method Integration Settings</td>
<td>Displays method integration settings.</td>
</tr>
<tr>
<td>Add Peak —or— Remove Peak —or— Cancel Add Peak</td>
<td>Adds a peak, removes a peak, or cancels an add peak operation in progress.</td>
</tr>
<tr>
<td>Confirming Ion List</td>
<td>Select the confirming ions to be viewed.</td>
</tr>
<tr>
<td>Peak Labels</td>
<td>Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).</td>
</tr>
<tr>
<td>Show Peak Info</td>
<td>Displays peak information for the selected compound. For example:</td>
</tr>
</tbody>
</table>

```
**methyltestosterone**

<table>
<thead>
<tr>
<th>Quan ion m/z:</th>
<th>267.10, 285.20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integration mode:</td>
<td>Method</td>
</tr>
<tr>
<td>Left RT:</td>
<td>1.87</td>
</tr>
<tr>
<td>Apex RT:</td>
<td>1.99</td>
</tr>
<tr>
<td>Right RT:</td>
<td>2.28</td>
</tr>
<tr>
<td>Data file:</td>
<td>steroids02</td>
</tr>
<tr>
<td>Filter:</td>
<td>+ c Full ms2 303.3@cid</td>
</tr>
<tr>
<td>Detector:</td>
<td>MS</td>
</tr>
<tr>
<td>Trace:</td>
<td>Mass range</td>
</tr>
</tbody>
</table>
```

Reset Scaling | Resets the original scaling after a zoom operation. |
Peak Detection Settings | Opens the Peak Detection Settings dialog box for the selected compound. |
Qualification

The Qualification pane displays the compound selected in the Quantification Data pane and Compounds pane.

The Qualification pane has five pages:

- Calibration Curve
- Spectra
- QED Spectra
- Confirming Ions
- Ion Overlay

Calibration Curve

The Calibration Curve page displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration.

Follow these procedures:

- To manually exclude a calibration point
- To zoom in on an area

For a description of commands on the shortcut menu, see “Calibration Curve Shortcut Menu” on page 329.
To manually exclude a calibration point

In the samples 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.

To zoom in on an area

1. In the Calibration Curve plot, drag your cursor to delineate a rectangle around an area.

   The delineated area expands to fill the view.

2. To restore the method default view, right-click the calibration curve plot and choose **Reset Scaling** from the shortcut menu.

   Changes to the calibration settings immediately apply to the entire results set, but you save them only when you save the batch.
Calibration Curve Shortcut Menu

The Calibration Curve shortcut menu includes the following commands:

**Table 66. Calibration Curve shortcut menu commands**

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard Type</td>
<td>Sets the standard type to External or Internal.</td>
</tr>
<tr>
<td>Calibration Curve Type</td>
<td>Sets the calibration curve type to one of the following:</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
<tr>
<td>Response Via</td>
<td>Sets the response to Area or to Height.</td>
</tr>
<tr>
<td>Weighting</td>
<td>Sets the weighting to equal, 1/X, 1/X^2, 1/Y, or 1/Y^2.</td>
</tr>
<tr>
<td>Origin</td>
<td>Sets the origin to Ignore, Force, or Include.</td>
</tr>
<tr>
<td>Units</td>
<td>Sets the units.</td>
</tr>
<tr>
<td>Done with Settings</td>
<td>Saves the calibration curve settings.</td>
</tr>
<tr>
<td>Reset Scaling</td>
<td>Resets the original scale in the calibration curve pane.</td>
</tr>
</tbody>
</table>

Spectra

The Spectra page displays a comparison of the spectra found in the data and the method reference.

To zoom in on an area

1. Drag your cursor to delineate a rectangle around an area.
   The delineated area expands to fill the view.
2. To restore the method default view, right-click the spectra plot and choose **Reset Scaling** from the shortcut menu.
QED Spectra

The QED spectra display the averaged QED spectra from the raw data file and the datastore match. If the sample contains no QED data, the page is blank.

To zoom in on an area

1. Drag your cursor to delineate a rectangle around an area.
   
   The delineated area expands to fill the view.

2. To restore the method default view, right-click the spectra plot and choose Reset Scaling from the shortcut menu.
Confirming Ions

The Confirming Ions page 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. A red border indicates that an ion ratio is outside of its window. Depending on the method option settings, another ion view is available on the Ion Overlay page. See “Ion Overlay” on page 335.

A red border indicates that an ion ratio is outside of its window.
Follow these procedures:

- To manually add a peak
- To remove a manually created peak
- To zoom in on a peak
- To change the displayed information for detected peaks
- To display the peak information window

For a description of commands on the shortcut menu, see “Confirming Ions Shortcut Menu” on page 334.

✹ To manually add a peak

1. Right-click the chromatogram plot and select **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 application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.

✹ To remove a manually created peak

Right-click the chromatogram plot, and choose **Remove Peak** from the shortcut menu.

The application removes the manually added peak.

✹ To zoom in on a peak

1. In the chromatogram plot, drag your cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the method default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.
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 quantification 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.

To display the peak information window

1. Right-click the quantification and confirming ion chromatogram plots.

2. Choose Show Peak Info from the shortcut menu.

   Information in this window includes the data stream processed for this ion, consisting of a particular detector, filter (if applicable), and trace. For example, an MS detector might show a filter of “+ c Full ms [35.00-500.00]” and a Mass Range trace.

   This window also shows the peak area and height, along with the retention times of the peak integration and the peak apex.
## Confirming Ions Shortcut Menu

The Confirming Ions shortcut menu includes the following commands:

**Table 67. Confirming ions shortcut menu commands**

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method Integration Settings</td>
<td>Displays method integration settings.</td>
</tr>
<tr>
<td>Add Peak - Remove Peak - Cancel Add Peak</td>
<td>Adds a peak, removes a manually added peak, or cancels an add peak operation in progress.</td>
</tr>
<tr>
<td>Range Calc Method: Manual</td>
<td>Selects the method used to calculate the ion ratio range windows: Manual, Average, Weighted average, or Level.</td>
</tr>
<tr>
<td>Range Calc Level</td>
<td>Range based on the calibration level.</td>
</tr>
<tr>
<td>Target Ratio:</td>
<td>Specifies the theoretical ratio of the confirming ion’s response to the quantification ion’s response.</td>
</tr>
<tr>
<td>Window Type:</td>
<td>Specifies the Absolute or Relative calculation approach for determining the acceptable ion ratio range.</td>
</tr>
<tr>
<td>Window: %</td>
<td>Specifies the acceptable ion ratio range as a percentage.</td>
</tr>
<tr>
<td>Peak Labels</td>
<td>Displays or hides the peak labels (Label area, Label retention time, Label height, or Label signal to noise).</td>
</tr>
</tbody>
</table>
| Show Peak Info            | Displays peak information for the selected compound. For example: methyltestosterone

| Quan ion m/z: | 267.10, 285.20 |
| Integration mode: | Method |
| Left RT:       | 1.87 | Area: | 684395 |
| Apex RT:       | 1.99 | Height: | 95311 |
| Right RT:      | 2.23 | Noise: | 530.01 |
| Data file:     | steroidst2 |
| Filter:        | + c Full ms2 303.3@cid |
| Detector:      | MS |
| Trace:         | Mass range |

| Reser Scaling | Resets the original scaling after a zoom operation.                      |
| Peak Detection Settings | Opens the Peak Detection Settings dialog box for the selected compound. See “Peak Detection Settings dialog box” on page 325. |
Ion Overlay

The Ion Overlay page represents an overlay of the entire ion set—quantification and qualifying/confirming—for the selected sample and compound. Use this page to graphically review the peak apex alignment and co-eluting peak profiles.

To zoom in on a peak

1. Drag your cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the method default view, right-click the chromatogram plot and choose Reset Scaling from the shortcut menu.
Qual Mode

Use the Qual Mode and the associated peaks pane to view qualitative information that complements the textual information for the selected Specimen/Qual 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 Specimen/Qual sample types.

In addition to the Quan Mode, the Qual Mode view displays data in the following panes:

- Peaks Pane
- Chromatogram Navigation Pane
- Qualitative Peak Pane
- Spectra Pane (Reference and Selected)
- Ranking Pane

**Tip** To resize the panes, drag the separators that divide the panes.
Peaks Pane

The peaks pane works with the samples list to display graphical values for a unique sample and peak combination. For detailed descriptions of parameters on the peaks pane, see “Peaks pane” on page 339.

❖ To display peaks for a specific compound

1. From the samples list, select a sample.

Note If you select a sample type other than Specimen/Qual, the TraceFinder application returns you to Quan Mode.

The peaks pane lists 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 189.

2. From the peaks pane, select a peak in the sample.

<table>
<thead>
<tr>
<th>Peak RT (min)</th>
<th>SI</th>
<th>RSI</th>
<th>MP</th>
<th>Library entry</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.01</td>
<td>844</td>
<td>847</td>
<td>33</td>
<td>o-Toluidine</td>
</tr>
<tr>
<td>5.46</td>
<td>892</td>
<td>894</td>
<td>38</td>
<td>2-Cyclohexen-1-one, 3,5,5-trimethyl-</td>
</tr>
<tr>
<td>8.00</td>
<td>937</td>
<td>937</td>
<td>80</td>
<td>Acenaphthene</td>
</tr>
<tr>
<td>8.84</td>
<td>259</td>
<td>549</td>
<td>0</td>
<td>Naphthalene, 1-methyl-</td>
</tr>
<tr>
<td>10.94</td>
<td>942</td>
<td>943</td>
<td>53</td>
<td>Fluoranthenne</td>
</tr>
</tbody>
</table>

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 peaks pane.
2. Right-click and choose Remove Selected Peak from the shortcut menu.

The TraceFinder application removes the selected peak from the peaks 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 340.
**Figure 84.** Peaks pane

![Filter: + c Full ms [35.00-500.00]](image)

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
</table>
| Filter           | Filter used to identify the peaks. Specified in the raw data file or the master method. When your raw data file is data-dependent, the filter indicates this with a “d”:

```
Filter: + c d Full ms2 179.15@cid35.00 [35.00-370.00]
```

<table>
<thead>
<tr>
<th>Data-dependent filter</th>
</tr>
</thead>
</table>

- **Peak RT (min)**: 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.

- **Library Entry**: 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 peaks pane displays a red marker. See “Chromatogram navigation pane” on page 341.

For a description of commands on the shortcut menu, see “Chromatogram navigation pane shortcut menu commands” on page 341.

❖ 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 make it easier to identify the peak you want to add to the results set.

   ![Diagram of chromatogram with peak marked]

2. Right-click the chromatogram navigation pane, and choose Add 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.

   ![Diagram showing peak marked with triangulated delimiter]

The TraceFinder application places the peak delimiter tags at the base point locations and automatically updates the peak values in the peaks pane and qualitative peak pane.
Figure 85. Qualitative peak pane with a manually added peak

![Manually added peak](image)

Manually added base points

<table>
<thead>
<tr>
<th>Peak RT (min)</th>
<th>SI</th>
<th>RSI</th>
<th>MP</th>
<th>Library entry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.93</td>
<td>930</td>
<td>933</td>
<td>94</td>
<td>Phenol, 2-fluoro-</td>
</tr>
<tr>
<td>3.18</td>
<td>834</td>
<td>845</td>
<td>96</td>
<td>Ethanamine, N-ethyl-N-nitroso-</td>
</tr>
<tr>
<td>5.01</td>
<td>800</td>
<td>903</td>
<td>5</td>
<td>Phenol, 3-methyl-</td>
</tr>
</tbody>
</table>

Table 69. Chromatogram navigation pane shortcut menu commands

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Add Peak</td>
<td>Adds a peak.</td>
</tr>
<tr>
<td>Reset Scaling</td>
<td>Resets the original scaling after a zoom operation.</td>
</tr>
</tbody>
</table>
Qualitative Peak Pane

The qualitative peak pane displays the selected peak. See “Qualitative peak pane” on page 344.

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 344.

❖ 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

m/z: 109.00, 279.10, 297.30
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.
The qualitative peak pane shortcut menu includes the following commands:

**Table 70. Qualitative peak pane shortcut menu commands**

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reset Scaling</td>
<td>Resets the original scaling after a zoom operation.</td>
</tr>
<tr>
<td>Method Integration</td>
<td>Displays method integration settings.</td>
</tr>
<tr>
<td>Peak Labels</td>
<td>Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).</td>
</tr>
<tr>
<td>Remove Peak</td>
<td>Removes the peak displayed in the Qual pane.</td>
</tr>
</tbody>
</table>
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 88.** 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” on page 347.

When you select a library entry other than the original entry, the TIC Report and TIC Summary Report indicate this with a “P” flag:

<table>
<thead>
<tr>
<th>Peak</th>
<th>Retention Time</th>
<th>Area</th>
<th>Height</th>
<th>Inj Estimate</th>
<th>In-sample Estimate</th>
<th>Flag</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naphthalene</td>
<td>7.96</td>
<td>13829174</td>
<td>10605061</td>
<td>0.000</td>
<td>0.000</td>
<td>P</td>
</tr>
</tbody>
</table>

For a detailed description of ranking pane parameters, see “Ranking pane parameters” on page 347.

❖ To change the library entry for a selected peak

In the ranking pane, select the check box for the library entry 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 peaks pane, the SI, RSI, MP, and Library Entry values update to reflect the selected library entry.
### Figure 89. Ranking pane

<table>
<thead>
<tr>
<th>Rank</th>
<th>SI</th>
<th>RSI</th>
<th>MP</th>
<th>Library entry</th>
</tr>
</thead>
<tbody>
<tr>
<td>☑</td>
<td>337</td>
<td>337</td>
<td>80</td>
<td>Acenaphthene</td>
</tr>
<tr>
<td>☐</td>
<td>665</td>
<td>668</td>
<td>11</td>
<td>Biphenyl</td>
</tr>
<tr>
<td>☐</td>
<td>656</td>
<td>656</td>
<td>8</td>
<td>Naphthalene, 2-ethyl-</td>
</tr>
</tbody>
</table>

### Table 71. Ranking pane parameters

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;Check box column&gt;</td>
<td>Indicates selected library entries for the selected peak.</td>
</tr>
<tr>
<td>Rank</td>
<td>Indicates the order of best matches between the selected peak and library entries.</td>
</tr>
<tr>
<td>SI</td>
<td>Search index method used to search the NIST library.</td>
</tr>
<tr>
<td>RSI</td>
<td>Reverse search index method used to search the NIST library.</td>
</tr>
<tr>
<td>MP</td>
<td>Match probability.</td>
</tr>
<tr>
<td>Library Entry</td>
<td>Library compound that matches the identified peak.</td>
</tr>
</tbody>
</table>
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.

This section includes the following topics:

- Viewing Reports
- Generating Reports
- Working with Reports
- Working with the Active View

Figure 90. 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” on page 349.

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 353.

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.
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. Click the Select a Report list.

The report list opens, displaying all configured report types.

<table>
<thead>
<tr>
<th>Report Name</th>
<th>Type</th>
<th>Requires</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alternate Batch Report</td>
<td>Custom</td>
<td>Batch</td>
</tr>
<tr>
<td>Alternate Confirmation</td>
<td>Custom</td>
<td>Sample</td>
</tr>
<tr>
<td>Batch Report</td>
<td>Standard</td>
<td>Batch</td>
</tr>
<tr>
<td>Blank Report</td>
<td>Standard</td>
<td>Sample</td>
</tr>
</tbody>
</table>

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 65.

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 you want to display in the report list, select any combination of report filter options in the Filter Reports area.
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 351.

- 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 351.

- 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 352.

---

**Table 72. Filter Reports options**

<table>
<thead>
<tr>
<th>Option</th>
<th>Behavior</th>
</tr>
</thead>
<tbody>
<tr>
<td>Only Show Automated Batch Reports</td>
<td>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 286.</td>
</tr>
<tr>
<td>Standard Reports</td>
<td>Displays Standard report types.</td>
</tr>
<tr>
<td>Custom Reports</td>
<td>Displays all generated Custom report types. Custom reports are not available for viewing until you have generated the report.</td>
</tr>
<tr>
<td>Target Screening Reports</td>
<td>Displays all generated Target Screening reports. Target Screening reports are not available for viewing until you have generated the report.</td>
</tr>
</tbody>
</table>

**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.
To select a sample

1. Click the Sample File list.

   The sample list displays all samples in the batch.

<table>
<thead>
<tr>
<th>Sample Name</th>
<th>Sample ID</th>
<th>Sample Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>level2</td>
<td>level 2 = 10 ng/μL</td>
<td>Specimen</td>
</tr>
<tr>
<td>level3</td>
<td>level 3 = 20 ng/μL</td>
<td>Specimen</td>
</tr>
</tbody>
</table>

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 QC samples.

   **Note** Click the column headers to sort the samples. The application maintains this sort order each time you open the Report View for this batch.

3. Double-click the name of the sample.

   The sample list closes. The Report View page displays the sample-level report.

To select a compound

1. Click the Compound list.

   The compound list displays the names and retention times of all compounds in the sample.

<table>
<thead>
<tr>
<th>RT</th>
<th>Compound Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>All Compounds</td>
<td></td>
</tr>
<tr>
<td>6.00</td>
<td>Acetamiprid</td>
</tr>
<tr>
<td>6.00</td>
<td>Atrazine D6</td>
</tr>
<tr>
<td>6.00,6.00</td>
<td>Benthiocarbamate</td>
</tr>
<tr>
<td>6.00</td>
<td>Benthalazine</td>
</tr>
</tbody>
</table>

2. Double-click a single compound or **All Compounds**.

   The compound list closes. The Report View page displays the compound-level report.
6 Using the Analysis Mode
Working in the Report View

To select a sample and a compound

1. Click the Sample File list.

   The sample list displays all samples in the batch.

<table>
<thead>
<tr>
<th>Sample Name</th>
<th>Sample ID</th>
<th>Sample Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>level2</td>
<td>level 2 = 10 ng/μL</td>
<td>Specimen</td>
</tr>
<tr>
<td>level3</td>
<td>level 3 = 20 ng/μL</td>
<td>Specimen</td>
</tr>
</tbody>
</table>

   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 QC samples.

   Tip: Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

3. Double-click the name of the sample.

   The sample list closes.

4. Click the Compound list.

   The compound list displays the names and retention times of all compounds in the sample.

<table>
<thead>
<tr>
<th>Compound:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>All Compounds</td>
<td></td>
</tr>
<tr>
<td>Acetamiprid</td>
<td></td>
</tr>
<tr>
<td>Anitraz</td>
<td></td>
</tr>
<tr>
<td>Altrazine D6</td>
<td></td>
</tr>
<tr>
<td>Betlubutanid</td>
<td></td>
</tr>
<tr>
<td>Benalaxyl</td>
<td></td>
</tr>
<tr>
<td>Benzophenone-3</td>
<td></td>
</tr>
</tbody>
</table>

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. Click the Select a Report list.

The report list opens.

<table>
<thead>
<tr>
<th>Report Name</th>
<th>Type</th>
<th>Requires</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blank Report</td>
<td>Standard</td>
<td>Sample</td>
</tr>
<tr>
<td>BlankReport</td>
<td>Custom</td>
<td>Sample</td>
</tr>
<tr>
<td>Alternate ConfirmationReport</td>
<td>Custom</td>
<td>Sample</td>
</tr>
<tr>
<td>Chromatogram Report</td>
<td>Standard</td>
<td>Sample</td>
</tr>
</tbody>
</table>

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 65.

If you have many reports, you can filter the list.
3. To limit the types of reports you want to display in the report list, select any combination of report filter check boxes in the Filter Reports area.

<table>
<thead>
<tr>
<th>Option</th>
<th>Behavior</th>
</tr>
</thead>
<tbody>
<tr>
<td>Only Show Automated Batch Reports</td>
<td>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 286. If you have only batch-level reports specified in the Batch View, selecting this option excludes all reports in the Report Name list.</td>
</tr>
<tr>
<td>Standard Reports</td>
<td>Displays sample-level Standard report types.</td>
</tr>
<tr>
<td>Custom Reports</td>
<td>Displays sample-level Custom report types.</td>
</tr>
<tr>
<td>Target Screening Reports</td>
<td>Displays sample-level Target Screening report types.</td>
</tr>
</tbody>
</table>

**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. Click the **Sample File** box.

The sample list displays all samples in the batch.

<table>
<thead>
<tr>
<th>Select</th>
<th>Sample Name</th>
<th>Sample ID</th>
<th>Sample Type</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Specimen</td>
<td>sample 1</td>
<td>Specimen</td>
</tr>
<tr>
<td></td>
<td>std_5</td>
<td>std = 5 ng/μL</td>
<td>Calibrator</td>
</tr>
<tr>
<td></td>
<td>std_50</td>
<td>std = 50 ng/μL</td>
<td>QC</td>
</tr>
<tr>
<td></td>
<td>blank</td>
<td>blank</td>
<td>Negative</td>
</tr>
<tr>
<td></td>
<td>sample1</td>
<td>sample 1</td>
<td>Specimen</td>
</tr>
</tbody>
</table>

2. To show only samples that would be included in the selected report, select the **Only Show Samples Relevant...** check box.

For example, if you selected the Quality Control Report, the sample list displays only QC samples.

**Note** Click the column headers to sort the samples. The application saves this sort order in the Report View for this batch.

3. Select the check box for each sample 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 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.

<table>
<thead>
<tr>
<th>Acquisition</th>
<th>Instrument</th>
<th>Devices</th>
<th>Queues</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>Acquisition Queue</strong> - Empty (Ready)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>Processing Queue</strong> - Empty (Ready)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>Reporting Queue</strong> - 1 batch (Ready)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>Batch4600</strong> - 1 sample</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>std_5</strong> - Reporting</td>
</tr>
</tbody>
</table>

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 349.

**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 buttons 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.

![Report View page screenshot](image)
3. Click the **Print Report** button, ![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 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** button, ![export_report_icon].

   The Export Report dialog box opens.

4. Locate the folder where you want to write the report file.

5. Type a file name for the exported report file.

6. Select a file type from the Save as Type list:

   ![Save as Type list]

   - PDF (*.pdf)
   - Character Separated Values (CSV) (*.csv)
   - Microsoft Excel (97-2003) (*.xls)
   - Microsoft Excel (97-2003) Data-Only (*.xle)
   - Microsoft Excel Workbook Data-Only (*.xlsx)
   - Microsoft Word (97-2003) (*.doc)
   - Microsoft Word (97-2003) - Editable (*.rtf)
   - Rich Text Format (RTF) (*.rtf)
   - XML (*.xml)

7. Click **Save**.

   The TraceFinder application saves the file as the specified file type and writes the report file to the specified folder.
To search for text

1. Select a report from the Select a Report list.
2. (Optional) Select a sample from the Sample File list.
   The application displays the report on the Report View page.
3. Click the Find Text button, .
   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 button, , and select a zoom scale.
Working with the Active View

Use the Active View page to view quantitative data for each sample in a report. Data in the Active View are labeled with flag information. These flags are based on a comparison of the batch data to criteria defined in the master method.

❖ To display the Active View page

Click the **Active View** tab.

The Active View page displays quantitative data and QAQC error flags for each sample. See “Active View page” on page 361.

❖ 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 and sample file](image)

❖ To filter which compounds to display

Click the Showing button to display either all compounds or only compounds that are flagged for failing a QAQC test.

![Showing options](image)
**Figure 91.** Active View page

![Active View page](image)

**Table 73.** Active View parameters (Sheet 1 of 4)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>View Only</td>
<td>The Active View pane is available only when View Only is selected.</td>
</tr>
<tr>
<td>Select A Report</td>
<td>Displays the report types created for the current batch.</td>
</tr>
<tr>
<td>Sample File</td>
<td>Used when the report type includes separate reports for each sample.</td>
</tr>
<tr>
<td>Total Rows</td>
<td>The number of compound rows currently displayed in the pane.</td>
</tr>
<tr>
<td>Showing</td>
<td>Displays all compounds or only the flagged compounds.</td>
</tr>
</tbody>
</table>
Table 73. Active View parameters (Sheet 2 of 4)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column headings</td>
<td>Many column headings are specific to individual reports. See “Active View Report Contents” on page 365.</td>
</tr>
<tr>
<td>Status</td>
<td>Indicates the status of the reported compound.</td>
</tr>
<tr>
<td></td>
<td>• A yellow check mark indicates one of the following conditions:</td>
</tr>
<tr>
<td></td>
<td>– The compound was manually integrated.</td>
</tr>
<tr>
<td></td>
<td>– Any of the confirming peaks was manually integrated.</td>
</tr>
<tr>
<td></td>
<td>– The compound has quan flags.</td>
</tr>
<tr>
<td></td>
<td>• A red check mark indicates that the QAQC checks failed.</td>
</tr>
<tr>
<td></td>
<td>• A green check mark indicates that none of these conditions exist.</td>
</tr>
<tr>
<td></td>
<td>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.</td>
</tr>
<tr>
<td>Compound Name</td>
<td>Alphanumeric name assigned to the compound.</td>
</tr>
<tr>
<td>Compound Type</td>
<td>Target Compound or Internal Standard.</td>
</tr>
<tr>
<td>QAQC Flags</td>
<td>Indicates that the QAQC check for the sample failed.</td>
</tr>
<tr>
<td></td>
<td>Manual Integration reports do not use the QAQC column.</td>
</tr>
<tr>
<td>Quan Flags</td>
<td>• Limit of Detection (LOD)</td>
</tr>
<tr>
<td></td>
<td>• Limit of Quantitation (LOQ)</td>
</tr>
<tr>
<td></td>
<td>• Limit of Reporting (LOR)</td>
</tr>
<tr>
<td></td>
<td>• Values between the limit of detection and the limit of quantitation, known as the J flag</td>
</tr>
<tr>
<td></td>
<td>• Upper Limit of Linearity (ULOL)</td>
</tr>
<tr>
<td></td>
<td>Quan flags do not apply to these sample types: Calibrator, QC, or Solvent.</td>
</tr>
<tr>
<td>Manual Flags</td>
<td>Indicates manually integrated peaks.</td>
</tr>
<tr>
<td></td>
<td>• M indicates a manually integrated quan peak.</td>
</tr>
<tr>
<td></td>
<td>• m indicates a manually integrated confirming peak.</td>
</tr>
<tr>
<td>Total Response</td>
<td>The sum of all Quan Peak Response values for the compound.</td>
</tr>
<tr>
<td>Quan Peak Response</td>
<td>Response of the quan peak.</td>
</tr>
<tr>
<td>Quan peak RT</td>
<td>Retention time for the quan peak.</td>
</tr>
<tr>
<td>Theoretical Amount</td>
<td>Theoretical amount of the compound. Reports N/A when not applicable.</td>
</tr>
<tr>
<td>Concentration</td>
<td></td>
</tr>
<tr>
<td>Confirming n Mass</td>
<td>Mass of the confirming peak.</td>
</tr>
</tbody>
</table>
Table 73. Active View parameters  (Sheet 3 of 4)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Confirming n Response</td>
<td>Response of the confirming peak.</td>
</tr>
<tr>
<td>Confirming n Manual Flag</td>
<td>Indicates a manually integrated confirming peak.</td>
</tr>
<tr>
<td>Confirming n Ion Ratio Flag</td>
<td>Indicates that the ion ratio is out of range.</td>
</tr>
<tr>
<td>Confirming n Ion Ratio</td>
<td>Actual ratio of the confirming ion response to the quan ion response.</td>
</tr>
<tr>
<td>Confirming n Range</td>
<td>Acceptable range for the confirming ion.</td>
</tr>
<tr>
<td>Retention Time</td>
<td>The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Quan Mass</td>
<td>The mass-to-charge ratio used to determine the peak area and peak height of the compound.</td>
</tr>
<tr>
<td>Injection Concentration</td>
<td>Calculated amount as the sample was injected, with no conversion applied.</td>
</tr>
<tr>
<td>Injection Units</td>
<td>Injection units specified on the Calibration page in Method Development mode. See “Calibration” on page 156.</td>
</tr>
<tr>
<td>Sample Concentration</td>
<td>The injected concentration multiplied by the conversion factor.</td>
</tr>
<tr>
<td>Sample Units</td>
<td>Sample units specified on the Calibration page in Method Development mode. See “Calibration” on page 156.</td>
</tr>
<tr>
<td>QIon</td>
<td>Mass range for the quan peak.</td>
</tr>
<tr>
<td>RT</td>
<td>Retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
</tbody>
</table>

**Manual Integration reports**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/z</td>
<td>Mass-to-charge ratio for the quan peak.</td>
</tr>
<tr>
<td>Method RT</td>
<td>Apex retention time for the method-integrated peak.</td>
</tr>
<tr>
<td>Method Peak Height</td>
<td>Height of the method-integrated peak.</td>
</tr>
<tr>
<td>Method Peak Area</td>
<td>Area of the method-integrated peak.</td>
</tr>
<tr>
<td>Manual RT</td>
<td>Apex retention time for the manually integrated peak.</td>
</tr>
<tr>
<td>Manual Peak Height</td>
<td>Height of the manually integrated peak.</td>
</tr>
<tr>
<td>Manual Peak Area</td>
<td>Area of the manually integrated peak.</td>
</tr>
</tbody>
</table>
### Table 73. Active View parameters  (Sheet 4 of 4)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Internal Standard reports</strong></td>
<td></td>
</tr>
<tr>
<td>Std Response</td>
<td>Average of the internal standard’s response as found in the calibration file.</td>
</tr>
<tr>
<td>Minimum Response</td>
<td>Minimum response time as specified on the ISTD page in Method Development mode. See “ISTD” on page 169.</td>
</tr>
<tr>
<td>Maximum Response</td>
<td>Maximum response time as specified on the ISTD page in Method Development mode. See “ISTD” on page 169.</td>
</tr>
<tr>
<td>Sample Response</td>
<td>Area found in the sample.</td>
</tr>
<tr>
<td>Std RT</td>
<td>Average retention time as found in the calibration file.</td>
</tr>
<tr>
<td>Min RT</td>
<td>Minimum retention time as specified on the ISTD page in Method Development mode. See “ISTD” on page 169.</td>
</tr>
<tr>
<td>Max RT</td>
<td>Maximum retention time as specified on the ISTD page in Method Development mode. See “ISTD” on page 169.</td>
</tr>
<tr>
<td>Sample RT</td>
<td>Retention time found in the sample.</td>
</tr>
<tr>
<td><strong>Graphical data</strong></td>
<td></td>
</tr>
<tr>
<td>Quan Peak 1</td>
<td></td>
</tr>
<tr>
<td>Calibration curve</td>
<td>Displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration.</td>
</tr>
<tr>
<td>Spectra</td>
<td>Displays a comparison of the spectra found in the data and the method reference.</td>
</tr>
<tr>
<td>QED Spectra</td>
<td>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.</td>
</tr>
<tr>
<td>Confirming Ions</td>
<td>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.</td>
</tr>
</tbody>
</table>
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 366.

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
- Quality Control Report Active View values
- Quantitation Report Active View columns
- Solvent Blank Report Active View columns
## Table 74. Common Active View report columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Status</td>
<td>Indicates the status of the reported compound.</td>
</tr>
<tr>
<td></td>
<td>• A yellow caution sign indicates one of the following conditions:</td>
</tr>
<tr>
<td></td>
<td>– The compound was manually integrated.</td>
</tr>
<tr>
<td></td>
<td>– Any of the confirming peaks was manually integrated.</td>
</tr>
<tr>
<td></td>
<td>– The compound has quan flags.</td>
</tr>
<tr>
<td></td>
<td>– The compound has a QAQC failure.</td>
</tr>
<tr>
<td></td>
<td>• A green check mark indicates that none of these conditions exists.</td>
</tr>
<tr>
<td></td>
<td>When the compound is an internal standard, warning flags are displayed only on the internal standard report.</td>
</tr>
<tr>
<td>Compound Name</td>
<td>Alphanumeric name assigned to the compound.</td>
</tr>
<tr>
<td>Compound Type</td>
<td>Target Compound or Internal Standard.</td>
</tr>
<tr>
<td>QAQC Flags</td>
<td>Indicates that the QAQC check for the sample failed.</td>
</tr>
<tr>
<td></td>
<td>The Method Validation and MDL reports do not use the QAQC column.</td>
</tr>
<tr>
<td>Quan Flags</td>
<td>• Limit of Detection (LOD)</td>
</tr>
<tr>
<td></td>
<td>• Limit of Quantitation (LOQ)</td>
</tr>
<tr>
<td></td>
<td>• Limit of Reporting (LOR)</td>
</tr>
<tr>
<td></td>
<td>• Values between the limit of detection and the limit of quantitation, known as the J flag</td>
</tr>
<tr>
<td></td>
<td>• Upper Limit of Linearity (ULOL)</td>
</tr>
<tr>
<td></td>
<td>Quan flags do not apply to these sample types: Calibrator, QC, or Solvent.</td>
</tr>
<tr>
<td></td>
<td>The Calibration report does not use the Quan Flags column. The Calibration Curve report does not use the Quan Flags column.</td>
</tr>
<tr>
<td>Manual Flags</td>
<td>Indicates manually integrated peaks.</td>
</tr>
<tr>
<td></td>
<td>• M indicates a manually integrated quan peak.</td>
</tr>
<tr>
<td></td>
<td>• m indicates a manually integrated confirming peak.</td>
</tr>
</tbody>
</table>

## Table 75. Blank Report Active View columns (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Retention Time</td>
<td>Retention time for the quan mass. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>Quan Mass</td>
<td>Mass range for the quan peak.</td>
</tr>
<tr>
<td>Response</td>
<td>Sum of all Quan Peak Response values for the compound.</td>
</tr>
<tr>
<td>Inj Conc</td>
<td>Calculated amount as the sample was injected, with no conversion applied.</td>
</tr>
</tbody>
</table>
### Table 75. Blank Report Active View columns (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inj Units</td>
<td>Injection units specified on the Calibration page in Method Development mode. See “Calibration” on page 156.</td>
</tr>
<tr>
<td>Sample Conc</td>
<td>Calculated amount multiplied by the conversion factor.</td>
</tr>
<tr>
<td>Sample Units</td>
<td>Sample units specified on the Calibration page in Method Development mode. See “Calibration” on page 156.</td>
</tr>
</tbody>
</table>

### Table 76. Calibration Report Active View columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Curve Type</td>
<td>The type of curve used when calibrating the compound (linear, quadratic, or average response factor).</td>
</tr>
<tr>
<td>Average RF</td>
<td>The average response factor. Applicable if curve type is Average RF.</td>
</tr>
<tr>
<td>Average Response</td>
<td>The average response for the internal standard across all calibration points. Applies only to Internal Standard sample types.</td>
</tr>
<tr>
<td>A0</td>
<td>The value with no X. Applies only to linear and quadratic curves.</td>
</tr>
<tr>
<td>A1</td>
<td>The X value. Applies only to linear and quadratic curves.</td>
</tr>
<tr>
<td>A2</td>
<td>The X^2 value. Applies only to quadratic curves.</td>
</tr>
<tr>
<td>R^2</td>
<td>The minimum correlation coefficient (r^2) for an acceptable calibration (when in linear or quadratic mode).</td>
</tr>
<tr>
<td>RSD</td>
<td>Relative standard deviation. Applies only to internal standards and targets calibrated with an average RF curve.</td>
</tr>
<tr>
<td>Level</td>
<td>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.</td>
</tr>
</tbody>
</table>

### Table 77. High Density Sample Report 1 and High Density Sample Report 1 Long Active View columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/z</td>
<td>Mass-to-charge ratio for the quan peak.</td>
</tr>
<tr>
<td>Total Response</td>
<td>The sum of all Quan Peak Response values for the compound.</td>
</tr>
<tr>
<td>Quan Peak Response</td>
<td>Response of the quan peak.</td>
</tr>
<tr>
<td>Quan Peak RT</td>
<td>Retention time for the quan peak.</td>
</tr>
<tr>
<td>T Amount</td>
<td>Theoretical amount of the compound. Reports N/A when not applicable.</td>
</tr>
<tr>
<td>Conc</td>
<td>Calculated (injected) amount.</td>
</tr>
</tbody>
</table>
### Table 79. High Density Sample Report 2 and High Density Sample Report 2 Long Active View columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/z</td>
<td>Mass-to-charge ratio for the quan peak.</td>
</tr>
<tr>
<td>Total Response</td>
<td>Sum of all Quan Peak Response values for the compound.</td>
</tr>
<tr>
<td>Quan Peak Response</td>
<td>Response of the quan peak.</td>
</tr>
<tr>
<td>Quan Peak RT</td>
<td>Retention time for the quan peak.</td>
</tr>
<tr>
<td>T Amount</td>
<td>Theoretical amount of the compound. Reports N/A when not applicable.</td>
</tr>
<tr>
<td>Conc</td>
<td>Calculated (injected) amount.</td>
</tr>
<tr>
<td>Confirming 1 Mass</td>
<td>Mass of the confirming peak.</td>
</tr>
<tr>
<td>Confirming 1 Response</td>
<td>Response of the confirming peak.</td>
</tr>
<tr>
<td>Confirming 1 Manual Flag</td>
<td>Indicates a manually integrated confirming peak.</td>
</tr>
<tr>
<td>Confirming 1 Ion Ratio Flag</td>
<td>Indicates that the ion ratio is out of range.</td>
</tr>
<tr>
<td>Confirming 1 Ion Ratio</td>
<td>Actual ratio of the confirming ion response to the quan ion response.</td>
</tr>
<tr>
<td>Confirming 1 Range</td>
<td>Acceptable range for the confirming ion.</td>
</tr>
</tbody>
</table>

### Table 80. High Density Sample Report 3 and High Density Sample Report 3 Long Active View columns (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/z</td>
<td>Mass-to-charge ratio for the quan peak.</td>
</tr>
<tr>
<td>Total Response</td>
<td>Sum of all Quan Peak Response values for the compound.</td>
</tr>
<tr>
<td>Quan Peak Response</td>
<td>Response of the quan peak.</td>
</tr>
<tr>
<td>Quan Peak RT</td>
<td>Retention time for the quan peak.</td>
</tr>
<tr>
<td>T Amount</td>
<td>Theoretical amount of the compound. Reports N/A when not applicable.</td>
</tr>
<tr>
<td>Conc</td>
<td>Calculated (injected) amount.</td>
</tr>
<tr>
<td>Confirming 1 Mass</td>
<td>Mass of the confirming peak.</td>
</tr>
<tr>
<td>Confirming 1 Response</td>
<td>Response of the confirming peak.</td>
</tr>
<tr>
<td>Confirming 1 Manual Flag</td>
<td>Indicates a manually integrated confirming peak.</td>
</tr>
<tr>
<td>Confirming 1 Ion Ratio Flag</td>
<td>Indicates that the ion ratio is out of range.</td>
</tr>
<tr>
<td>Confirming 1 Ion Ratio</td>
<td>Actual ratio of the confirming ion response to the quan ion response.</td>
</tr>
<tr>
<td>Confirming 1 Range</td>
<td>Acceptable range for the confirming ion.</td>
</tr>
<tr>
<td>Confirming 2 Mass</td>
<td>Mass of the confirming peak.</td>
</tr>
<tr>
<td>Confirming 2 Response</td>
<td>Response of the confirming peak.</td>
</tr>
<tr>
<td>Confirming 2 Manual Flag</td>
<td>Indicates a manually integrated confirming peak.</td>
</tr>
<tr>
<td>Confirming 2 Ion Ratio Flag</td>
<td>Indicates that the ion ratio is out of range.</td>
</tr>
</tbody>
</table>
Table 80. High Density Sample Report 3 and High Density Sample Report 3 Long Active View columns (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Confirming 2 Ion Ratio</td>
<td>Actual ratio of the confirming ion response to the quan ion response.</td>
</tr>
<tr>
<td>Confirming 2 Range</td>
<td>Acceptable range for the confirming ion.</td>
</tr>
</tbody>
</table>

Table 81. Internal Standard Summary Report Active View columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Std Response</td>
<td>Average of the internal standard’s response as found in the calibration file.</td>
</tr>
<tr>
<td>Minimum Response</td>
<td>Minimum response time as specified on the ISTD page in Method Development mode. See “ISTD” on page 169.</td>
</tr>
<tr>
<td>Maximum Response</td>
<td>Maximum response time as specified on the ISTD page in Method Development mode. See “ISTD” on page 169.</td>
</tr>
<tr>
<td>Sample Response</td>
<td>Area found in the sample.</td>
</tr>
<tr>
<td>Std RT</td>
<td>Average retention time as found in the calibration file.</td>
</tr>
<tr>
<td>Min RT</td>
<td>Minimum retention time as specified on the ISTD page in Method Development mode. See “ISTD” on page 169.</td>
</tr>
<tr>
<td>Max RT</td>
<td>Maximum retention time as specified on the ISTD page in Method Development mode. See “ISTD” on page 169.</td>
</tr>
<tr>
<td>Sample RT</td>
<td>Retention time found in the sample.</td>
</tr>
</tbody>
</table>

Table 82. Ion Ratio Failure Report Active View columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quan Ion</td>
<td>The ion for quan peak.</td>
</tr>
<tr>
<td>Qual Ion</td>
<td>The ion for the confirming peak.</td>
</tr>
<tr>
<td>Quan Ion Response</td>
<td>Response of the quantitation ion.</td>
</tr>
<tr>
<td>Qual Ion Response</td>
<td>Response of the qualitative ion.</td>
</tr>
<tr>
<td>Ratio</td>
<td>The ratio of the confirming ion response to the quan ion response.</td>
</tr>
<tr>
<td>Range</td>
<td>The acceptable range.</td>
</tr>
</tbody>
</table>

Table 83. Manual Integration Report Active View columns (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/z</td>
<td>Mass-to-charge ratio for the quan peak.</td>
</tr>
<tr>
<td>Method RT</td>
<td>Apex retention time for the method-integrated peak.</td>
</tr>
<tr>
<td>Method Peak Height</td>
<td>Height for the method-integrated peak.</td>
</tr>
<tr>
<td>Method Peak Area</td>
<td>Area for the method-integrated peak.</td>
</tr>
</tbody>
</table>
6 Using the Analysis Mode
Working in the Report View

Table 83. Manual Integration Report Active View columns (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manual RT</td>
<td>Apex retention time for the manually integrated peak.</td>
</tr>
<tr>
<td>Manual Peak Height</td>
<td>Height of the manually integrated peak.</td>
</tr>
<tr>
<td>Manual Peak Area</td>
<td>Area of the manually integrated peak.</td>
</tr>
</tbody>
</table>

Table 84. Manual Integration Report Active View columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m/z</td>
<td>Mass-to-charge ratio for the quan peak.</td>
</tr>
<tr>
<td>Method RT</td>
<td>Apex retention time for the method-integrated peak.</td>
</tr>
<tr>
<td>Method Peak Height</td>
<td>Height for the method-integrated peak.</td>
</tr>
<tr>
<td>Method Peak Area</td>
<td>Area for the method-integrated peak.</td>
</tr>
<tr>
<td>Manual RT</td>
<td>Apex retention time for the manually integrated peak.</td>
</tr>
<tr>
<td>Manual Peak Height</td>
<td>Height of the manually integrated peak.</td>
</tr>
<tr>
<td>Manual Peak Area</td>
<td>Area of the manually integrated peak.</td>
</tr>
</tbody>
</table>

Table 85. Quality Control Report Active View values

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Curve Type</td>
<td>L - Linear</td>
</tr>
<tr>
<td></td>
<td>A - Average RF</td>
</tr>
<tr>
<td></td>
<td>Q - Quadratic</td>
</tr>
<tr>
<td>Daily RF</td>
<td>The response factor value for Average RF curve types. For all other curve types, this column is blank.</td>
</tr>
<tr>
<td>Mean RF</td>
<td>The average response factor as found in the calibration file. Displayed for Average RF curve types. For all other curve types, this column is blank.</td>
</tr>
<tr>
<td>Min RF</td>
<td>Minimum QC response factor as found on the QC Check page in the method.</td>
</tr>
<tr>
<td>RF % D</td>
<td>Percent difference between daily and average response factor.</td>
</tr>
<tr>
<td>Max RF Diff (%)</td>
<td>Maximum QC response factor as found on the QC Check page in the method.</td>
</tr>
<tr>
<td>QC Amount</td>
<td>The amount defined by the level for the compound.</td>
</tr>
<tr>
<td>Calculated Amount</td>
<td>Reportable amount of concentration.</td>
</tr>
<tr>
<td>Amount % Difference</td>
<td>Percentage difference between the calculated amount and the QC amount. Use the injected concentration to calculate this value.</td>
</tr>
<tr>
<td>Max Amount % Difference</td>
<td>Maximum allowed percentage difference between the calculated amount and the QC amount.</td>
</tr>
</tbody>
</table>
### Table 86. Quantitation Report Active View columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time for the peak. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>QIon</td>
<td>Mass range for the quan peak.</td>
</tr>
<tr>
<td>Response</td>
<td>Sum of all quan peak response values for the compound.</td>
</tr>
<tr>
<td>Injected Concentration</td>
<td>Calculated amount as the sample was injected, with no conversion applied.</td>
</tr>
</tbody>
</table>

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 156. |
| 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 156. |

### Table 88. Solvent Blank Report Active View columns

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>Retention time for the quan peak. The time after injection when the compound elutes. The total time that the compound is retained on the column.</td>
</tr>
<tr>
<td>QIon</td>
<td>Mass range for the quan peak.</td>
</tr>
<tr>
<td>Response</td>
<td>Sum of all Quan Peak Response values for the compound.</td>
</tr>
<tr>
<td>Method</td>
<td>Method of evaluation defined in the method.</td>
</tr>
<tr>
<td>Upper Limit</td>
<td>Defined in the method.</td>
</tr>
</tbody>
</table>
Working in the Local Method View

A local method is a copy of a master method associated with a batch. You can edit only the local copy of the method, or you can edit the master method and overwrite the local copy with the edited master method.

In the Local Method view, you can edit the local method parameters. A local method is a copy of a master method associated with a batch. Local methods are named 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 94.

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 92. Local Method View

Local Method View - BatchA_MethodA

Master method: MethodA

Lab name: Default Laboratory
Assay type: Assay name
Injection volume: 1.00
Ion range calc method: Manual

Instrument method: Anabolic Steroids

Qualitative peak processing template: Default

Background subtraction range option: None
Number of scans to subtract: 1
Stepoff value: 0

Set chromatogram reference sample: None
Set Reference sample:

Mass Tolerance: 500.0 MMU PPM

Edit Update Select Apply
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. 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 294.

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 380.

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 380.

❖ **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 46.

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, +.

The application adds a new, Specimen sample to the end of the sample list.

To insert a sample into the list

1. Select the sample above which you will insert a new, Specimen sample.
2. Right-click and choose Insert Sample from the shortcut menu.

The application inserts a new, Specimen sample above the selected sample.

To copy a sample

1. Select the sample 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 you want to remove.
   Use the SHIFT or CTRL keys to select multiple samples.
2. Right-click and choose Remove Selected Samples from the shortcut menu, or click the Remove Sample icon, –.

The application removes the selected samples from the list.

To edit sample values

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

<table>
<thead>
<tr>
<th>Sample type</th>
<th>Level</th>
<th>Sample ID</th>
<th>Sample name</th>
<th>Comment</th>
<th>Repeat sample count</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specimen</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Negative</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

**Available sample types**

- Specimen
- Specimen/Qual
- QC
- Solvent
- Calibrator
- Hydrolysis
- Unextracted
- Negative
2. For each QC or Calibrator sample, click the Level cell and select a level from the list.

   The calibration and QC levels were defined in the master method. If there is nothing to select in the Level list, do the following:
   a. Close the Batch Template Editor.
   b. Return to the Method Development mode.
   c. Open the master method.
   d. Click the **Compounds** tab.
   e. Click the **Calibration Levels** tab.
   f. Add the levels.
   g. Save the method.
   h. Return to the Analysis mode, and begin this batch template again.

   You must close your original batch template without saving it and start a new template.

   For detailed instructions, see “Editing a Master Method” on page 110.

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 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.

      ![Copy Down option](image)

      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:

- Copying selected output formats from the first sample

Duplicate the selected output formats to all samples in the batch
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 you want to identify 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.
Figure 93. Batch Template Editor

Table 89. Batch Template Editor parameters (Sheet 1 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Template Method Information</strong></td>
<td></td>
</tr>
<tr>
<td>Project</td>
<td>The top-level project for the batch.</td>
</tr>
<tr>
<td>Subproject</td>
<td>The lower-level project for the batch.</td>
</tr>
<tr>
<td>Method</td>
<td>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.</td>
</tr>
</tbody>
</table>
Table 89. Batch Template Editor parameters (Sheet 2 of 2)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Assay Type</td>
<td>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.</td>
</tr>
</tbody>
</table>

**Column values**

- **Sample Type**: Defines how the application processes the sample data. Each sample is classified as one of the following sample types: Specimen, Specimen/Qual, QC, Solvent, Calibrator, Hydrolysis, Unextracted, or Negative.
- **Level**: The level defined for a calibration sample or quality control sample.
- **Sample ID**: A user-defined alphanumeric string that identifies a sample.
- **Sample Name**: A user-defined name that identifies a sample.
- **Comment**: A user-defined comment for the sample.
- **Repeat Sample Count**: Number of samples to create for this sample type.

**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**: Exports reports in XML format. Available only for standard reports.
- **Create XLSM**: Exports 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 65.

For detailed information about specifying reports when you create a method in the Method Development mode, see “Editing the Reports Page” on page 175.

For detailed information about viewing batch reports in the Acquisition mode, see “Selecting and Reviewing Reports” on page 238.
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 Summary Report
- Calibration Report
- Calibration Curve Report
- Chromatogram Report
- Compound Calibration Report
- Compound Calibration Report - Alternate
- Confirmation Report
- High Density Calibration Report
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- Manual Integration Report
- Method Report
- Negative Report
- Qualitative Peak Report
- Qualitative Summary Report
- Quality Control Report
- Quantitation Report
- Quantitation Report - 2
- Sample Report
- Sample Report Long
- Solvent Blank Report

To view an example of each type of standard report, see “Sample Standard Reports” on page 387.
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 to create separate reports for each sample. Rather than creating separate reports for each sample, this method uses data from only the last sample to create a single report for the entire batch.

The TraceFinder application includes the following 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

- Target Screening Long Report
- Target Screening Summary Report
Report Flags

When generating or viewing a report, you might see one of the following quantification or calibration flags listed on the page.

### Table 90. Quantification flags

<table>
<thead>
<tr>
<th>Flag</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>b</td>
<td>Compound was observed at a concentration in a Matrix Blank sample above the specified limit.</td>
</tr>
<tr>
<td>s</td>
<td>Compound was observed at a response in a solvent blank sample above the specified limit.</td>
</tr>
<tr>
<td>J</td>
<td>Compound was observed at a concentration above the limit of detection, but below the limit of quantitation.</td>
</tr>
<tr>
<td>I or *</td>
<td>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.</td>
</tr>
<tr>
<td>C</td>
<td>Compound was observed at a concentration above the specified carryover limit.</td>
</tr>
<tr>
<td>?</td>
<td>Compound was observed at a concentration above the specified linearity limit.</td>
</tr>
<tr>
<td>D</td>
<td>Compound was observed at a concentration below the specified limit of detection.</td>
</tr>
<tr>
<td>Q</td>
<td>Compound was observed at a concentration below the specified limit of quantitation.</td>
</tr>
<tr>
<td>POS</td>
<td>Compound was observed at a concentration above the specified cutoff.</td>
</tr>
</tbody>
</table>

### Table 91. Calibration flags

<table>
<thead>
<tr>
<th>Flag</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>Calibration for this compound exceeded the specified maximum percent relative standard deviation (%RSD).</td>
</tr>
<tr>
<td>F</td>
<td>Response factor for this compound was below the specified minimum response factor (Min RF).</td>
</tr>
<tr>
<td>R</td>
<td>Calibration for this compound was below the specified minimum correlation coefficient ($r^2$).</td>
</tr>
<tr>
<td>A</td>
<td>Back calculation of the calibration points for this compound exceeded the specified maximum percent difference (Max %D).</td>
</tr>
<tr>
<td>X</td>
<td>Calibration point for this compound was excluded from the overall calibration by manual selection.</td>
</tr>
<tr>
<td>X(ISNF)</td>
<td>Calibration point for this compound was excluded from the overall calibration because its associated internal standard was not found.</td>
</tr>
</tbody>
</table>

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
- 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
- Quality Control 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.
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<th>File Name</th>
<th>Date/Time</th>
<th>Sample ID</th>
<th>Sample Name</th>
<th>Level</th>
<th>Sample Type</th>
<th>Val Pol</th>
<th>Inf Vol</th>
<th>Conv Factor</th>
<th>Comment</th>
</tr>
</thead>
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Flag legend: LOD=+LOQ; IR=Ion ratio failure; CR=Carryover; L=Linewty limit; D=Detection limit; Q=Quant limit; POS=POS limit; blank = Solvent blank
## Calibration Report

<table>
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<tr>
<th>Compound</th>
<th>Manually Integrated</th>
<th>Curve Type</th>
<th>y-Intercept</th>
<th>Slope</th>
<th>% RSD</th>
<th>Flag</th>
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**Curve Type:** A=Average RF; L=Linear; Q=Quadratic (Internal standard) **Note:** Amounts displayed for internal standards represent the ISSTD Response.

**Calibration Report:** A=Response factor; F=Response factor; R=RF2; A=Amount(X=Excluded, X=ISSTD)=Excluded because ISSTD wasn't found.
A Reports
Sample Standard Reports

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/

Thermo Scientific

TraceFinder User Guide

393


### Sample Standard Reports

#### Calibration Report

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<th>Level</th>
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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=Ratio; F=Response factor; R=Reagent; A=Amount[X=Excluded; X][BNF]=Excluded because ISTD wasn't found.

Manually integrated
Calibration Density Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMERjamie.humphries
Batch: Preview2
Method: Preview2_EPA536-Triazines
Cali File: Preview2.calx
## Check Standard Report

**Lab Name:** Thermo Lab  
**Instrument:** TQVID  
**User:** TQVID  
**Batch:** 01HPR1  
**Method:** 01HPR1_POP_040511  
**Call File:** 01HPR1_calls

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<th>Max RF %</th>
<th>QC Amt</th>
<th>Calb Amt</th>
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Manually Integrated:  
* = Fail; Curve Type: A=Average RF; L=Linear; Q=Quadratic; R=Recovery limits exceeded
Chromatogram Report

Lab Name: Thermo Lab
Instrument: TQU0637
User: TQ0637
Batch: 01HFLR1
Method: 01HFLR1_PDP_040511
Call File: 01HFLR1.rlsk

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![Chromatogram Graph]
Compound Name: nicotine

Quadratic Pare

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Manually Integrated: [ ]

Calibration Flags: D = RSD, F = Response factor, R = R Squared, A = Amount
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Manually Integrated: [ ]

Calibration Flags: D = RSD, F = Response factor, R = R Squared, A = Amount
## Compound Calibration Report - Alternate

### Compound Name:
Dinitrafin

![Graph showing calibration curve with equation: Y = -3.798e+02 * X^2 + 8.976e+04 * X, R^2 = 0.99985. Origin: 0; Units: Area; Area range: 0 to 45,000,000.](image)

<table>
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<th>Std Area</th>
<th>IS Amount</th>
<th>IS Area</th>
<th>Response factor</th>
<th>Calc Amt</th>
<th>Units</th>
<th>Min Range</th>
<th>Max Range</th>
<th>% RSD</th>
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### Table Notes:
- **Manually Integrated:** [ ]
- **Calibration Flags:** D = RSD, F = Response factor, R = R Squared, A = Amount

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**Lab Name:** Thermo Lab  
**Instrument:** TQX01.37  
**User:** TQX01.37/PC  
**Batch:** 0116PR1
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<td>3/7/2011 7:06:17 PM</td>
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Confirmation Report

Lab Name: Thermo Lab
Instrument: TQ00637
Method: 011HPLR1_PDP_040511
User: TQ00637_RPC
Batch: 011HPLR1
Cal File: 011HPLR1.cal

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<td>3/17/2011 8:06:03 PM</td>
<td></td>
</tr>
</tbody>
</table>

**Dinofuran**

- **Injected**: 642.34 PPB
- **Sample**: 642.34 PPB

**Retention Time**: 4.52
**Area**: 41994838
**Height**: 8893885

**Calibration Curve**

**MS-Data**

**MS-Reference**

**Overlay**

Flag legend: LOD=LOQ; L-ion ratio failure; C=Carryover; T=Linearity limit; D=Detection limit; Q=Quant limit; P0S=Post limit; b=Blank; e=Solvent blank

**Quan Ion 1: 203.111-199.14**

**Qual Ion 1: 203.111-199.14**

Ratio: 72.29% Range: 92.28% - 92.28%
Confirmation Report 2

Lab Name: Thermo Lab
Instrument: TQX00637
Method: 01HPR1_LDF_040511
User: TQX00637_RPC
Batch: 01HPR1
Call File: 01HPR1_call.

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Compound Name: Dinitfuran
Injection Conc: 642.34 PPB
Sample Conc: 642.34 PPB
Retention Time: 4.52
Area (Quan): 41994838
Height (Quan): 8853885
Qual Ratio 1: Pass
Qual Ratio 2: Pass

Quan Ion: 203.11->129.14

Quan Ion 1: 203.11->114.15
Ratio: 72.29% Range: 52.26 - 92.28%

MS-Data

MS-Reference: normalTraceFinder1.1\Projects\Default\Default01HPR1\Data\L32XLOQ_HPS1711.raw

Overlay
High Density Internal Standard Report

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<td>level 1</td>
<td>Drug_A</td>
<td>4/17/2008 5:05:47 PM</td>
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</tbody>
</table>

**Drug_A**

- Quan m/z: 371.20
- Total Area: 2275661
- Peak Area: 2275661
- RT: 1.95 min (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 % - 25.49 %

**Qual m/z: 488.20**

- Area: 32066
- Ratio: 14.09 %
- Range: 11.43 % - 17.14 %

**int Std**

- Quan m/z: 380.20
- Total Area: 673044
- Peak Area: 678044
- RT: 1.95 min (1.95)
- Amount: 15,000 ng/mL

Flag legend: LO=LOQ; ?=Ratio failure; C=Carryover; L=Linearity limit; D=Detection Limit; Q=Quan limit; P=Positive; N=Negative; B=Solvent blank; H=Hydrolysis
High Density Internal Standard Report Long

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER/jamie.humphries
Batch: Drug_A
Method: Drug_A
Cal File: Drug_A.calx

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<thead>
<tr>
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<th>Sample Name</th>
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<td>level 1</td>
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</tr>
</tbody>
</table>

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: 473.26
Area: 62641
Ratio: 27.53 %
Range: 22.33 % - 33.49 %

Qual m/z: 486.20
Area: 32086
Ratio: 14.69 %
Range: 11.43 % - 17.14 %

nl Std
Quan m/z: 380.20
Total Area: 679044
Peak Area: 678044
RT: 1.93min (1.94)
Amount: 15.000 ng/mL

Flag legend: LLOQ: Low Limit of Quantitation; CR: Carryover; PLL: Linearity limit; DL: Detection limit; C: Quan limit; PC: Peak cutoff; N: Negative; SB: Solvent blank
H: Hydrolysate
# High Density Sample Report 1

**Lab Name:** Thermo Lab  
**Instrument:** TQD00537  
**Method:** 01HJR.L1_PDP_040511  
**User:** TQD00537PNC  
**Batch:** 01HJR.L1

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Flag legend: LOD=LOQ; <m>ionic ratio failure; <n>Carynover; <f>linear limit; <d>Deletion limit; <q>Quan limit; <p>S=Res limit; <b>Blank; <s>Solute blank

---

**Thermo Scientific**

**TraceFinder User Guide**
High Density Sample Report 1 Long

Lab Name: Thermo Lab
Instrument: TQ00637
User: TQ00637PWC
Batch: 0111HPR1
Method: PDP04511

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<table>
<thead>
<tr>
<th>Compound</th>
<th>Quan m/z</th>
<th>Total Area</th>
<th>Peak Area</th>
<th>RT (min)</th>
<th>TAmount</th>
<th>Amount (PPB)</th>
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<tbody>
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<td>Osamyl, Ozone</td>
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<td>Dinethane</td>
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<td>Aldicarb, SO2</td>
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<td>1920.00</td>
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<td>199.00</td>
<td>46009719</td>
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Flag legend: LLOD=LLOQ; H=foo ratio failure; C=Carryover; 5=Linearly limit; D=Detection limit; Q=Quan limit; POS=POS limit; B=Blank; S=Solute blank
# High Density Sample Report 2

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**Oxanfloracetam**
- Quan m/z: 183.04
- Total ion: 47920271
- Peak Area: 47882071
- RT: 4.39 min (4.34)
- Amount: 158.40 PPM
- TAmount: 158.40 PPM

**Ox acetate**
- Quan m/z: 80.08
- Area: 8274971
- %: 120 - 27.25%
- Range: 13.69 - 93.49%

**Aldochlor_S0**
- Quan m/z: 132.05
- Total ion: 43053255
- Peak Area: 43053255
- RT: 5.95 min (4.52)
- Amount: 6.29 PPM
- TAmount: 6.29 PPM

**Aldochlor_S02**
- Quan m/z: 148.04
- Total ion: 74393259
- Peak Area: 74393259
- RT: 6.07 min (4.68)
- Amount: 160.15 PPM
- TAmount: 160.00 PPM

**Aldochlor_S02**
- Quan m/z: 84.00
- Area: 43918555
- %: 99.46%
- Range: 40.81 - 80.81%

**Eprosarten**
- Quan m/z: 130.00
- Total ion: 23040792
- Peak Area: 23040792
- RT: 2.04 min (4.03)
- Amount: 656.38 PPM
- TAmount: 656.38 PPM

**COMS**
- Quan m/z: 139.00
- Total ion: 40474319
- Peak Area: 40474319
- RT: 8.07 min (5.07)
- Amount: 320.14 PPM
- TAmount: 320.00 PPM

**Ultra RQ**
- Quan m/z: 108.85
- Area: 32190012
- %: 97.69%
- Range: 29.22 - 89.22%

---

Flag legend: LO=LOQ; m=Mon failure; O=Carrier; T=Intensity limit; D=Detection limit; Q=Quan limit; P05=Rt limit; B=Blank; s=Solute blank.
## High Density Sample Report 2 Long

**Lab Name:** Thermo Lab  
**Instrument:** QIqU05X7  
**Method:** 011HPL.R1_PDP_040511  
**User:** QIqU05X7PC  
**File Name:** L32XLOG_HPS07111  
**Location:** L32XLOG  
**Sample Name:** L32XLOG_HPS07111  
**File Date:** 31/07/2011 8:06:03 PM  

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<th>Level</th>
<th>Sample Name</th>
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<th>Comment</th>
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<tbody>
<tr>
<td>1</td>
<td>8</td>
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</tr>
</tbody>
</table>

### TraceFinder User Guide Thermo Scientific

*Flag legend: LDP=LOQ; Ion ratio failure; C=Caryover; L=Linearly limit; D=Detection limit; Q=Quan limit; POS=Pos limit; B=Blank; p=Solvent blank*
High Density Sample Report 3

Lab Name: Thermo Lab
Instrument: TQ00637
User: TQ00637PQC
Batch: 01HPLR1
Method: 01HPLR1_PDP_040511
File Date: 3/17/2011 8:06:03 PM

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<tr>
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<td>8</td>
<td>L32XLOG_HPI031711</td>
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<td>3/17/2011 8:06:03 PM</td>
<td></td>
</tr>
</tbody>
</table>

**Amitriptyline**

- Quan ID: 72.10
- Total Area: 113824994
- Peak Area: 113824994
- RT: 6.331 min (4.19)
- Amount: 128.03 PPB
- TAmount: 128.00 PPB

**Omeprazole**

- Quan ID: 163.04
- Total Area: 47590371
- Peak Area: 47590371
- RT: 6.538 min (4.58)
- Amount: 58.19 PPB
- TAmount: 58.00 PPB

**Formaldehyde**

- Quan ID: 184.10
- Total Area: 213812129
- Peak Area: 213812129
- RT: 6.356 min (4.36)
- Amount: 96.246 PPB
- TAmount: 96.00 PPB

**Dinitofuran**

- Quan ID: 126.14
- Total Area: 409943438
- Peak Area: 409943438
- RT: 6.439 min (4.51)
- Amount: 62.34 PPB
- TAmount: 62.00 PPB

**Aldicarb_SO**

- Quan ID: 132.05
- Total Area: 459525255
- Peak Area: 459525255
- RT: 6.653 min (6.53)
- Amount: 61.26 PPB
- TAmount: 60.00 PPB

**Propamocarb**

- Quan ID: 103.00
- Total Area: 233040768
- Peak Area: 233040768
- RT: 6.531 min (4.53)
- Amount: 69.19 PPB
- TAmount: 60.00 PPB

Flag legend: L0D=L1LOG: H/on ratio failure; C=Caryover; T=Linearity limit; D=Detection limit; Q=Quan limit; POB=POS limit; b=Blank; s=Solvent blank
# High Density Sample Report 3 Long

<table>
<thead>
<tr>
<th>Yel Pre</th>
<th>Sample ID</th>
<th>File Name</th>
<th>Level</th>
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<th>File Data</th>
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<tbody>
<tr>
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<td>L32XLOQ_HPO31711</td>
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<td>3/17/2011 8:06:03 PM</td>
<td></td>
</tr>
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**Oxymethyl-Oxime**

- Quan m/z: 90.06
- Area: 6374691
- Ratio: 7.24%
- Range: 0.00% - 27.25%
- RT: 4.32 min (4.31)
- Amount: 1280.93 PBP
- TAmount: 1280.00 PBP

**Omethoide**

- Quan m/z: 133.03
- Area: 5655012
- Ratio: 74.28%
- Range: 53.49% - 93.49%
- RT: 4.34 min (4.34)
- Amount: 158.19 PBP
- TAmount: 158.00 PBP

**Formanilide**

- Quan m/z: 120.00
- Area: 3352305
- Ratio: 5.02%
- Range: 0.00% - 28.09%
- RT: 4.39 min (4.38)
- Amount: 842.49 PBP
- TAmount: 842.00 PBP

---

Flag legend: LOD=LODQ; I=non ratio failure; C=Carryover; T=Lowerly limit; D=Detection limit; Q=Quan limit; POS+P(at) limit; B=Blank; s=Solvent blank
## Internal Standard Summary Report

**Lab name:** Thermo Fisher Laboratory  
**Instrument:** Thermo Scientific Instrument  
**User:** AMER.jamie.humphries  
**Batch:** Drug_A  
**Method:** Drug_A, Drug_A  
**Call File:** Drug_A.calx

<table>
<thead>
<tr>
<th>Vial Pos</th>
<th>Sample ID</th>
<th>Filename</th>
<th>Level</th>
<th>Sample Name</th>
<th>File Date</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>cal 1 = 6 ng/mL</td>
<td>cal_1</td>
<td>level 1</td>
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<td>4/17/2008 5:05:47 PM</td>
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<table>
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<th>Compound</th>
<th>Std Response</th>
<th>Min</th>
<th>Max</th>
<th>Sample Response</th>
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</thead>
<tbody>
<tr>
<td>Int_Seq</td>
<td>655596</td>
<td>327798(50.00%)</td>
<td>983394(150.00%)</td>
<td>678044</td>
</tr>
<tr>
<td></td>
<td>Std RT</td>
<td>Min</td>
<td>Max</td>
<td>Sample RT</td>
</tr>
<tr>
<td></td>
<td>1.93</td>
<td>1.68(-0.25)</td>
<td>2.18(+0.25)</td>
<td>1.93</td>
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* = Fail  
Manually integrated
## Ion Ratio Failure Report

**Lab Name:** Thermo Lab  
**Instrument:** TQD-9037  
**User:** TQD-9037/FRPC  
**Batch:** 019FRLR1  
**Method:** 019FRLR1_TP3_04.05.11  
**Call File:** 019FRLR1_cal

### Table: Ion Ratio Failure Report

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<th>Level</th>
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<th>File Date</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
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<td>L3_20LGQ_HPD3_1711</td>
<td>32_NLGQ</td>
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<td>3/17/2011 8:06:03 PM</td>
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<table>
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<th>Quan Response</th>
<th>Qual Ion</th>
<th>Qual Response</th>
<th>Ratio</th>
<th>Range</th>
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<tbody>
<tr>
<td>Salbutamol, I</td>
<td>Area</td>
<td>178.02</td>
<td>40020.74</td>
<td>220.05</td>
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<td>74.25</td>
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<td>308610.95</td>
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<td>421.88</td>
<td>3.69-9-409.96</td>
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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 displays as zeros.

<table>
<thead>
<tr>
<th>Pos</th>
<th>Sample ID</th>
<th>Filename</th>
<th>Level</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Tray1:15</td>
<td>SampleID008</td>
<td>5ppb-001</td>
<td>N/A</td>
<td>D008</td>
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<td>New Dilutions 6/26/2007 I</td>
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**SampleID002**

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<th>Spike Amt</th>
<th>Lower Limit %</th>
<th>Upper Limit %</th>
<th>LCSD Conc</th>
<th>% Rec</th>
<th>RPD</th>
<th>Max RPD</th>
<th>Rec Fails</th>
<th>RPD Fails</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIA</td>
<td>0.500</td>
<td>50.00</td>
<td>150.00</td>
<td>4.712</td>
<td>0.00</td>
<td>50.00</td>
<td>50.00</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DEA</td>
<td>0.500</td>
<td>50.00</td>
<td>150.00</td>
<td>5.065</td>
<td>0.00</td>
<td>50.00</td>
<td>50.00</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Cyanazine</td>
<td>0.500</td>
<td>50.00</td>
<td>150.00</td>
<td>5.127</td>
<td>0.00</td>
<td>50.00</td>
<td>50.00</td>
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</tr>
<tr>
<td>Simazine</td>
<td>0.500</td>
<td>50.00</td>
<td>150.00</td>
<td>4.826</td>
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<td>50.00</td>
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<tr>
<td>Atrazine</td>
<td>0.500</td>
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<td>150.00</td>
<td>5.184</td>
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<tr>
<td>Propazine</td>
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**SampleID008**

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<th>% Rec</th>
<th>Lower Limit %</th>
<th>Upper Limit %</th>
<th>LCSD Conc</th>
<th>% Rec</th>
<th>RPD</th>
<th>Max RPD</th>
<th>Rec Fails</th>
<th>RPD Fails</th>
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<tbody>
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<td>DIA</td>
<td>0.500</td>
<td>4.754</td>
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<td>50.00</td>
<td>150.00</td>
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<td>50.00</td>
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<td>0</td>
</tr>
<tr>
<td>DEA</td>
<td>0.500</td>
<td>4.960</td>
<td>0.00</td>
<td>50.00</td>
<td>150.00</td>
<td>5.065</td>
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<td>50.00</td>
<td>50.00</td>
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<td>0</td>
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<tr>
<td>Cyanazine</td>
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<td>5.218</td>
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Manually integrated
Manual Integration Report

Lab Name: Thermo Lab
Instrument: TQI00037
Method: G11HPLRI_PDP_040511
User: TQI00037_RPC
Batch: 01HPLR1
Call File: G11HPLR1.call

<table>
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<tr>
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<th>Sample ID</th>
<th>File Name</th>
<th>Level</th>
<th>Sample Name</th>
<th>File Date</th>
<th>Comment</th>
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<tbody>
<tr>
<td>8</td>
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<td>3/17/2011 8:06:03 PM</td>
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</tbody>
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3-OH Carbofuran
m/z: 183.08

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  
Cali File: Preview2.cali

<table>
<thead>
<tr>
<th>Compound</th>
<th>Avg Conc</th>
<th>Std Dev</th>
<th>t-stat</th>
<th>% RSD</th>
<th>MDL</th>
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<tbody>
<tr>
<td>DIA D-5</td>
<td>290218</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>IS</td>
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<tr>
<td>DEA D-7</td>
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<td>0.00</td>
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<td>DEA</td>
<td>0.065</td>
<td>0.000</td>
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Manually integrated
**Lab name:** Thermo Fisher Laboratory  
**Instrument:** Thermo Scientific Instrument  
**User:** AMER\jamie.humphries  
**Batch:** Preview2

**Method Detection Limit Report**

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<thead>
<tr>
<th>Compound</th>
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<td>Simazine D-10</td>
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<td>Simazine</td>
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<td>826</td>
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Method: Preview2_EPA536-Triazines  
Cali File: Preview2.calx
Method Detection Limit Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER/jamie.humphries
Batch: Preview2

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<th>Level</th>
<th>Sample Name</th>
<th>File Date</th>
<th>Comment</th>
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Manually integrated
Method Report

Method name: Drug_A_Drug_A
Master method name: Drug_A
Current calibration file: Drug_A.cax
Assay type: Drug_A
Inj vol: 1.000
Instrument method: 20x

Compound Identification:

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<th>RT</th>
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<th>View width</th>
<th>Use as reference</th>
<th>Reference compound</th>
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</thead>
<tbody>
<tr>
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Method Report

Method name: Drug_A_Drug_A
Master method name: Drug_A
Current calibration file: Drug_A.cax
Assay type: Drug_A
Inj vol: 1.000
Instrument method: 20x

Compound Calibration:

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<th>Calibration</th>
<th>Curve type</th>
<th>Weighting</th>
<th>Origin</th>
<th>Units</th>
<th>ISTD Name</th>
<th>ISTD Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drug_A</td>
<td>Area</td>
<td>Internal</td>
<td>Linear</td>
<td>Equal</td>
<td>Ignore</td>
<td>ng/mL</td>
<td>Int_Std</td>
<td>ng/mL</td>
</tr>
</tbody>
</table>

Method Report

Method name: Drug_A_Drug_A
Master method name: Drug_A
Current calibration file: Drug_A.cax
Assay type: Drug_A
Inj vol: 1.000
Instrument method: 20x

QAQC Limits:

<table>
<thead>
<tr>
<th>Compound</th>
<th>LOD</th>
<th>LOQ</th>
<th>Cutoff</th>
<th>ULOL</th>
<th>Carryover</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drug_A</td>
<td>1.500</td>
<td>1.500</td>
<td>15.000</td>
<td>100.000</td>
<td>1000.000</td>
</tr>
</tbody>
</table>

Method Report

Method name: Drug_A_Drug_A
Master method name: Drug_A
Current calibration file: Drug_A.cax
Assay type: Drug_A
Inj vol: 1.000
Instrument method: 20x

Groups
Method Report

Method name: Drug_A_Drug_A
Master method name: Drug_A
Current calibration file: Drug_A.caix
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

Quan options
- Sort Qual results by: Search Index
- Enable limiting peaks: False
- Limit Peaks to :

ToxLab Forms settings
- Quan flags
- Flag values below LOD: True
- Flag values below LOQ: True
- Flag values above Cutoff: True
- Flag values above ULLOQ: True
- Flag values above Carryover: True
- Flag values between LOD and LOQ: True

User interface options
- Shade row when sample is outside of evaluation criteria: False
- Separation overlay display : True
- Use alternative calibration report format: False
- Display quan flags and legend: True

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
Master method name: Drug_A
Current calibration file: Drug_A.caix
Assay type: Drug_A
Inj vol: 1.000
Instrument method: 20x

QAQC QC Check:

Compound | Max RF diff (%) | Min RF
Drug_A | 20.00 | 0.000
## Sample Standard Reports

### Method Report

| Method name: | Drug_A_Drug_A | Master method name: | Drug_A | Current calibration file: | Drug_A.calix | Assay type: | Drug_A | Ion range calc method: | Average | Inj vol: | 1.000 | Instrument method: | 20x |

### QAQC Negative:

| Compound | Drug_A | Criterion | % of LOD | Max value | 1.500 |

### Method Report

| Method name: | Drug_A_Drug_A | Master method name: | Drug_A | Current calibration file: | Drug_A.calix | Assay type: | Drug_A | Ion range calc method: | Average | Inj vol: | 1.000 | Instrument method: | 20x |

### QAQC ISTD:

| Compound | Int_Std | Min recovery (%) | 50.00 | Max recovery (%) | 150.00 | Min RT (+min) | 0.25 | Max RT (+min) | 0.25 |

### Method Report

| Method name: | Drug_A_Drug_A | Master method name: | Drug_A | Current calibration file: | Drug_A.calix | Assay type: | Drug_A | Ion range calc method: | Average | Inj vol: | 1.000 | Instrument method: | 20x |

### QAQC Solvent Blank:

| Compound | Int_Std | Drug_A | Selection Method | None | Upper Limit % | 0 |

### Method Report

| Method name: | Drug_A_Drug_A | Master method name: | Drug_A | Current calibration file: | Drug_A.calix | Assay type: | Drug_A | Ion range calc method: | Average | Inj vol: | 1.000 | Instrument method: | 20x |

### QAQC Hydrolysis:

| CompoundName | Drug_A | EvaluationMethod | Range | LowerLimit | 15.000 | UpperLimit | 23.000 |
## Method Validation Report

<table>
<thead>
<tr>
<th>Compound</th>
<th>Avg Conc</th>
<th>Theo Conc</th>
<th>% Diff</th>
<th>Min Conc</th>
<th>Max Conc</th>
<th>% RSD</th>
<th>Max % RSD</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIA D-5</td>
<td>295652</td>
<td>0.358</td>
<td>-28.34</td>
<td>0.250</td>
<td>0.750</td>
<td>0.00</td>
<td>20.00</td>
</tr>
<tr>
<td>DEA D-7</td>
<td>1778658</td>
<td>0.602</td>
<td>20.45</td>
<td>0.250</td>
<td>0.750</td>
<td>0.00</td>
<td>20.00</td>
</tr>
<tr>
<td>Cyanazine D-5</td>
<td>2224244</td>
<td>0.565</td>
<td>12.90</td>
<td>0.250</td>
<td>0.750</td>
<td>0.00</td>
<td>20.00</td>
</tr>
<tr>
<td>Simazine D-10</td>
<td>505462</td>
<td>0.607</td>
<td>21.49</td>
<td>0.250</td>
<td>0.750</td>
<td>0.00</td>
<td>20.00</td>
</tr>
<tr>
<td>Atrazine D-5</td>
<td>2334865</td>
<td>0.512</td>
<td>2.46</td>
<td>0.250</td>
<td>0.750</td>
<td>0.00</td>
<td>20.00</td>
</tr>
<tr>
<td>Atrazine</td>
<td></td>
<td>0.757</td>
<td>51.41</td>
<td>0.250</td>
<td>0.750</td>
<td>0.00</td>
<td>20.00 &lt;&lt;&lt;</td>
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<tr>
<td>Propazine D-14</td>
<td>272050</td>
<td>0.00</td>
<td>IS</td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>
**Lab name:** Thermo Fisher Laboratory

**Instrument:** Thermo Scientific Instrument

**User:** AMER/jamie.humphries

**Batch:** Preview2

### Method Validation Report Data

<table>
<thead>
<tr>
<th>Compound</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIA D-5</td>
<td>295652</td>
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<tr>
<td>DIA</td>
<td>0.358</td>
</tr>
<tr>
<td>DEA D-7</td>
<td>1778658</td>
</tr>
<tr>
<td>DEA</td>
<td>0.602</td>
</tr>
<tr>
<td>Cyanazine D-5</td>
<td>2224244</td>
</tr>
<tr>
<td>Cyanazine</td>
<td>0.565</td>
</tr>
<tr>
<td>Simazine D-10</td>
<td>505462</td>
</tr>
<tr>
<td>Simazine</td>
<td>0.607</td>
</tr>
<tr>
<td>Atrazine D-5</td>
<td>2334865</td>
</tr>
<tr>
<td>Atrazine</td>
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<td>Propazine</td>
<td>0.757</td>
</tr>
<tr>
<td>Propazine D-14</td>
<td>272050</td>
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**Manually integrated**

>>> = Failure
**Method Validation Report**

<table>
<thead>
<tr>
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<th>Sample ID</th>
<th>Filename</th>
<th>Level</th>
<th>Sample Name</th>
<th>File Date</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tray1:10</td>
<td>SampleID003</td>
<td>500ppt-003</td>
<td>N/A</td>
<td>D003</td>
<td>6/26/2007 10:18:49 PM</td>
<td>New Dilutions 6/26/2007</td>
</tr>
</tbody>
</table>

Manually integrated     

<<< = Failure
MSMSD Report

Lab name: Thermo Fisher Laboratory
Instrument: Thermo Scientific Instrument
User: AMER/jamie.humphries
Batch: Preview2
Cali File: Preview2.cals

<table>
<thead>
<tr>
<th>Pos</th>
<th>Sample ID</th>
<th>Filename</th>
<th>Level</th>
<th>Sample Name</th>
<th>File Date</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tray1:1</td>
<td>SampleID2021</td>
<td>DACTTest001</td>
<td>N/A</td>
<td>D021</td>
<td>6/27/2007 11:42:07 AM</td>
<td>New dilution of DACT</td>
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SampleID021

<table>
<thead>
<tr>
<th>Compound</th>
<th>Unknown Concentration</th>
<th>Spike Concentration</th>
<th>MS Concentration</th>
<th>% Rec</th>
<th>Lower Limit %</th>
<th>Upper Limit %</th>
<th>Rec Fails</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIA</td>
<td>0.000</td>
<td>0.500</td>
<td>0.000</td>
<td>0.00</td>
<td>50.00</td>
<td>150.00</td>
<td>0</td>
</tr>
<tr>
<td>DEA</td>
<td>0.000</td>
<td>0.500</td>
<td>0.000</td>
<td>0.00</td>
<td>50.00</td>
<td>150.00</td>
<td>0</td>
</tr>
<tr>
<td>Cyanazine</td>
<td>0.000</td>
<td>0.500</td>
<td>0.000</td>
<td>0.00</td>
<td>50.00</td>
<td>150.00</td>
<td>0</td>
</tr>
<tr>
<td>Simazine</td>
<td>0.000</td>
<td>0.500</td>
<td>0.000</td>
<td>0.00</td>
<td>50.00</td>
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<td>0.000</td>
<td>0.00</td>
<td>50.00</td>
<td>150.00</td>
<td>0</td>
</tr>
</tbody>
</table>
## Quality Control Report

**Lab name:** Thermo Fisher Laboratory  
**Instrument:** Thermo Scientific Instrument  
**User:** AMER/jamie.humphries  
**Batch:** Drug_A  
**Method:** Drug_A, Drug_A  
**Cal File:** Drug_A.calx

<table>
<thead>
<tr>
<th>Vial Pos</th>
<th>Sample ID</th>
<th>Filename</th>
<th>Level</th>
<th>Sample Name</th>
<th>File Date</th>
<th>Comment</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>qc 40% = 6 ng/mL</td>
<td>qc_40</td>
<td>level 40</td>
<td></td>
<td>4/17/2008 5:07:57 PM</td>
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### Compound: Drug_A

<table>
<thead>
<tr>
<th>Curve Type</th>
<th>Daily RF</th>
<th>Mean RF</th>
<th>Min RF</th>
<th>RF %</th>
<th>Max RF % D</th>
<th>QC amt</th>
<th>Calc amt</th>
<th>Amt %C</th>
<th>Max Amt %C Flag</th>
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</thead>
<tbody>
<tr>
<td>L</td>
<td>0.00</td>
<td>6.00</td>
<td>5.603</td>
<td>-6.62</td>
<td>20.00</td>
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### Internal standard summary:

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<tr>
<th>Compound</th>
<th>Std Response</th>
<th>Min</th>
<th>Max</th>
<th>Sample Response</th>
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</thead>
<tbody>
<tr>
<td>Int_Std</td>
<td>655596</td>
<td>327798(50.00%)</td>
<td>983394(150.00%)</td>
<td>639922</td>
</tr>
<tr>
<td></td>
<td>Std RT</td>
<td>Min</td>
<td>Max</td>
<td>Sample RT</td>
</tr>
<tr>
<td>Int_Std</td>
<td>1.93</td>
<td>1.68(-0.25)</td>
<td>2.18(+0.25)</td>
<td>1.93</td>
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</tbody>
</table>

Manually integrated \[= Fails\] Curve Type: A=Average RF; L=Linear; Q=Quadratic; R=Recovery limits exceeded
<table>
<thead>
<tr>
<th>Sample ID</th>
<th>File Name</th>
<th>Level</th>
<th>Sample Name</th>
<th>File Date</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>L32XLQQ_HPI031711</td>
<td>325,000</td>
<td>L32XLQQ_HPI031711</td>
<td>3/7/2011 8:06:03 PM</td>
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</table>

**Quantitation Report**

**Lab Name:** Thermo Lab  
**Instrument:** QTR0637  
**User:** QTR0637WRC  
**Batch:** 01/04/2011  
**Call File:** 01/04/2011.caas

**Surrogates**

<table>
<thead>
<tr>
<th>Sample</th>
<th>RT</th>
<th>Qion</th>
<th>Response</th>
<th>Curve Type</th>
<th>Average RF/Response Ratio</th>
<th>Injected Con</th>
<th>Units</th>
<th>Calculated Con</th>
<th>Units</th>
<th>Flags</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propiskin (S)</td>
<td>7.70</td>
<td>111.10</td>
<td>135063122</td>
<td>Quadratic</td>
<td>0.00</td>
<td>6.40</td>
<td>/</td>
<td>6.40</td>
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</table>

**Target Compounds**

<table>
<thead>
<tr>
<th>Sample</th>
<th>RT</th>
<th>Qion</th>
<th>Response</th>
<th>Curve Type</th>
<th>Average RF/Response Ratio</th>
<th>Injected Con</th>
<th>Units</th>
<th>Calculated Con</th>
<th>Units</th>
<th>Flags</th>
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</thead>
<tbody>
<tr>
<td>Quinolone</td>
<td>4.32</td>
<td>72.10</td>
<td>115624924</td>
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<td>1280.33</td>
<td>PPB</td>
<td>1280.33</td>
<td>PPB</td>
<td>/</td>
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<tr>
<td>Omeprazole</td>
<td>4.34</td>
<td>183.04</td>
<td>47/992071</td>
<td>Quadratic</td>
<td>0.00</td>
<td>158.19</td>
<td>PPB</td>
<td>158.19</td>
<td>PPB</td>
<td>/</td>
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<tr>
<td>Formotereine</td>
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<td>165.10</td>
<td>418152129</td>
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<td>6.42</td>
<td>PPB</td>
<td>6.42</td>
<td>PPB</td>
<td>/</td>
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<tr>
<td>Dinutelurin</td>
<td>4.52</td>
<td>129.14</td>
<td>47/984836</td>
<td>Quadratic</td>
<td>0.00</td>
<td>6.42</td>
<td>PPB</td>
<td>6.42</td>
<td>PPB</td>
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<tr>
<td>Aldicarb,SO</td>
<td>4.52</td>
<td>132.05</td>
<td>46655255</td>
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<tr>
<td>Propamocarb</td>
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<td>102.00</td>
<td>233304788</td>
<td>Quadratic</td>
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<td>6.38</td>
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<tr>
<td>Pyridostigmine</td>
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<td>105.40</td>
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<td>6.40</td>
<td>PPB</td>
<td>6.40</td>
<td>PPB</td>
<td>/</td>
</tr>
</tbody>
</table>

Flag legend: LQD=LOD; LOQ=LOQ; >LOM ratio failure; O=Carryover; I=Linearity limit; D=Detection limit; G=Quant limit; P=OLP limit; B=Blank; S=Solvent blank

Manually Integrated

Thermo Scientific
### Quantitation Report - 2

**MS Intag Parameters:**
- PDQP_04/03/11

**Quant Method:**
- 0194PLR_1_PDP_04/03/11

**Title:**
- Assay

**Last Update:**
- 6/2/2011 9:47:56 AM

**Data Acq Method:**
- PDQP_04/04/11

**Operator:**
- TQO008003AC

**Instr:**
- TQO008003AC

**Response Via:**
- PDQP_04/04/11

**Quant Time:**
- 4/19/2011 3:39:05 PM

**Data File:**
- L32XLQG_HP031711

**Acq On:**
- 3/17/2011 8:06:30 PM

**Sample:**
- L32XLQG_HP031711

**Comment:**
- Vial: 5

**Multiplier:**
- 1.00

**Quant Results File:**
- C:\Thermo\TraceFinder\0.1\Projects\Default\Default01\HPUR\1\Data\L32XLQG_HP031711.DQS

#### Bngsagts

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>RT</th>
<th>Qian</th>
<th>Response</th>
<th>Conc</th>
<th>Units</th>
<th>Dev (min)</th>
<th>Spike Amt</th>
<th>Recovery</th>
<th>Flag</th>
</tr>
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<tbody>
<tr>
<td>28 Propriol (5)</td>
<td>7.70</td>
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#### Target Compounds

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>RT</th>
<th>Qian</th>
<th>Response</th>
<th>Conc</th>
<th>Units</th>
<th>Dev (min)</th>
<th>Spike Amt</th>
<th>Recovery</th>
<th>Flag</th>
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</thead>
<tbody>
<tr>
<td>1 Oxamyl, Oxime</td>
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<td>72.10</td>
<td>11862493</td>
<td>1280.03</td>
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<td>0.01</td>
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<tr>
<td>2 Cyantranilipyr</td>
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<td>183.04</td>
<td>47692071</td>
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<td>PPR</td>
<td>0.01</td>
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<tr>
<td>3 Imidacloprid</td>
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<td>0.01</td>
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<tr>
<td>4 Dinofuran</td>
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<td>129.14</td>
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<tr>
<td>5 Atrazine</td>
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<td>152.06</td>
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<tr>
<td>6 Ip-toxim</td>
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<td>162.02</td>
<td>22304076</td>
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<td>PPR</td>
<td>0.01</td>
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<td></td>
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<tr>
<td>7 Pyrimethanil</td>
<td>4.57</td>
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## Quantitation Report - 2

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## Solvent Blank Report

**Lab Name:** Thermo Lab  
**Instrument:** TQD00037  
**User:** TQD00037/RPC  
**Batch:** 011HPLR1  
**Method:** 011HPLR1_PDP_040511  
**Call File:** 011HPLR1_calx

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### Burp tubes

**Propoxy (S)**  
- RT: 7.69  
- Clon: 111.10  
- Response: 1553885  
- Method: None

### Target Compounds

**Oxamyl, Oxtene**  
- RT: 4.32  
- Clon: 72.10  
- Response: 1291350  
- Method: None

**Omeprazole**  
- RT: 4.34  
- Clon: 163.04  
- Response: 540538  
- Method: None

**Formotranide**  
- RT: 4.35  
- Clon: 165.10  
- Response: 440852  
- Method: None

**Dinofuran**  
- RT: 4.52  
- Clon: 129.14  
- Response: 608336  
- Method: None

**Aldicarb, SG**  
- RT: 4.51  
- Clon: 132.05  
- Response: 538697  
- Method: None

**Propamocarb**  
- RT: 4.53  
- Clon: 102.00  
- Response: 750160  
- Method: None

**Pyrimethone**  
- RT: 4.56  
- Clon: 105.10  
- Response: 231305  
- Method: None

**Aldicarb, SO2**  
- RT: 4.68  
- Clon: 148.04  
- Response: 840601  
- Method: None

**Oxamyl**  
- RT: 4.77  
- Clon: 90.00  
- Response: 408081  
- Method: None

**Methomyl**  
- RT: 4.98  
- Clon: 88.10  
- Response: 973424  
- Method: None

**Flonicamid**  
- RT: 5.05  
- Clon: 203.00  
- Response: 121206  
- Method: None

**ODMS**  
- RT: 5.07  
- Clon: 169.00  
- Response: 495002  
- Method: None

**5-OH, TBZ**  
- RT: 5.12  
- Clon: 147.10  
- Response: 427244  
- Method: None

**Thiamethoxam**  
- RT: 5.12  
- Clon: 181.10  
- Response: 149534  
- Method: None

**Monocrotophos**  
- RT: 5.26  
- Clon: 190.00  
- Response: 820046  
- Method: None

**Imidacloprid**  
- RT: 5.66  
- Clon: 209.06  
- Response: 611636  
- Method: None

**Clothianidin**  
- RT: 5.71  
- Clon: 169.10  
- Response: 218332  
- Method: None

**Thiabendazole**  
- RT: 5.87  
- Clon: 131.10  
- Response: 692435  
- Method: None

**3-OH, Carbocuran**  
- RT: 6.03  
- Clon: 163.08  
- Response: 1717688  
- Method: None

**Acarathrin**  
- RT: 6.07  
- Clon: 126.10  
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- Method: None

**Cymoxanil**  
- RT: 6.38  
- Clon: 128.14  
- Response: 108494  
- Method: None

**Thiacloprid**  
- RT: 6.51  
- Clon: 126.10  
- Response: 299625  
- Method: None

**Methidathion, OA**  
- RT: 6.75  
- Clon: 145.00  
- Response: 1537066  
- Method: None

**Aldicarb**  
- RT: 6.94  
- Clon: 116.05  
- Response: 563453  
- Method: None

**Azinphos, Me, OA**  
- RT: 6.95  
- Clon: 132.00  
- Response: 485885  
- Method: None

**Methucon**  
- RT: 7.65  
- Clon: 187.16  
- Response: 437173  
- Method: None

**Simazine**  
- RT: 7.69  
- Clon: 104.10  
- Response: 182755  
- Method: None

**Primicarb**  
- RT: 7.71  
- Clon: 182.08  
- Response: 6027105  
- Method: None

**Manually Integrated**
# Surrogate Recovery Report

**Lab Name:** Thermo Lab

**Instrument:** TQU00037

**User:** TQU00037/RPC

**Batch:** 01HPLR1

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<td>L32XLOG, HP031711</td>
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**Compound** | **Conc Added** | **Conc Recovered** | **% Recovered** | **Limits** |
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Manually Integrated: 

Recovery limits exceeded: R
### TIC Report

**Lab Name:** Default Laboratory  
**Instrument:** Thermo Scientific Instrument  
**User:** MS110434UTQ  
**Batch:** jbe_test_5

**File Name:** Sample Standard Reports

**Method:** jbe_test_5, jbe_test_q2c1

**Cal File:** jbe_test_5_cal.txt

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**Compound**  
- 1,3-Benzenediol, o-(2-furyl)-o'- (2-trifluoromethylbenzoyl): 0, mainlib: 128603, entry: 6, match prob: 556, search index: 975, formula: C19H11F3O5, weight: 376

---

**Graphs:**
- **m-Methoxybenzoic acid, hexadecyl ester**
- **4-Methoxyphenyl octadecyl ether**
- **1,3-Benzenediol, o-(2-furyl)-o'-(2-trifluoromethylbenzoyl)**
## TIC Summary Report

### Lab Name: Default Laboratory

### Instrument: Thermo Scientific instrument

### User: MS110434/ITQ

### Batch: jbe_test_5

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### Qualitatively-Identified Compounds

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<th>Conc</th>
<th>Units</th>
<th>Injected</th>
<th>Sample</th>
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- 8-Chloro-5-quino[1]necarboxylic acid: 2.78, 566067, 0.000, 0.000
- 8-Chloro-5-quino[1]necarboxylic acid: 2.90, 164769, 0.000, 0.000
- Cyclohexylidenehexamethylene, hexamethyl-: 3.07, 213699, 0.000, 0.000
- Cyclohexylidenehexamethylene, octamethyl-: 4.46, 1139812, 0.000, 0.000
- Benzylamine, 2,6-dimethyl- (methylamine): 5.44, 10912, 0.000, 0.000
- Benzene, 3,5-dimethyl- (methylamine): 5.80, 87135, 0.000, 0.000
- 2-Hydroxy-1,4-dioxane, 2,2-dimethyl-: 7.18, 14550, 0.000, 0.000
- Quinoline, 2,6-dimethyl-: 7.74, 10864, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 8.43, 10854, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 9.40, 10900, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 11.02, 200098, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 11.02, 27413, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 11.08, 69527, 0.000, 0.000
- Cyclohexylidenehexamethylene, hexamethyl-: 11.13, 313964, 0.000, 0.000
- Cyclohexylidenehexamethylene, hexamethyl-: 11.33, 35676, 0.000, 0.000
- Padimate O: 11.44, 843015, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 11.52, 13886, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 11.91, 413305, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 11.96, 523574, 0.000, 0.000
- 1,1,3,5,5,5-Hexamethyltrisiloxane: 12.07, 206827, 0.000, 0.000
- 5-Acetamido-4,7-dioxo-4,7-dihydrobenzofurazan: 12.11, 91590, 0.000, 0.000
- 5-Acetamido-4,7-dioxo-4,7-dihydrobenzofurazan: 12.13, 43177, 0.000, 0.000
- 5-Acetamido-4,7-dioxo-4,7-dihydrobenzofurazan: 12.33, 15408, 0.000, 0.000
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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, and Comment 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.

   ![Selected vs Not Selected](image)

2. Right-click and choose **Copy Down** from the shortcut menu.

   The value is copied to all rows below the selected row.

**To automatically enter sequential column values**

1. Enter a value for the first row of the fill down sequence.

   This does not have to be the first sample row. You can begin the fill down procedure from any row in the sequence.
2. Select the cell whose value is the first in the fill down sequence. Observe the difference between a selected and nonselected cell.

3. Right-click and choose Fill Down from the shortcut menu.

The application enters sequential column values starting with the value in the selected row and ending with the last row in the column.

You can repeatedly use the Fill Down command to create multiple sequences.

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.
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 button, ▼, 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 442.

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 94.** Enter Filter Criteria dialog box

![Enter Filter Criteria dialog box](image)

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<td>Requires meeting all filter criteria.</td>
</tr>
<tr>
<td>Or Conditions</td>
<td>Requires meeting any of the specified filter criteria.</td>
</tr>
<tr>
<td>Add A Condition</td>
<td>Adds a new, empty condition to the filter criteria.</td>
</tr>
<tr>
<td>Delete Condition</td>
<td>Deletes the selected condition. Click the box at the left of the row to select the condition.</td>
</tr>
<tr>
<td>Operator</td>
<td>The mathematical function applied to the operand.</td>
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<tr>
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