TraceFinder Analysis Quick Reference Guide

This quick reference guide describes the Analysis mode tasks assigned to the Technician role in the Thermo TraceFinder™ 3.0 analytical software.

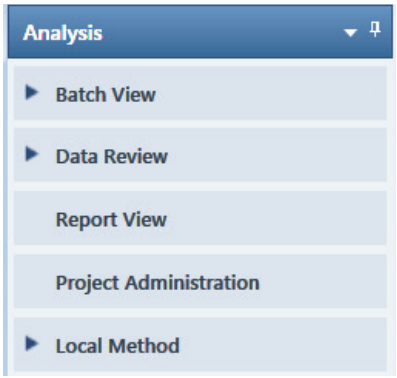
For detailed descriptions of all procedures described in this quick reference guide, refer to the "Using the Analysis Mode" chapter of the *TraceFinder User Guide*.

Contents

❖ To open the Analysis mode

Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.



Revision A XCALI-97502

Thermo SCIENTIFIC

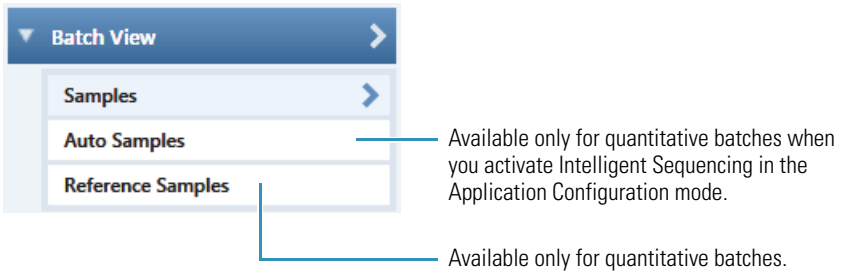
Batch View

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

❖ To open the Batch View

Click **Batch View** in the navigation pane.

The Batch View navigation pane opens.



The Batch View includes the following pages:

- Samples Page
- Auto Samples Page
- Reference Samples Page

Samples Page

Use the Samples page to create a new batch. Follow these procedures:

- To open the Samples page
- To create a 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 submit samples

❖ To open the Samples page

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

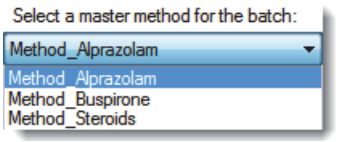
The Samples page opens.

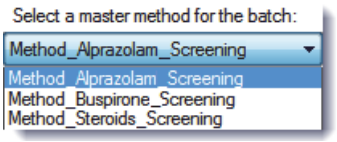
❖ To create a batch

1. Choose **File > New > Batch**.

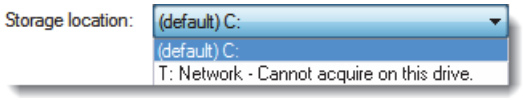
   The Create a New Batch dialog box opens.
2. Select to create either a quantitative batch or a screening batch.
3. Select a master method from the Method list.

   The application displays all available quantitative or screening methods.





4. Select a drive from the Storage Location list.



Tip The application does not display drives that do not have a project and subproject.

The project list displays all projects, subprojects, and batches on the selected drive.

You cannot use network drives to acquire data. For more information about network drives, refer to the "Using the Application Configuration Mode" chapter in the *TraceFinder User Guide*.

5. Select a project and a subproject, and then enter a name for your new batch.

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

6. Click **Save**.

A new batch opens with one Specimen sample. The batch name in the title bar indicates that you are creating a quantitative or screening batch.

❖ To add samples to the list

Select the number of sample rows to add and click the **Add Sample** icon,  .

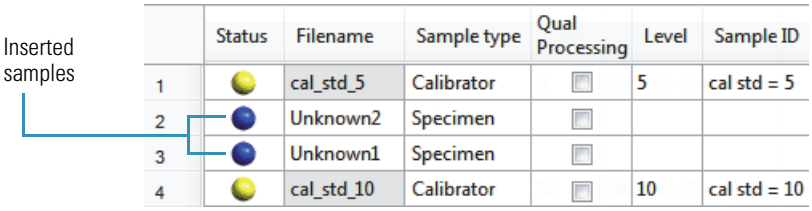
Tip To quickly add a sample row, right-click the sample list and choose **Add Sample** from the shortcut menu.

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

❖ To insert samples into the list

1. Select the sample above which you will insert new samples.
2. Select the number of samples to insert and click the **Insert Sample** icon,  .

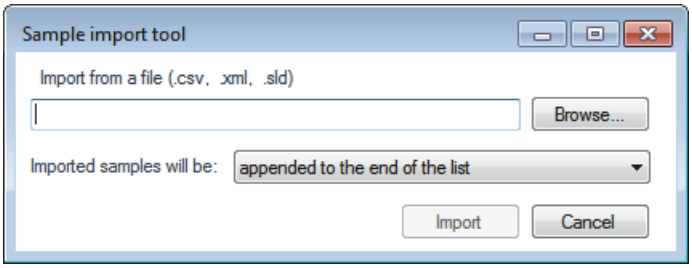
The application inserts the Specimen samples above the selected sample.



❖ To import samples into the list

1. Click the **Import Samples** icon,  .

The Sample Import Tool dialog box opens.



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

4. Click **Import**.

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

   When you import samples from an Xcalibur™ sequence file, the TraceFinder application makes the following column name and sample type substitutions.

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

Xcalibur sample type	TraceFinder sample type
Blank	Negative
Std Bracket	Calibrator

❖ To remove samples from the list

1. Select the samples that you want to remove.

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

2. Right-click and choose **Remove Selected Samples** from the shortcut menu.

❖ To copy a sample

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

   The TraceFinder application inserts the copy above the selected sample.

❖ To reinject a sample

1. In the Sample list, select the sample that you want to reinject.
2. Right-click and choose **Reinject This Sample** from the shortcut menu.

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

❖ To edit sample values

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

   Type a new file name over the current file name.

   –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.

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

Available sample types		
Specimen	Hydrolysis	QC
Solvent	Calibrator	
Unextracted	Negative	

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

   The sample levels are defined in the master method. If there are no levels to select from the Level list, do the following:

   a. Return to the Method Development mode.
   b. Open the method.
   c. Click the **Compounds** tab.
   d. Click the **Calibration Levels** tab.
   e. Add the levels.
   f. Save the method.
   g. Return to the Analysis mode, and then click **Update**.

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

4. (Optional) Enter or edit the values for the remaining columns.

> **Note** When you use the horizontal scroll bar at the bottom of the sample list, the Status, Filename, Sample Type, and Level columns stay fixed while the other columns scroll right and left.

❖ To submit samples

1. Do one of the following:
   - To submit all samples in the batch, click the **Submit Batch** icon, .
   - To submit specific samples, select the samples and click the **Submit Selected Samples** icon, .

   The Submit Options dialog box opens.

2. Select the tasks that you want to perform: acquire data, process data, or create reports.

> **Note** By default, the application acquires and processes data when you submit the batch.

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

Auto Samples Page

The Auto Samples page identifies the Solvent or Negative samples to use for any Auto Sample or Auto Sample and Reinject failure actions as specified on the Intelligent Sequencing page of the method.

❖ To open the Auto Samples page

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

The Auto Samples page opens.

	Sample Type	Injection Volume	Injections Used	Number of Injections	Vial Position
	Solvent	1.0	0	1	10
	Matrix Blank	1.0	0	10	11
	Matrix Blank	1.0	0	10	12

❖ To add an auto sample type

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

   The application adds a Solvent sample to the sample list.

   You can add, insert, or remove samples from this list as you would any sample list. See "Samples Page" on page 2.

2. To change the sample type to a Negative, click the Sample Type column and select Negative from the list.
3. In the Injection Volume column for the sample, type a volume.

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

4. In the Number of Injections column, type the number of injections available in the designated Solvent or Negative vial.

   After auto sample injections have occurred, you can return to this page to view the number of injections used in each vial.
5. In the Vial Position column, type the vial position for the Solvent or Negative sample.

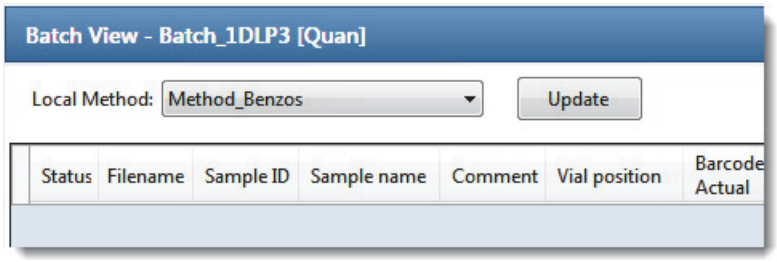
Reference Samples Page

The Reference Samples page displays the reference samples selected for this batch.

❖ **To specify a chromatogram reference sample**

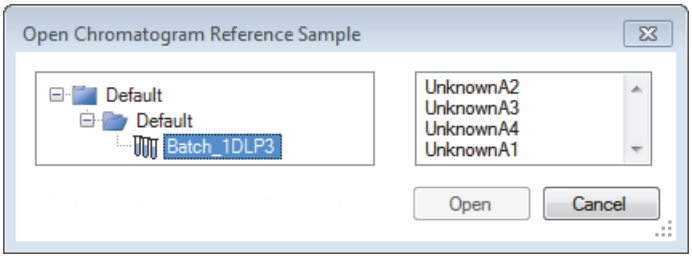
1. In the Batch View, click **Reference Samples**.

   An empty reference sample table opens.



2. Click the **Add Reference Sample** icon,  , or right-click and choose **Add Reference Sample** from the shortcut menu.

   The Open Chromatogram Reference Sample dialog box opens.



   Note If you are using a new method, no reference samples appear here. You must first process a batch using the current method to see the reference samples in this list.

3. Select a project from the list of projects.
4. Select a subproject from the list of subprojects.
5. Select a batch from the list of batches.

   The application displays only batches that were created using the current master method.
6. Select a sample from the list of processed samples.

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

Data Review

Use the Data Review to verify the data generated by a quantitative or target screening master method before you generate reports.

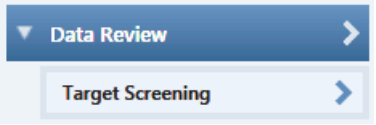
❖ **To open the Data Review view**

Click **Data Review** in the navigation pane.

The Data Review navigation pane opens.

Data Review for quantitative methods

Data Review for target screening methods



- Data Review for Quantitative Methods
- Data Review for Target Screening Methods

Data Review for Quantitative Methods

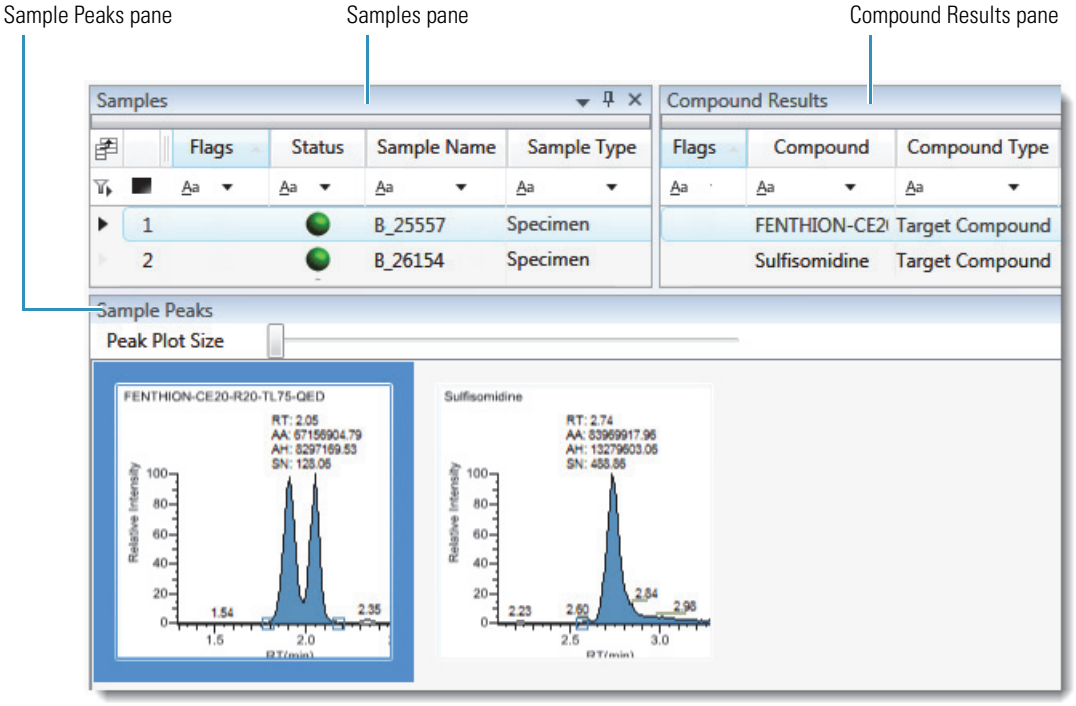
The Data Review for quantitative methods includes the following:

- Sample View
- Compound View
- Qualitative View

Sample View

The Sample View displays a list of all samples in the current batch, the compound results for all compounds in the method, and peak plots for all compounds found in the currently selected sample.

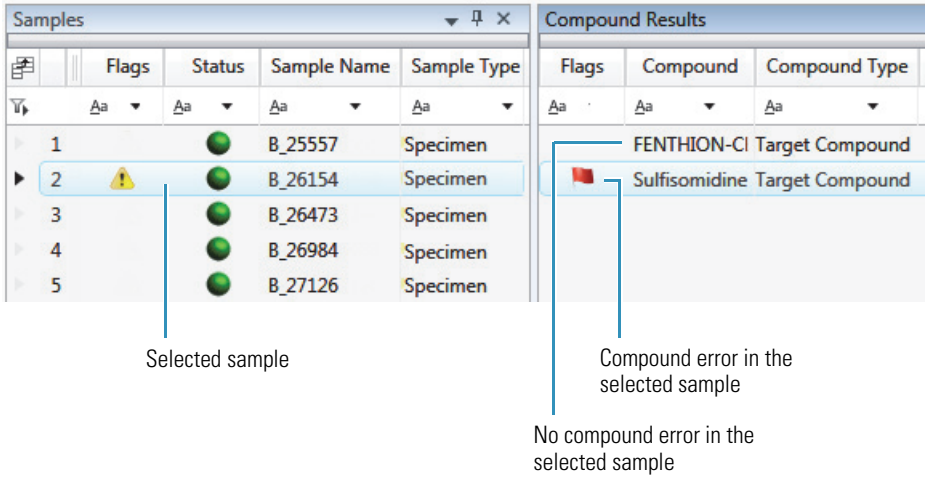
These are the default panes and their locations:



When you select a sample in the Samples pane, the associated Compound Results pane flags any compound with errors in the selected sample. The associated Sample Peaks pane displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the selected sample. The Sample Peaks pane highlights the compound selected in the Compound Results pane.

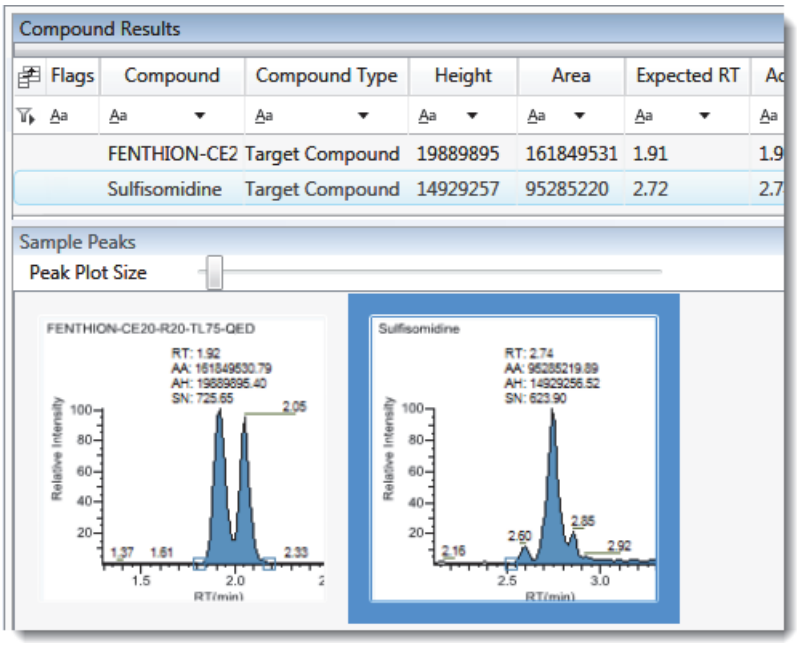
- Samples pane

  Use the Samples pane to select a specific sample. The associated Compound Results pane displays all compounds in the method and flags any compound with errors in the selected sample.



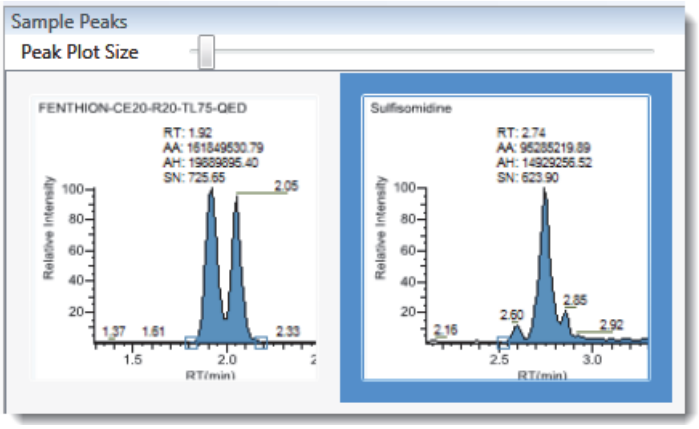
- Compound Results pane

  Use the Compound Results pane to select a specific compound in the selected sample. The associated Sample Peaks pane highlights the selected compound.



- Sample Peaks pane

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



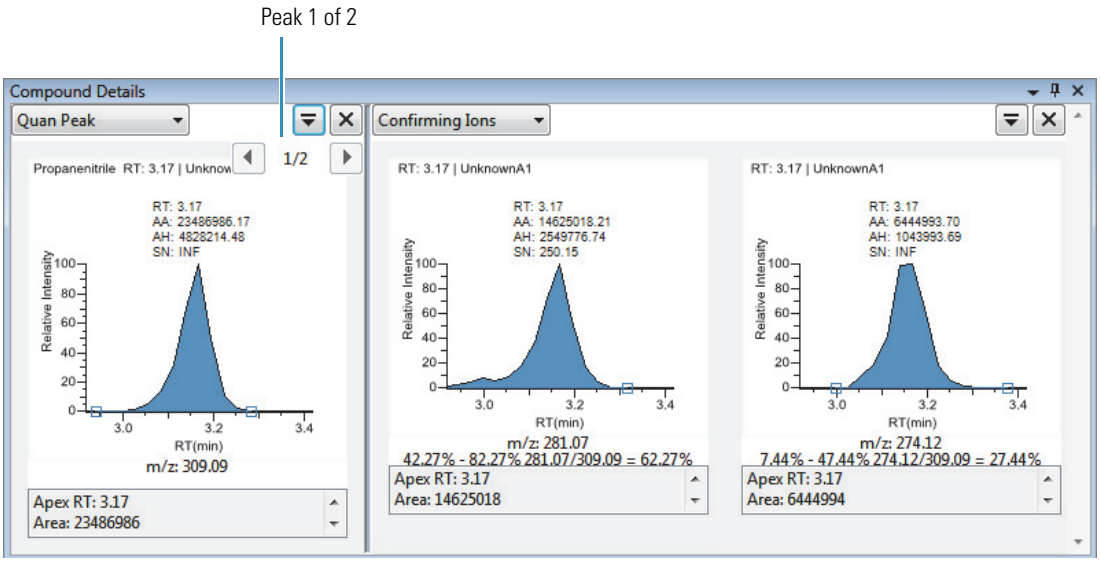
❖ To display details for a compound

Double-click the chromatogram in the Sample Peaks pane.

The Compound Details pane displays information about the **Quan Peak**, **Calibration Curve**, **Confirming Ions**, **ISTD**, **Reference Peak**, **Ion Overlay**, and **Spectra** for the compound.

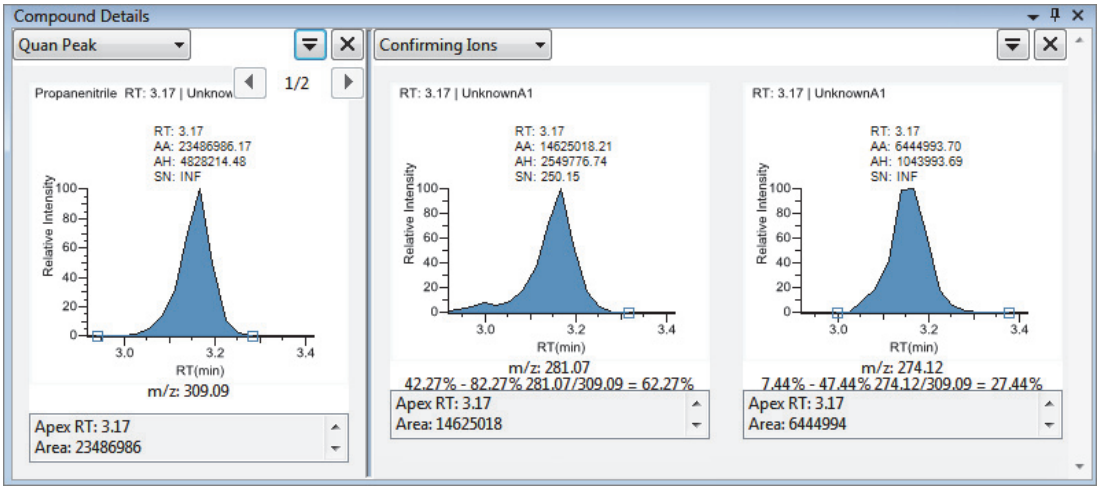
Quan Peak

You can switch between quantitative peaks, but you cannot view multiple quantitative peaks at the same time. The indicator in the upper right corner of the Quan Peak pane displays which of the multiple quantitative peaks you are viewing.



Confirming Ions

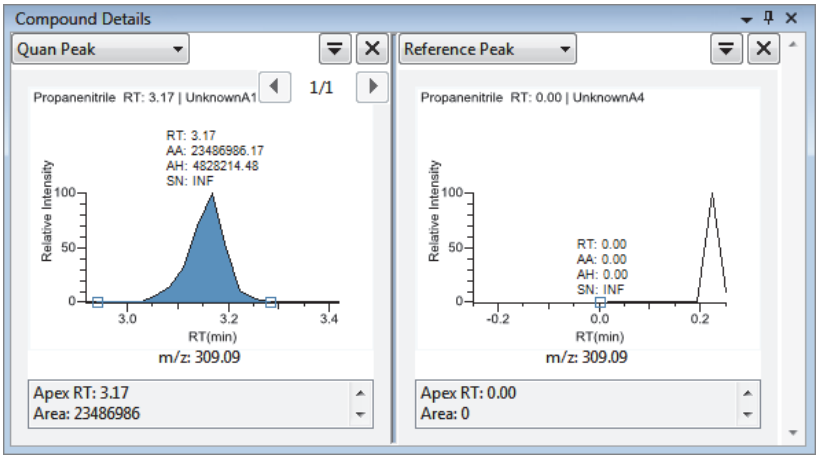
Quantitative peak with multiple confirming ions.



Note For compounds with an analog detection type, the application displays "No Confirming Ions are Enabled" in the Confirming Ions pane.

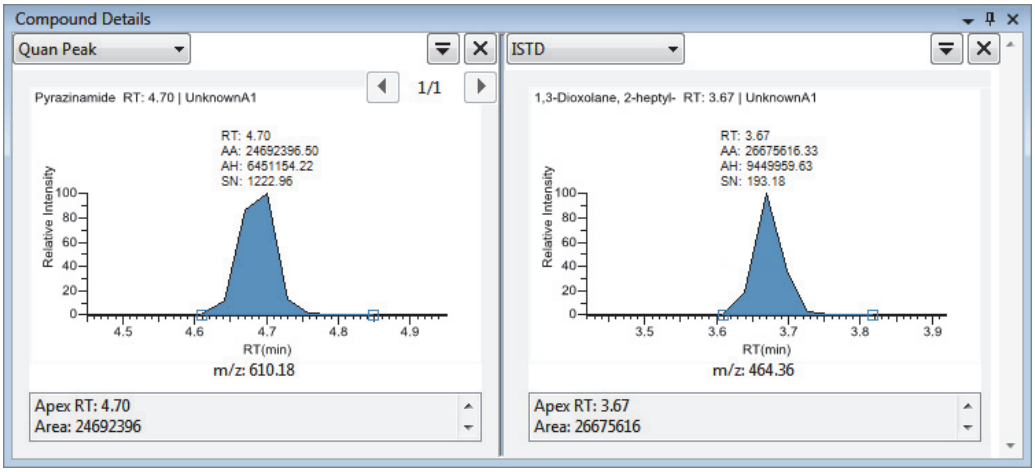
Reference Peak

Quantitative peak with a reference peak.



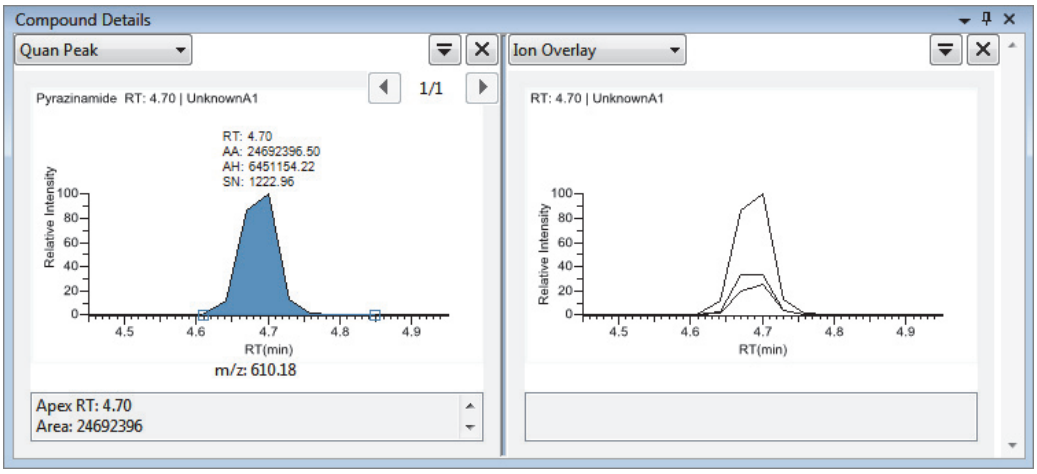
ISTD

Quantitative peak with an internal standard.



Ion Overlay

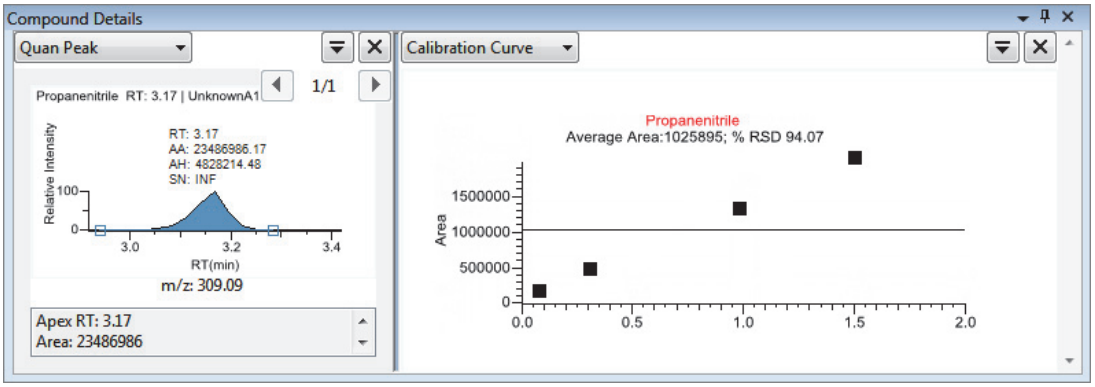
Quantitative peak with a confirming ion overlay.



Note For compounds with an analog detection type, the application displays "No Data" in the Ion Overlay pane.

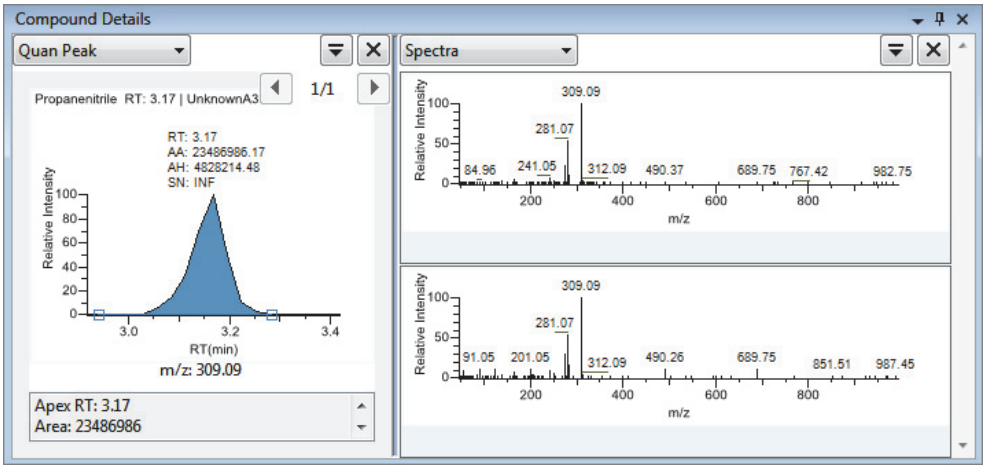
Calibration Curve

Quantitative peak with a calibration curve plot.



Spectra

Quantitative peak with data and reference spectra.

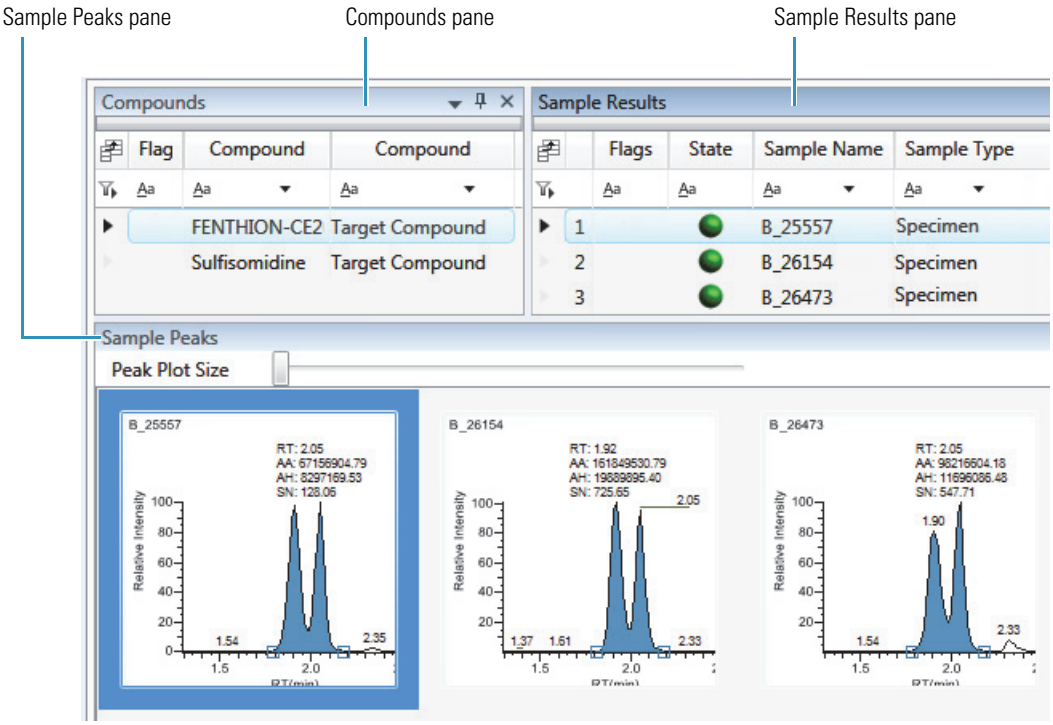


Note For compounds with an analog detection type, the application displays "Not Available" in the Spectra pane.

Compound View

The Compound View displays a list of all compounds available in the method, all samples in the current batch, and the peak plots for all compounds found in each sample.

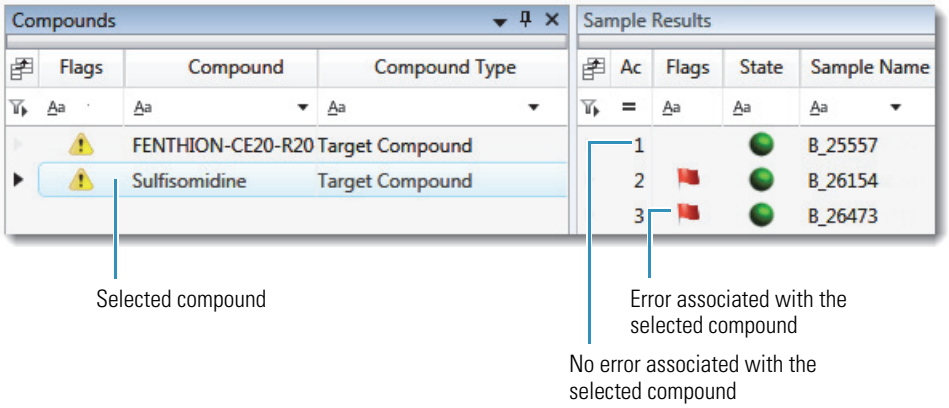
These are the default panes and their locations:



When you select a compound in the Compounds pane, the Sample Results pane flags any sample that contains errors with the selected compound. The Sample Peaks pane highlights the selected compound and displays the name of the sample in which the compound was found and the following information about the compound: chromatogram, retention time, area, height, and signal-to-noise ratio.

- Compounds pane

  Use the Compounds pane to select a specific compound. The Sample Results pane displays all samples in the batch and flags any sample that contains errors with the selected compound.



- Sample Results pane

  Use the Sample Results pane to select a specific compound in a specific sample. The Sample Peaks pane highlights the selected compound and displays the name of the sample in which the compound was found and the following information about the compound: chromatogram, retention time, area, height, and signal-to-noise ratio.

Qualitative View

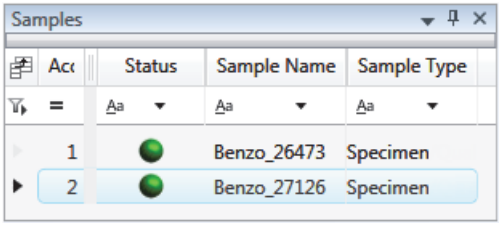
The Qualitative View displays qualitative information for the selected sample. To see processed data for a sample in the Qualitative View, you must select the Qual Processing parameter for that sample in the Batch View before you process the batch.

These are the default panes and their locations:

When you select a sample in the Samples pane, the associated Peaks pane displays all peaks found in the sample.

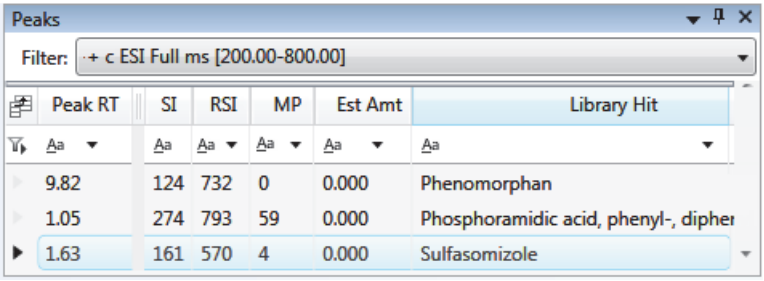
- Samples pane

  Use the Samples pane to select a specific sample.



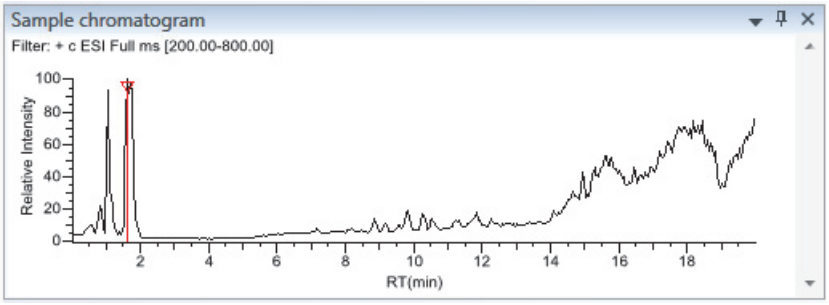
- Peaks pane

  The Peaks pane works with the Samples pane to display graphical values for a unique sample and peak combination.



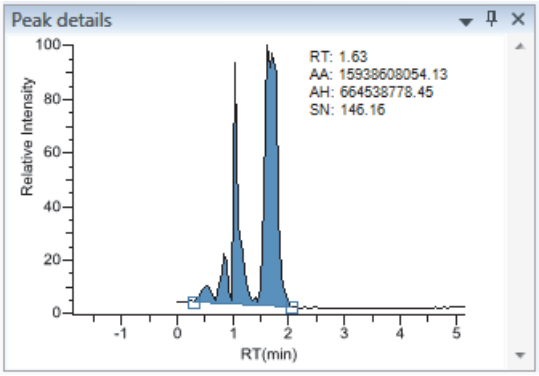
- Sample Chromatogram pane

  The Sample Chromatogram pane displays all peaks in the selected sample. The peak selected in the Peaks pane displays a red marker.



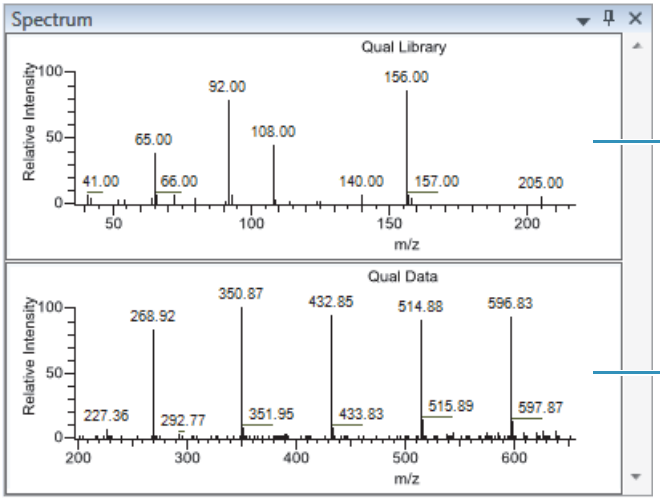
- Peak Details pane

  The Peak Details pane displays the selected peak.



- Spectrum pane

  The Spectrum pane displays the reference spectrum from the library and the spectrum data for the selected sample. The top pane displays the spectrum for the identified compound found in the reference library; the bottom pane displays the actual spectrum data for the selected peak.

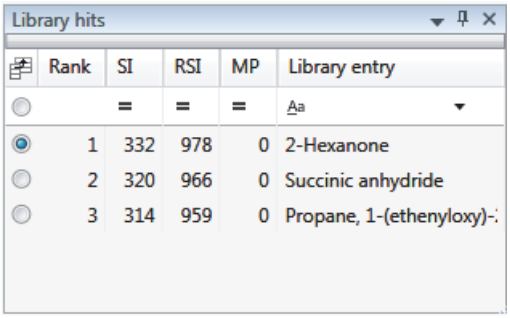


Reference spectrum from the library

Actual spectrum data for the compound

- Library Hits pane

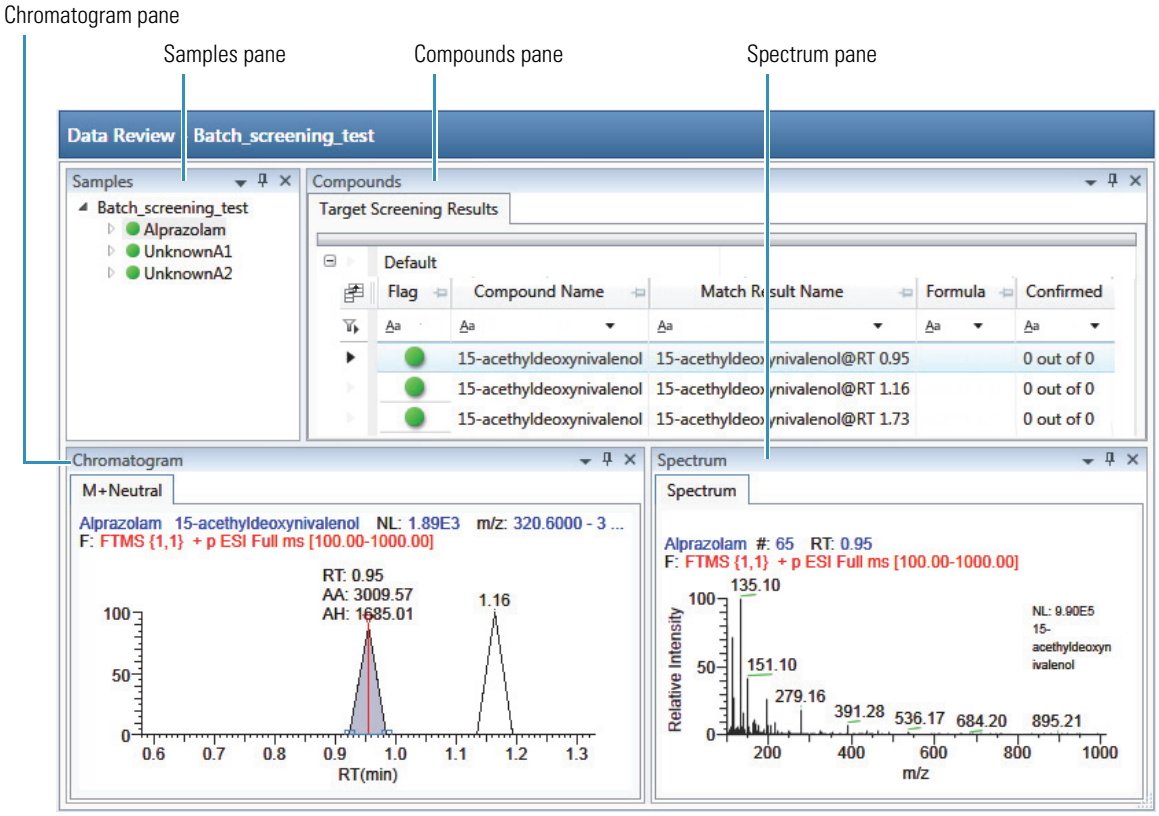
  The Library Hits pane displays the best library matches for the selected peak. Use this pane to select a different library entry for the peak.



Data Review for Target Screening Methods

In the target screening display, the application displays a list of all samples in the current batch, the compound results for all compounds in the method, and chromatogram and spectrum plots for all compounds found in the currently selected sample.

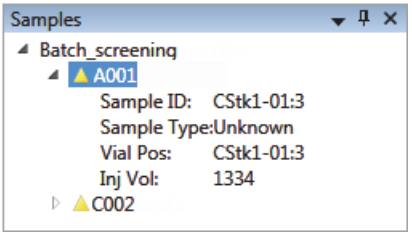
These are the default panes and their locations:



When you select a sample in the Samples pane, the associated Compounds pane flags any compound with errors in the selected sample. The associated Chromatogram pane displays the chromatogram, retention time, area, height, and signal-to-noise ratio for all compounds in the selected sample. The Spectrum pane highlights the compound selected in the Compounds pane. You can display, hide, or move any of these panes.

Samples Pane

Use the Samples pane to select a specific sample in the batch. The associated Compounds Pane displays all compounds in the method and flags any compound with errors in the selected sample.

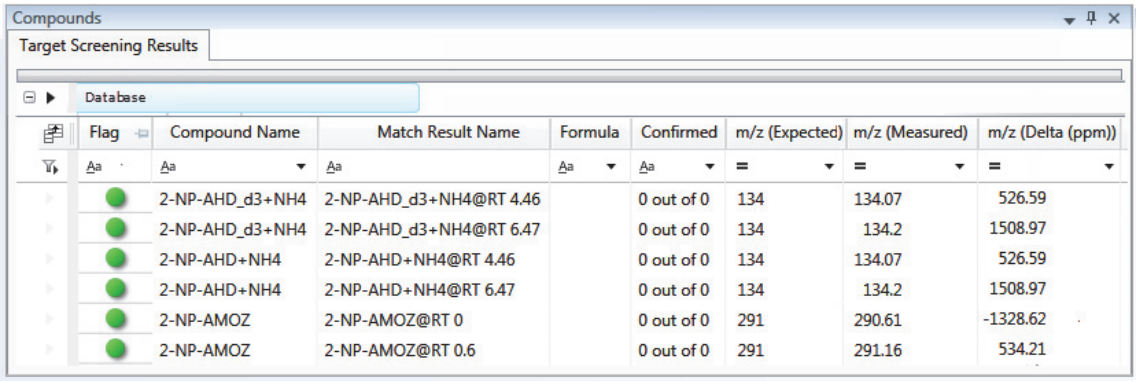


Flags in the Samples pane indicate one of the following:

- A green circle when the sample/compound/peak combination is identified and fully confirmed.
- A yellow triangle when the sample/compound/peak combination is identified but not fully confirmed.
- A red square when the sample/compound/peak combination is not identified.

Compounds Pane

The Compounds pane displays all found peaks in the selected sample and flags any compound with errors. The Target Screening Results grid reflects the identified compounds found in the compound database and the results of the method processing criteria.

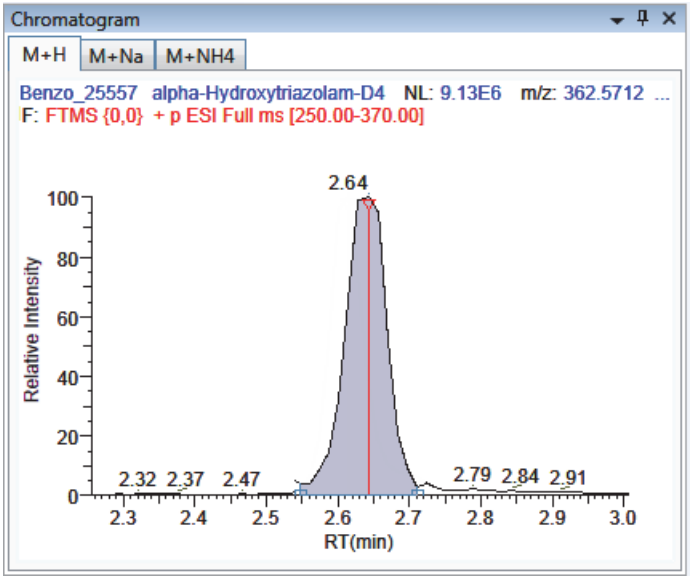


Flag	Compound Name	Match Result Name	Formula	Confirmed	m/z (Expected)	m/z (Measured)	m/z (Delta (ppm))
	2-NP-AHD_d3+NH4	2-NP-AHD_d3+NH4@RT 4.46		0 out of 0	134	134.07	526.59
	2-NP-AHD_d3+NH4	2-NP-AHD_d3+NH4@RT 6.47		0 out of 0	134	134.2	1508.97
	2-NP-AHD+NH4	2-NP-AHD+NH4@RT 4.46		0 out of 0	134	134.07	526.59
	2-NP-AHD+NH4	2-NP-AHD+NH4@RT 6.47		0 out of 0	134	134.2	1508.97
	2-NP-AMOZ	2-NP-AMOZ@RT 0		0 out of 0	291	290.61	-1328.62
	2-NP-AMOZ	2-NP-AMOZ@RT 0.6		0 out of 0	291	291.16	534.21

Chromatogram Pane

Use the Chromatogram pane to display all extracted chromatograms of all adducts of the selected compound.

The first tab displays the most intense target adduct for the peak result. Additional (optional) tabs display extracted ion chromatograms for other adducts for the target compound at the same retention time in order of intensity. If no signal exists for an adduct, it displays the XIC of the expected *m/z* within the specified retention and chromatogram windows. When you do not specify a retention time or window, the application displays the full time range.



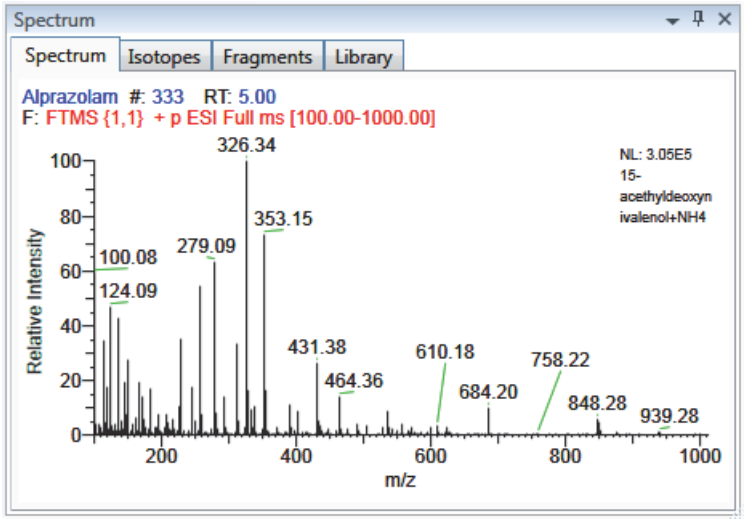
Spectrum Pane

Use the Spectrum pane to display the spectrum, isotopes, fragments, and library search information for the selected adduct in the Chromatogram pane. The Spectrum pane displays only the identification and confirmation criteria specified in the method. The confirmations are based only on the most intense adduct.

The Spectrum pane includes the following pages of information (when available) for each selected sample/compound/peak combination:

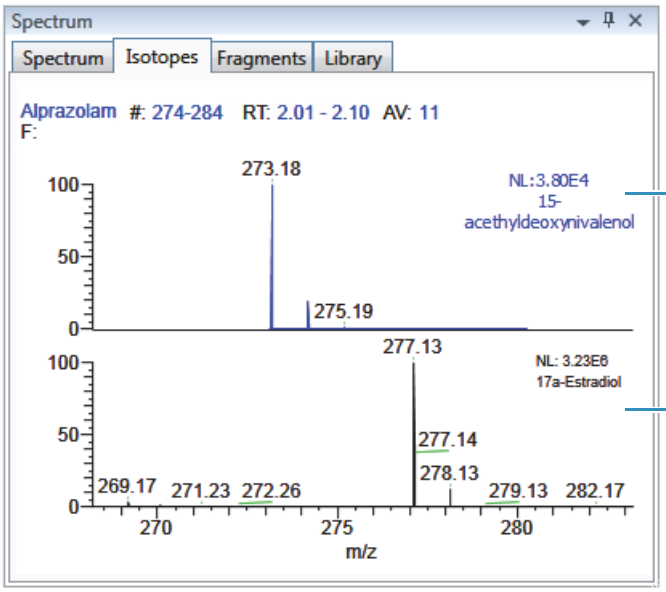
- Spectrum

  The application displays the neutral loss (NL) and compound/peak name information on the right side of the Spectrum page. When data is available, the plot width is the full mass range in the raw data file. Otherwise, the application scales the width to the scan range.



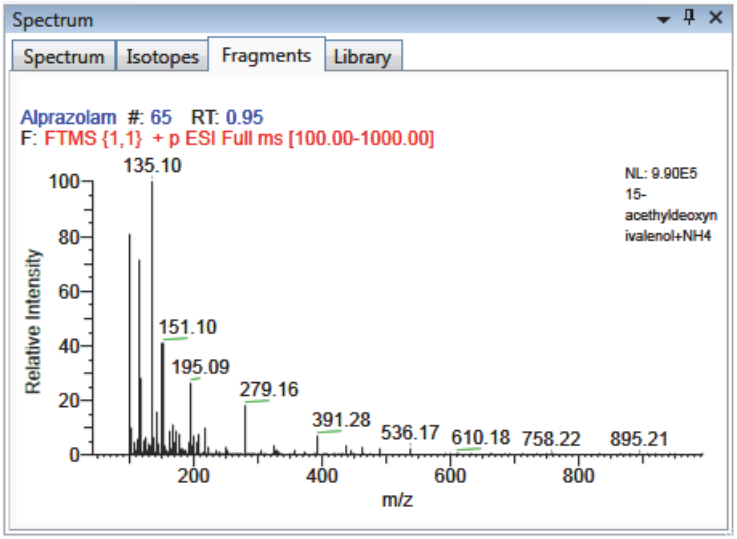
- Isotopes

  The isotopes page displays isotopic pattern results according to the threshold and deviation parameters defined in the screening method. To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage. An isotope peak is not found if its intensity, relative to the monoisotopic ion's intensity, is more than the specified intensity deviation percentage away from the theoretical relative intensity of the isotope ion. An isotope peak is found if its measured *m/z* is less than the specified mass deviation amount away from its expected *m/z*.



- Fragments

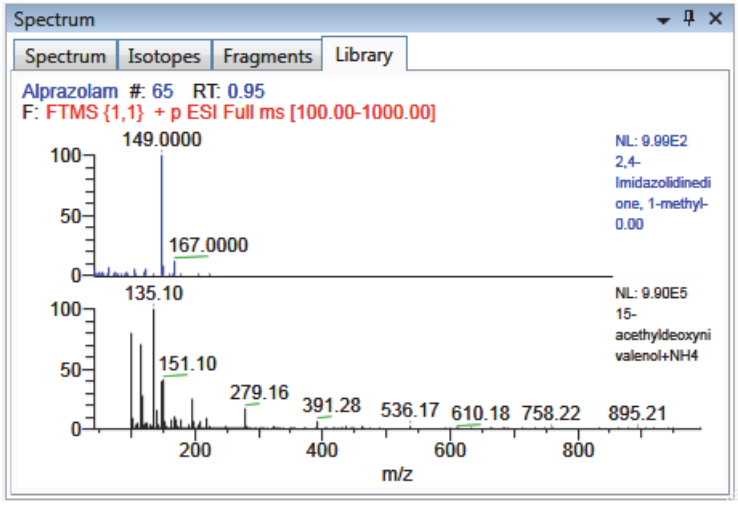
  The Fragments page displays the maximum number of fragments as specified in the screening method. You must define fragments in the screening library.



- Library

  The Library page displays the matching library spectrum (in blue) and the experimental spectrum (in black). The resulting score percentage from a library search match must be higher than your specified threshold value to identify or confirm the presence of a compound.

  The application scales both the matched library spectrum and the highest peak in the experimental spectra at 100 percent intensity and displays the resulting neutral loss (NL) value for the matched library entry name on the right of the plot.



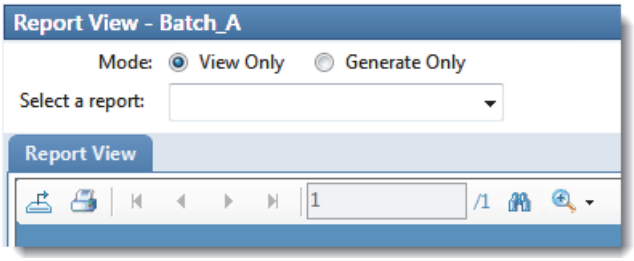
Report View

In the Report View of the Analysis mode, you can display or generate reports for the currently selected batch. You must process each sample in the batch before you can view or generate a sample-level report for that sample.

❖ To open the Report View

Click **Report View** in the navigation pane.

From the Report View, you can view reports or generate reports for your batch.



- **View Only**: Displays a PDF file or Microsoft™ Excel™ spreadsheet preview of the selected report type for the batch, sample, or compound. See "Viewing Reports."

  Preview reports for all Standard report types are always available. You must generate Custom and Target Screening report types before you can view them.

  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 report. See "Generating Reports" on page 24.

❖ To refresh the Report View

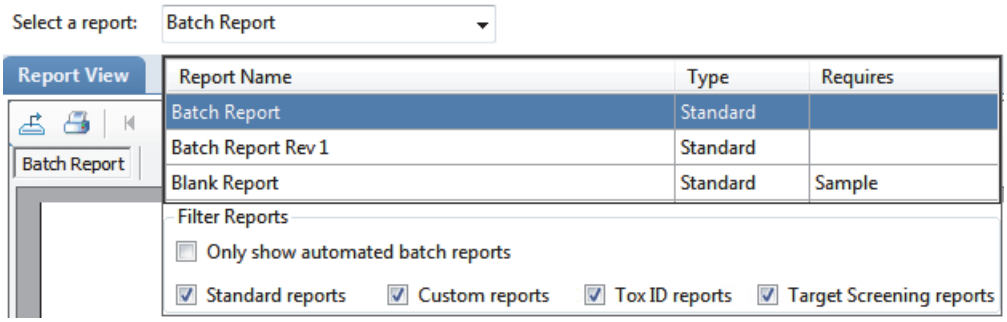
If you make changes to your reports, click **New Data Available - Refresh**.

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.

❖ To select a report

1. Select the **View Only** option.
2. Open the Select a Report list to display all configured report types.



These reports reflect the Displayed Reports selections in the Application Configuration mode.

(Optional) To sort the reports, you can click the column headers. The application maintains this sort order each time you open the Report View for this batch.

(Optional) To help organize your reports, you can filter the list.

(Optional) You can select any combination of filtering options.

Table 1. Filter Reports options

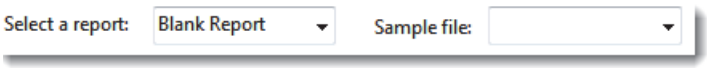
Option	Behavior
Only Show Automated Batch Reports	Displays only reports that have an output format specified in the Automated Batch Reports area in the Batch View.
Standard Reports	Displays the Standard report types.
Custom Reports	Displays the Custom report types. Custom reports are not available for viewing until you have generated the report.
ToxID Reports	Displays the ToxID report types. ToxID reports are not available for viewing until you have generated the report.
Target Screening Reports	Displays the Target Screening report types.

3. Double-click the name of the report.

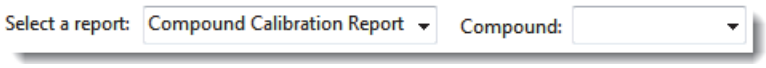
   The report list closes.

   - When the selected report is a batch-level report, the application displays the report on the Report View page.

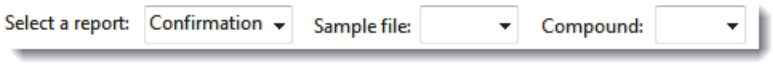
     When the selected report includes separate reports for each sample, you must select a sample file. Follow the procedure "To select a sample."

   - When the selected report includes separate reports for each compound, you must select a compound. Follow the procedure "To select a compound."

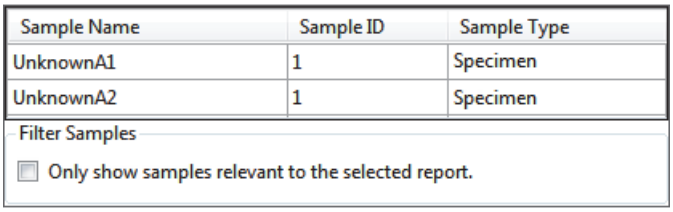
     

   - When the selected report includes separate reports for each sample and each compound in the sample, you must select both a sample file and a compound. Follow the procedure "To select a sample and a compound."

❖ To select a sample

1. Open the Sample File list to display all samples in the batch.

   To show only samples 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.

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

2. Double-click the name of the sample.

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

❖ To select a compound

1. Open the Compound list to display the names and retention times of all compounds in the sample.

RT	Compound Name
	All Compounds
3.14	Propanenitrile
3.15	Pyrazinamide

2. Double-click one of the compounds or double-click **All Compounds**.

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

❖ To select a sample and a compound

1. Open the Sample File list to display all samples in the batch.

Sample Name	Sample ID	Sample Type
UnknownA1	1	Specimen
UnknownA2	1	Specimen

Filter Samples

☐ Only show samples relevant to the selected report.

2. To show only samples that are 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.

   You can sort the reports by clicking the column headers. 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.

4. Open the Compound list to display the names and retention times of all compounds in the sample.

RT	Compound Name
	All Compounds
3.14	Propanenitrile
3.15	Pyrazinamide

5. Double-click one compound or **All Compounds**.

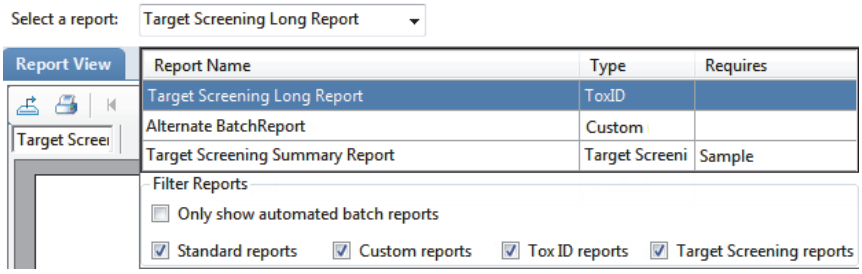
   The Compound list closes. The Report View page displays the compound-level report for the selected sample and compound.

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.

❖ To select a report

1. Select the **Generate Only** option.
2. Open the Select a Report list to display the available reports.



The application displays only configured sample-level report types in the list. You cannot generate batch-level or compound-level reports from this view.

If you have many reports, you can filter the list.

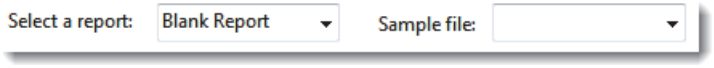
3. To limit the types of reports displayed in the report list, select any combination of report filter options in the Filter Reports area.

For a description of the Filter Reports options, see "Filter Reports options" on page 22.

4. Double-click the name of the report.

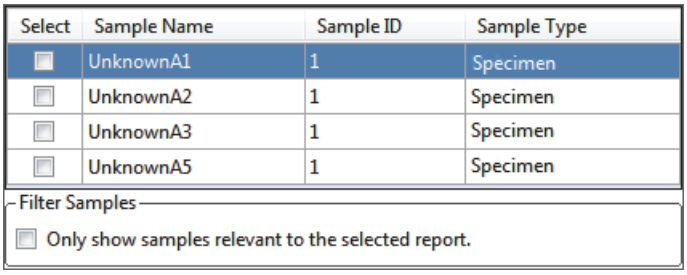
The report list closes.

- When the selected report is a batch-level report, the application generates the report and displays the report on the Report View page.
- When the selected report includes separate reports for each sample, you must select a sample file.



❖ To select a sample

1. Open the Sample File list to display all samples in the batch.



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

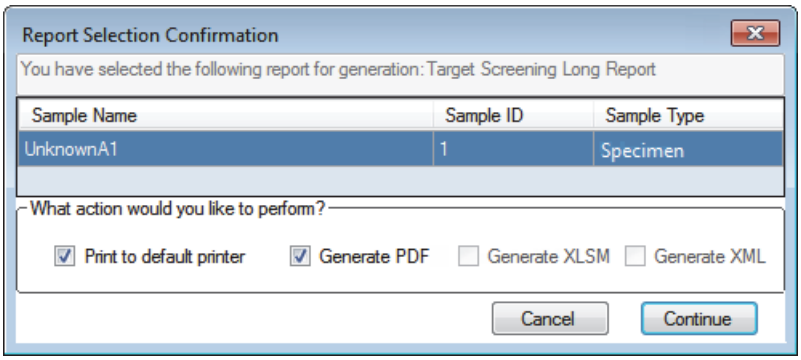
For example, when you select the Quality Control Report, the sample list displays only QC samples.

You can sort the reports by clicking the column headers. The application maintains this sort order each time you open the Report View for this batch.

3. Select the check box for each sample that you want to include in the report.

4. Click **Generate**.

   The Report Selection Confirmation dialog box opens.



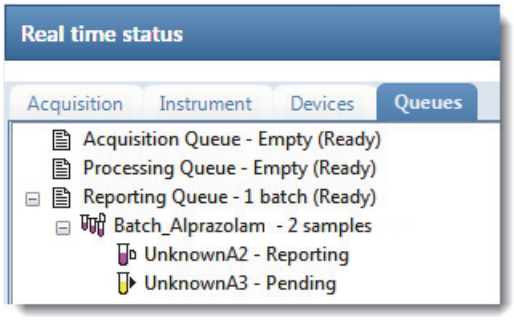
5. In the What Action Would You Like to Perform area, select the types of reports to create.

   Note The application automatically selects required output formats. These options are not editable.

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

6. Click **Continue**.

   The application submits the selected samples to the report queue.



   When you have already generated this report in the Batch View or Acquisition Mode, the application time-stamps the new report to differentiate it from the original report.

Working with Reports

Use the buttons on the Report View page to view, print, or export a report.

- A PDF file 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 generated with the Generate XLSM option selected.

❖ To print a standard or target screening report

1. Select the report to print from the Select a Report list.
2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.
3. Click the **Print Report** icon, .

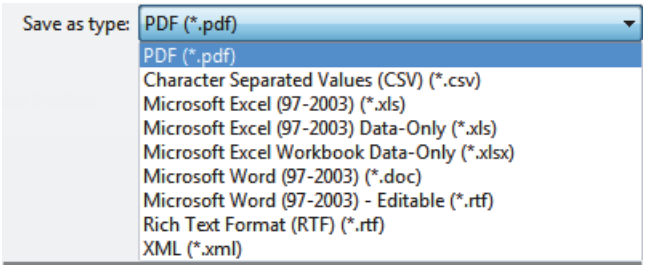
   The Print dialog box for your default printer opens.
4. Follow the typical procedure to print from your printer.

   Landscape reports automatically rotate to fit the paper.

❖ To export a standard report

1. Select the report that you want to print from the Select a Report list.
2. (Optional) Select a sample from the Sample File list.

   The application displays the report on the Report View page.
3. Click the **Export Report** button, .
4. In the Export Report dialog box, locate the folder where you want to write the report file.
5. Type a file name for the exported report file.
6. Select a file type from the Save as Type list.



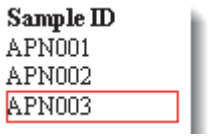
7. Click **Save**.

   The TraceFinder application saves the file as the specified file type and writes the report file to the specified folder.

❖ To search for text

1. Select a report from the Select a Report list.
2. Click the **Find Text** icon, .
3. In the Find Text dialog box, type your text and click **Find Next**.

   The TraceFinder application encloses the search results in a red box.

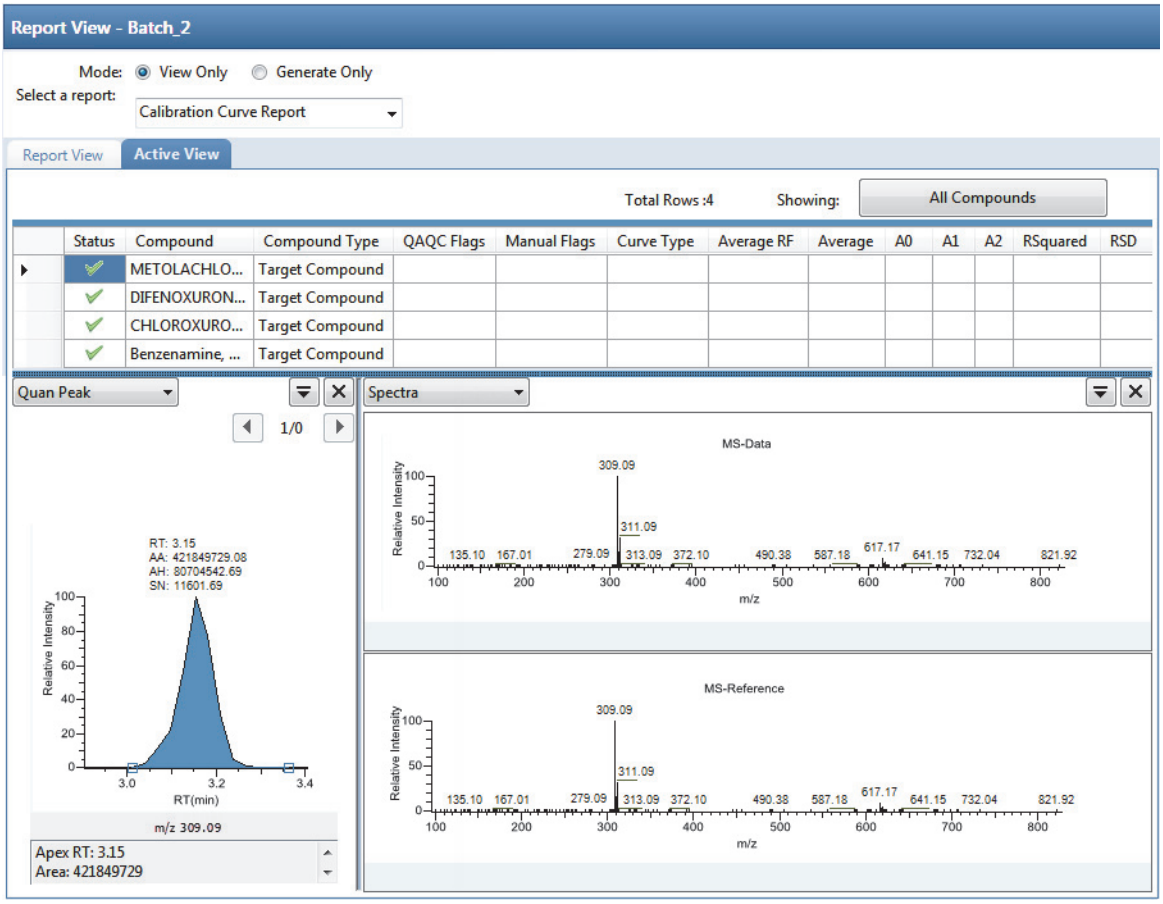


❖ To enlarge the report text

1. Select a report from the Select a Report list.
2. Click the **Zoom** icon, , and select a zoom scale.

Active View

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



Not all reports support the Active View feature. For descriptions of all the functions and parameters on the Active View page for each report that supports Active View, refer to the "Using the Analysis Mode" chapter of the *TraceFinder User Guide*.

❖ To display the Active View page

Click the **Active View** tab.

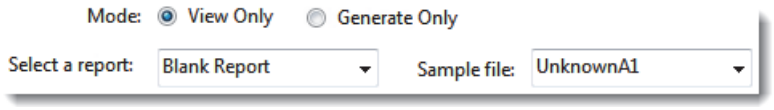
The Active View page displays quantitative data and QAQC error flags for each sample.

❖ To display a report

1. Select a report type from the Select a Report list.

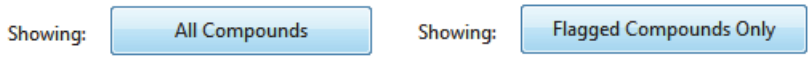
   The list displays only the report types created for the current batch.

2. (Optional) When the report type includes separate reports for each sample, select a sample file.



❖ To filter the compounds to display using the Showing toggle button

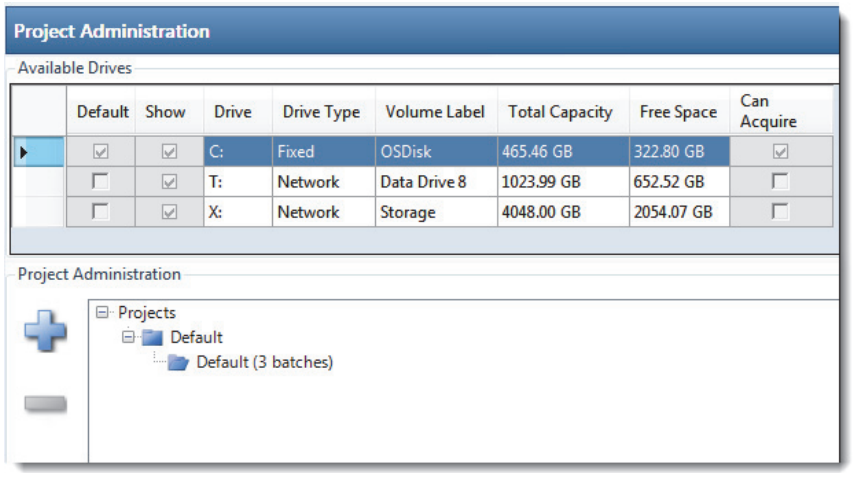
Click the Showing toggle button to switch the display to either all compounds or only compounds that are flagged for failing a QAQC test.



Project Administration

In the Project Administration view, you can create and manage projects and subprojects.

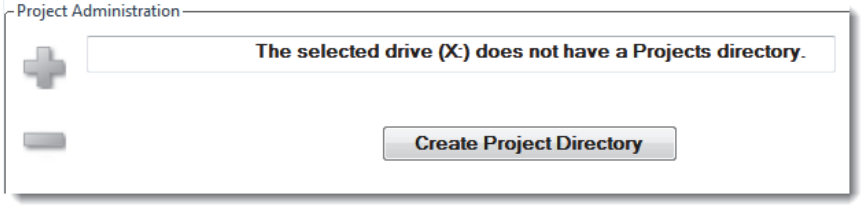
To open the Project Administration view, click **Project Administration** in the Analysis navigation pane.



❖ To choose a drive

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

   If you have not created a Projects directory on this drive, you see this message:



2. Click **Create Project Directory**.

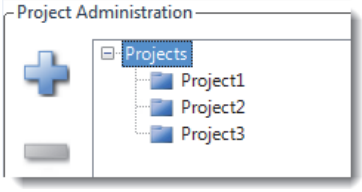
   The TraceFinder application adds a new Projects directory to the selected drive.

❖ To add a project or subproject

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 activates the plus sign icon, , indicating that you can create a folder within the selected folder.



2. Click the plus sign.

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

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

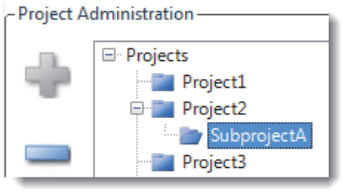
   Project names are limited to 30 characters and can contain spaces and special characters, except for the following special characters: \ / : * ? " < > |

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

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

❖ To delete projects or subprojects

1. Select the project or subproject that you want to delete.



   You can delete projects that do not have subprojects. You can delete subprojects that do not have batches. When the selected project or subproject is available for deletion, the application activates 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.

Local Method

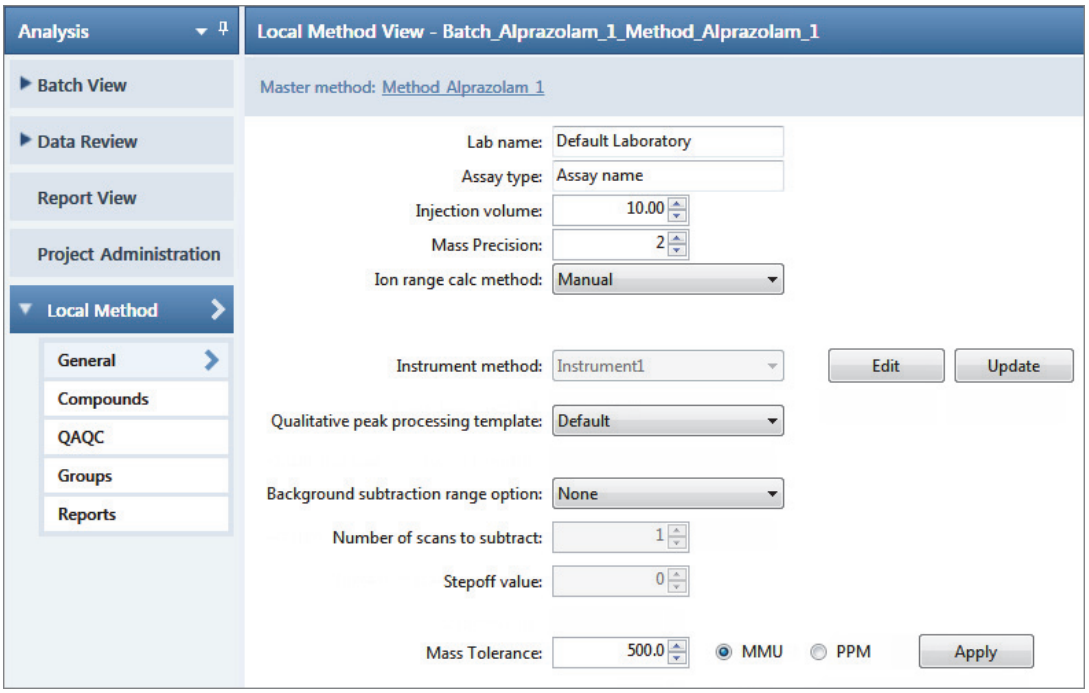
In the Local Method view of the Analysis mode, you can edit only the local copy of the method, or you can edit the master method and overwrite the local copy with the edited master method. A local method is a copy of a master method associated with a batch. Editing the local method does not affect parameters in the master method.

❖ To open the Local Method view

Click **Local Method** in the Analysis navigation pane.

The General page of the Local Method view opens. From the Local Method view, access the method parameters just as you would for a master method.

Local methods are named *BatchName_MasterMethodName*.



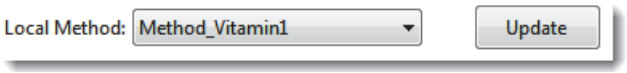
❖ To edit a local method

1. Enter any changes to the local method.

   For instructions for editing a method, refer to the "Using the Method Development Mode" chapter in the *TraceFinder User Guide*.
2. Choose **File > Save**.
3. 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.

Quick Acquisition

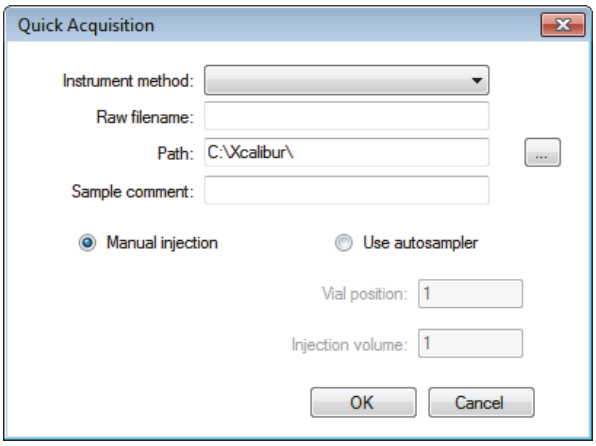
Use the quick acquisition feature to quickly submit a single sample from any page of the Acquisition mode.

Note The Quick Acquisition feature is available only when you activate it in the Application Configuration mode.

❖ 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. For the path, browse to a folder where you want to write the acquired raw data file.
5. Select either the manual injection or the autosampler option:
   - To perform manual injection, do the following:
     i. Select the **Manual Injection** option.
     ii. Click **OK**.

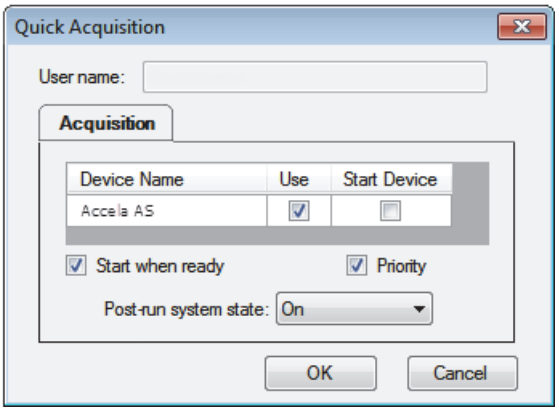
   The application submits the sample to the Acquisition queue.

   - To perform autosampler injection, do the following:
     i. Select the **Use Autosampler** option.
     ii. In the Vial Position box, type a vial position.
     iii. In the Injection Volume box, type an injection volume.

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

     iv. Click **OK**.

     The Quick Acquisition dialog box opens.



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

   This is usually the autosampler.

vi. (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.

vii. (Optional) Select the **Priority** check box to place the sample immediately after any currently acquiring sample.

viii. (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.

ix. Click **OK**.

The application submits the sample to the Acquisition queue.

Trademarks