TraceFinder Analysis Quick Reference Guide

This quick reference guide describes tasks using the Analysis mode in the Thermo TraceFinder™ 5.0 application.

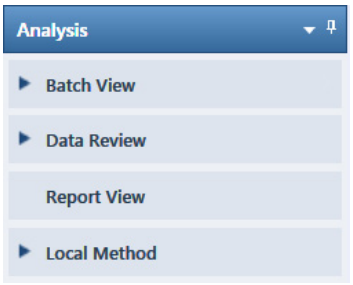
For detailed descriptions of all procedures described in this quick reference guide, refer to the appropriate Analysis mode chapter in the *TraceFinder User Guide*.

Contents

❖ To open the Analysis mode

Click **Analysis** in the navigation pane.

The Analysis navigation pane opens.



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 data, process data, 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 (all batch types)
- Auto Samples Page (quantitation batches with intelligent sequencing only)
- Reference Sample Page (quantitation batches only)
- Threshold Samples Page (quantitation batches only)

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Samples Page

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

❖ To open the Samples page

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

❖ To create a new batch

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

   The Create New Batch dialog box opens.
2. Select a repository from the list.

   Tip The application displays all configured and enabled repositories.

   The project list displays all projects, subprojects, and batches in the selected repository.
3. Select the folder where you want to store your batch.
4. Type a batch name in the New Batch box.
5. To select a master method, do the following:
   a. Select either **Quan**, **Screening**, or **Unknown Only** from the Type list.
   b. Select a repository from the Repository list.
   c. Select a master method from the Name list.

      The Name list displays all available methods for the selected method type.
6. Click **Create**.

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

   A new batch opens with one Unknown sample. The batch name in the title bar indicates that you are creating either a quantitation, a target screening, or an unknown screening batch.

❖ To add samples to the list

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

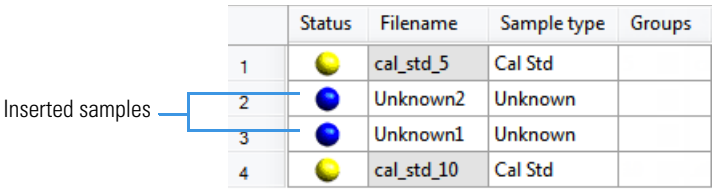
Tip To add a single sample row, right-click the sample list and choose **Add Sample**.

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,  .

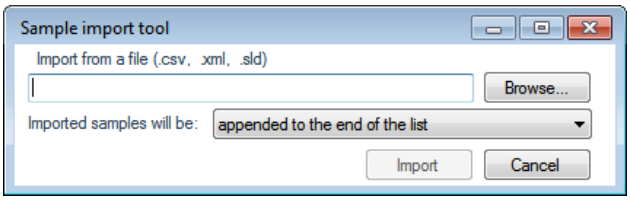
   The application inserts the Unknown samples above the selected sample.



❖ To import samples into the list

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

   The Sample Import Tool dialog box opens.



2. Browse to 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	Matrix Blank
Std Bracket	Cal Std

❖ 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**.

❖ To copy a sample

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

   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**.

   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.
   - Double-click the Filename column and locate a raw data file to use for the sample.

   –or–
   - Right-click and choose **Browse in Raw File**, and then locate a raw data file to use for the sample.
2. For each sample, click the Sample Type column and select a sample type from the list.

Available sample types				
Matrix Blank	Solvent	QC	Unknown	Cal Std

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

   The sample levels are defined in the master method. If there are no levels to select 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 scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening) Level, Sample ID, and Sample Name, while the other columns scroll right and left.

❖ To create a group

1. For each sample, click the Groups column and type the name of a group.
2. Repeat step 1 for each sample that you want to include in a group.
3. Create as many groups as you want.

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

❖ 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. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.
3. To process the submitted samples, select the **Process Data** check box.

   The application displays options for the type of method that the batch uses: Quantitation, Target Screening, or Unknown Screening. If a quantitation method or target screening method includes unknown screening features, the application also displays unknown screening options.

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

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

   Quantitate: Performs quantitation.

   Identify: Performs identification for unknown screening.

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

   With RT Alignment: Performs retention time alignment for unknown screening. This produces the heat map and group averages data in the Unknown Screening View.
5. (Optional) Select the **Create Reports** check box.
6. To start the selected processes, click **OK**.

Auto Samples Page

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

❖ 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

❖ To add an auto sample type

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

   The application adds a Solvent sample to the sample list.

   You can add, insert, or remove samples from this list as you would any sample list. See Samples Page.
2. To change the sample type to a Matrix Blank, click the Sample Type column and select Matrix Blank 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 Matrix Blank vial.

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

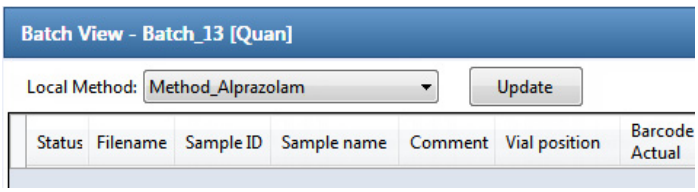
Reference Sample Page

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

❖ To specify a chromatogram reference sample

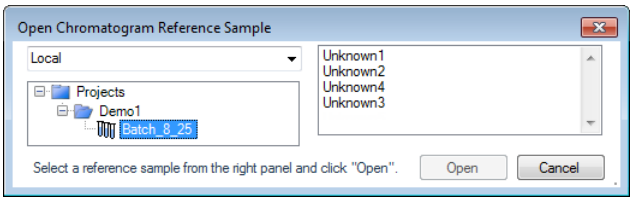
1. Click **Reference Sample** in the Batch View navigation pane.

   An empty reference sample table opens.



2. Right-click the table and choose **Add Reference Sample**, or click the **Add Reference Sample** icon,  .

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. From the right panel, select a sample from the list of processed samples.

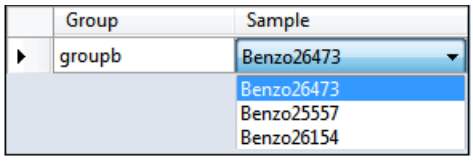
   The application displays all the processed samples in the selected batch. Before using a sample as a reference sample, you must have processed the sample with the current master method.
7. Click **Open**.

Threshold Samples Page

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

❖ To specify a threshold sample

1. In the navigation pane, click **Threshold Samples**.
2. Open the Sample list for each group and select a sample in the group to be the threshold sample.



The Comparative View uses the threshold method and amount you specified in the method, the group you created on the Samples page, and the threshold sample that you selected on this page to define the threshold guide that it displays on the sample peak plots.

See also To create a group and Comparative View.

Data Review

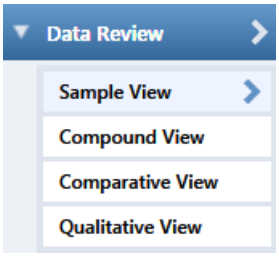
Use Data Review to verify the data generated by a quantitation, a target screening, or an unknown screening master method before you generate reports.

- Data Review for Quantitation Batches
- Data Review for Target Screening Batches
- Data Review for Unknown Screening Batches

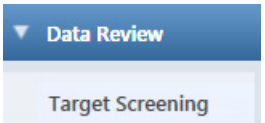
❖ To open the Data Review view

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

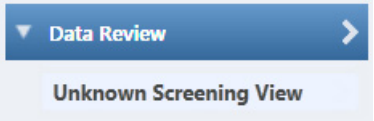
Data Review for quantitation batches



Data Review for target screening batches



Data Review for unknown screening batches



Data Review for Quantitation Batches

The Data Review for quantitation batches includes the following:

- Survey Mode
- Sample View
- Compound View
- Comparative View
- Qualitative View

Note If the quantitation method for the batch includes unknown screening features, the Data Review also includes an Unknown Screening View. See Data Review for Unknown Screening Batches.

Survey Mode

Whether you are assigned strict or loose Survey View permission, only Cal Std and QC sample types are displayed during processing; and the Sample View, Compound View, and Comparative View headers show **Survey Mode** or **Survey Mode - Loose Restrictions**, respectively. If you are assigned loose Survey View permission, however, all sample types are available to you after processing is completed.

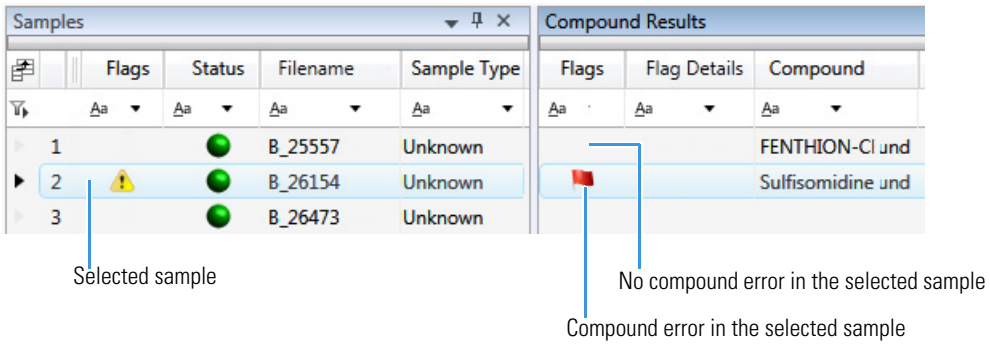
Sample View

Tip (Animation) To view "Using the Sample View," choose **Help > Animations**.

The Sample View displays a list of all samples in the current batch (Samples pane), the compound results for all compounds in the method (Compound Results pane), and peak plots for all compounds found in the currently selected sample (Sample-centric Plot pane).

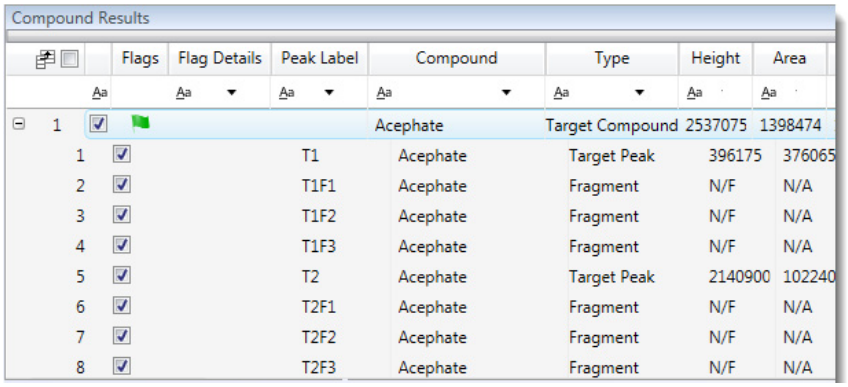
- **Samples pane**

  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.



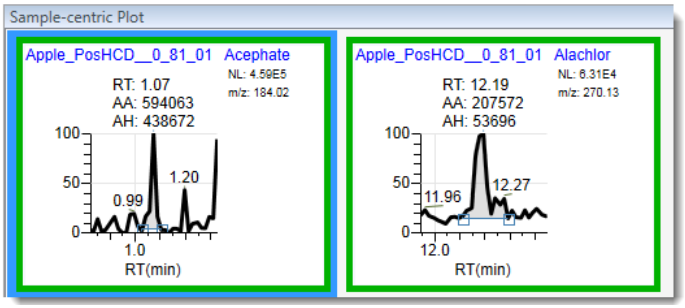
- **Compound Results pane**

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



- **Sample-centric Plot pane**

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



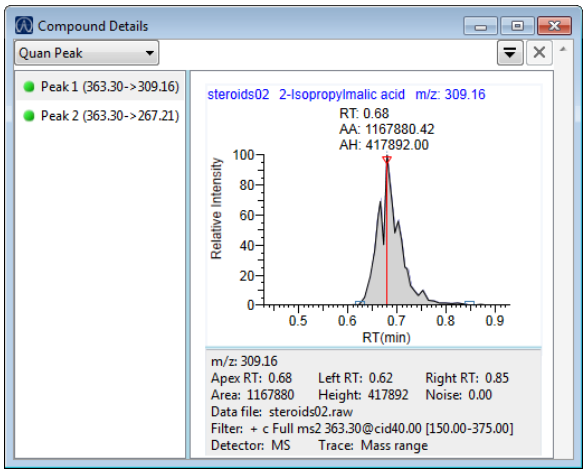
❖ To display details for a compound

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

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

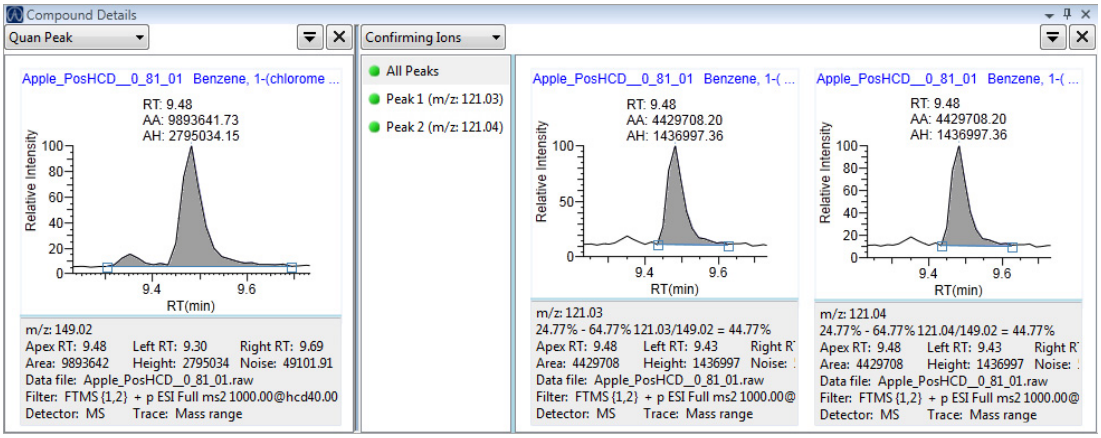
Quan Peak

A compound can have multiple quantitative peaks. You can switch between quantitative peaks, but you cannot view multiple quantitative peaks at the same time.



Confirming Ions

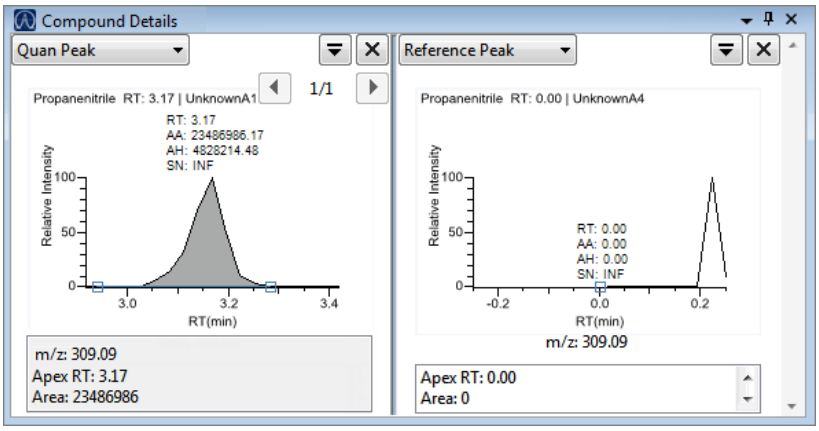
Figure 1. Quantitative peak with multiple confirming ions



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

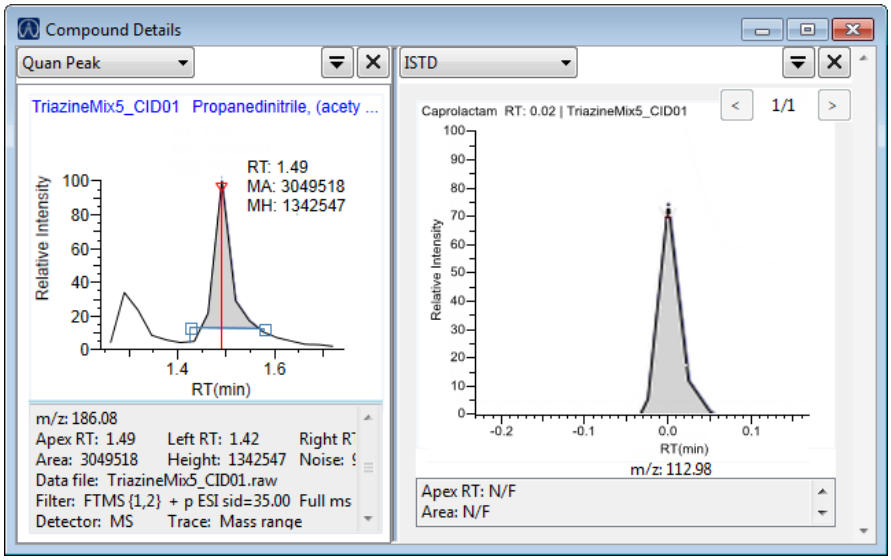
Reference Peak

Figure 2. Quantitative peak with a reference peak



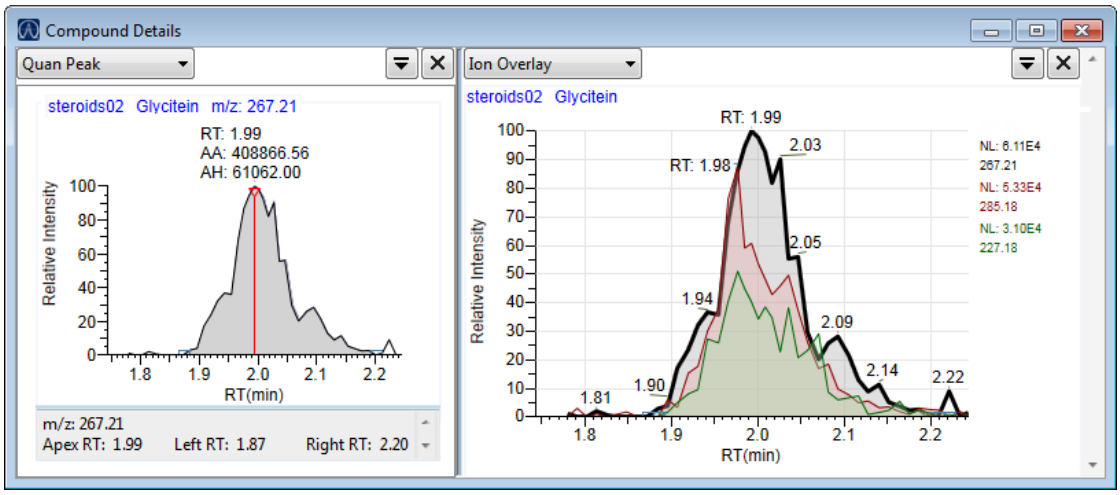
ISTD

Figure 3. Quantitative peak with an internal standard



Ion Overlay

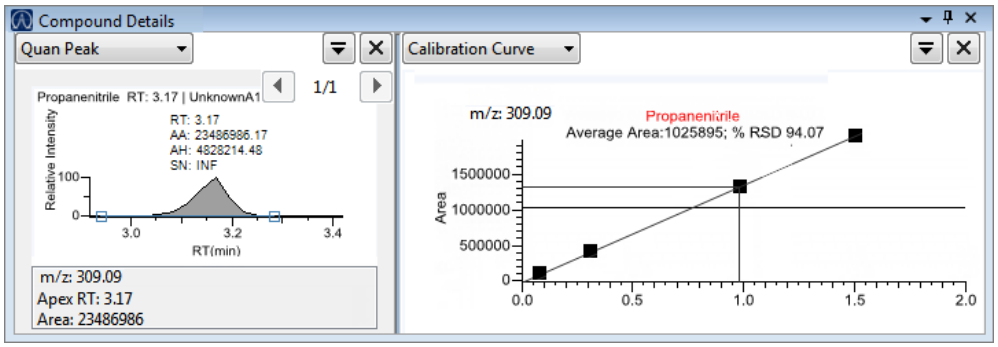
Figure 4. Quantitative peak with a confirming ion overlay



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

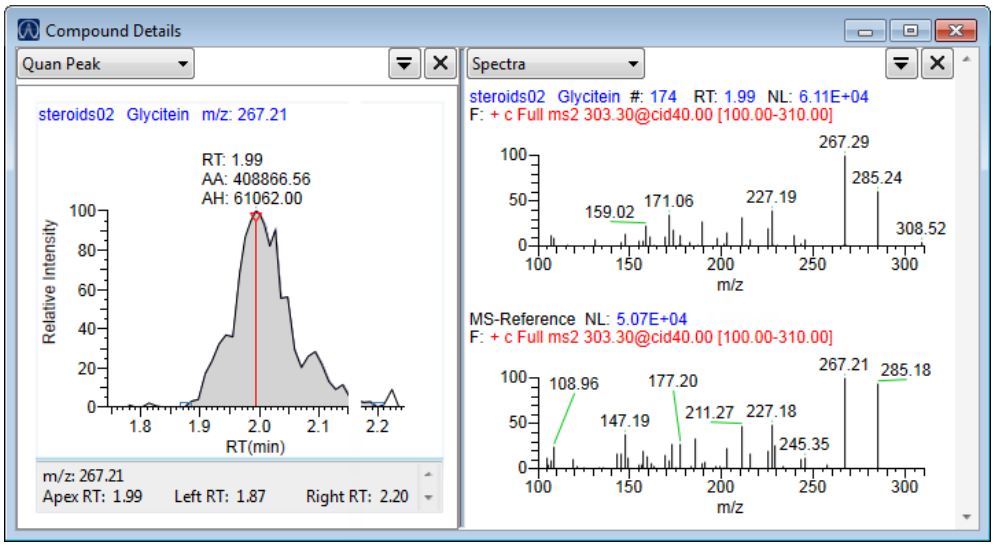
Calibration Curve

Figure 5. Quantitative peak with a calibration curve plot



Spectra

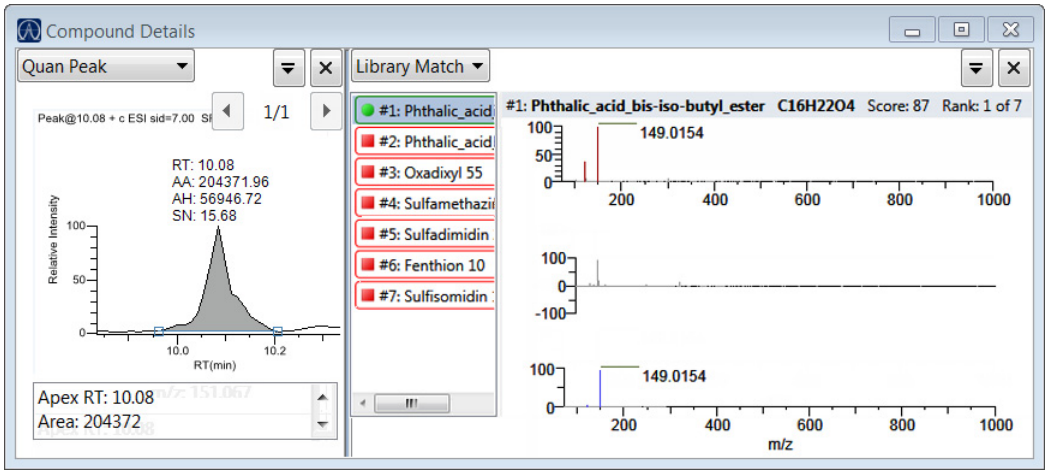
Figure 6. Quantitative peak with data and reference spectra



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

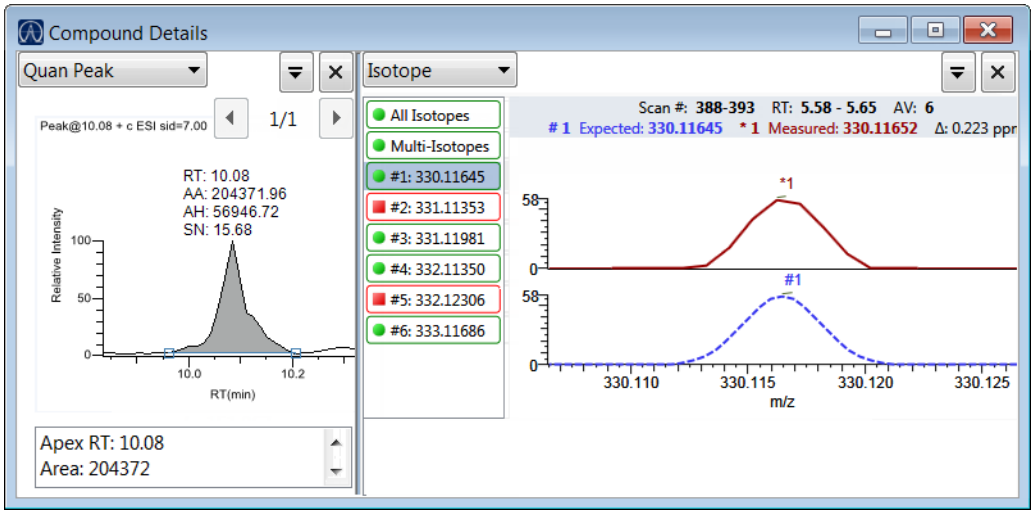
Library Match

Figure 7. Quantitative peak with a library match



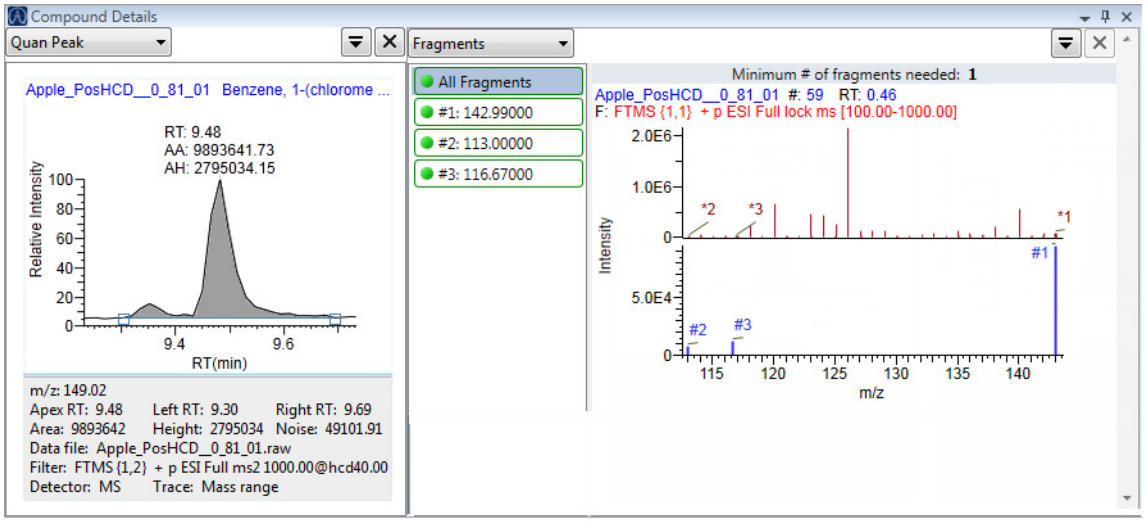
Isotope

Figure 8. Quantitative peak with isotopes



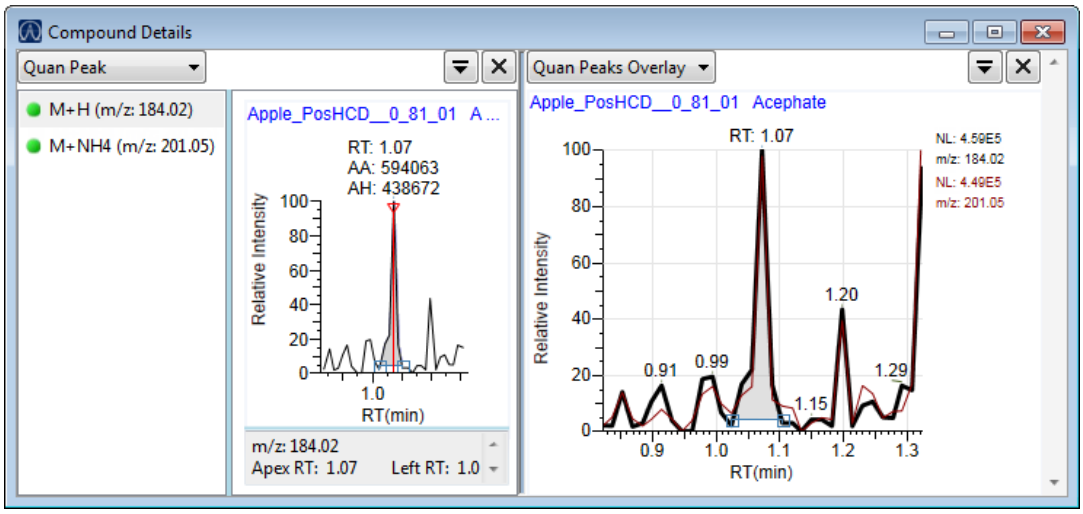
Fragments

Figure 9. Quantitative peak with fragments



Quan Peaks Overlay

Figure 10. Quantitative peak with a quan peaks overlay

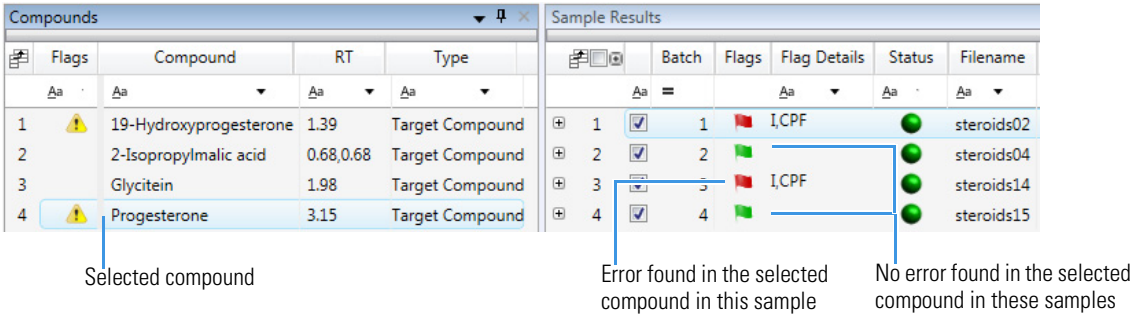


Tip (Animation) To view "Using the Compound View," choose **Help > Animations**.

The Compound View displays a list of all compounds available in the method (Compounds pane), all samples in the current batch (Sample Results pane), the peak plots for all compounds found in each sample (Compound-centric pane), Group Averages pane, and a Retention Time Summary pane.

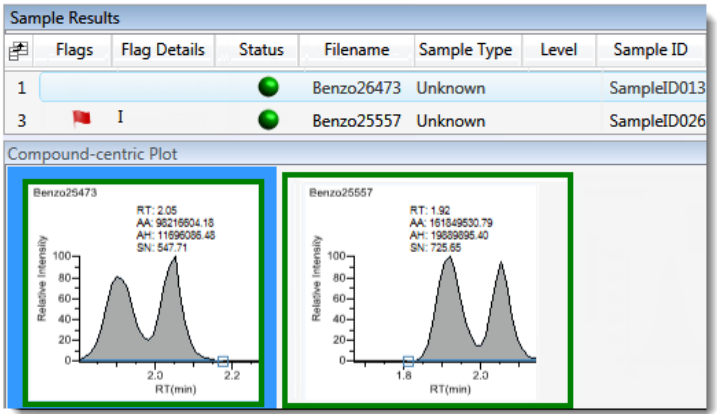
- **Compounds pane**

  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 associated with the selected compound.



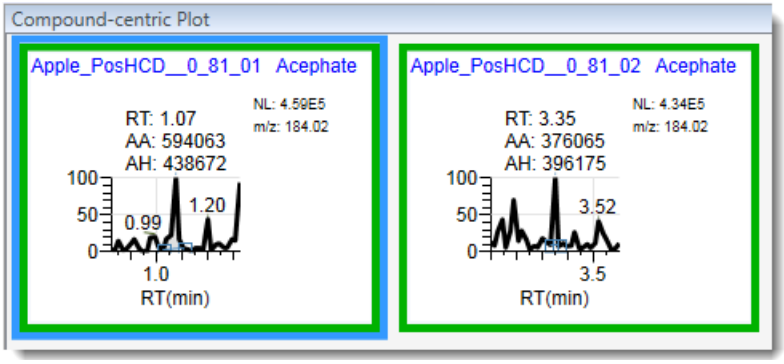
- **Sample Results pane**

  Use the Sample Results pane to select a compound in a specific sample. The **Compound-centric Plot 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: the chromatogram, retention time, area, height, and signal-to-noise ratio.



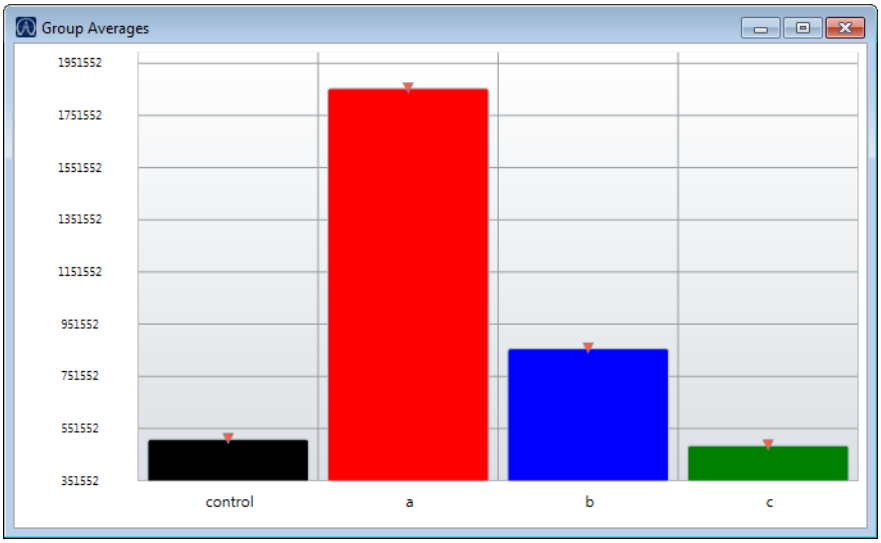
- **Compound-centric Plot pane**

  Use the Compound-Centric Plot pane to view an overlay of the quantitation and confirming peaks for each sample in the batch. The Compound-Centric Plot pane displays the compound chromatograms for the selected compound in each sample in the batch. A blue border indicates the compound in the sample that is currently selected in the **Sample Results pane**.



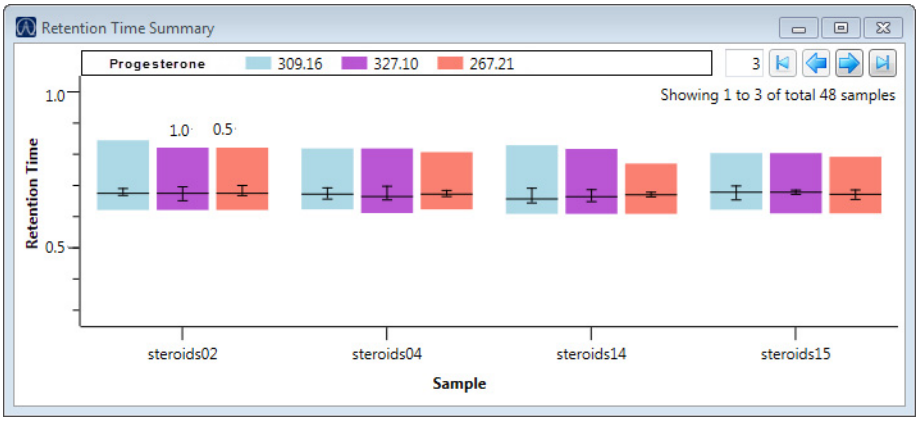
- **Group Averages pane**

  Use the Group Averages pane to compare the peak areas of different samples to a control group of samples. You must define at least two groups, and one group must be a control group.



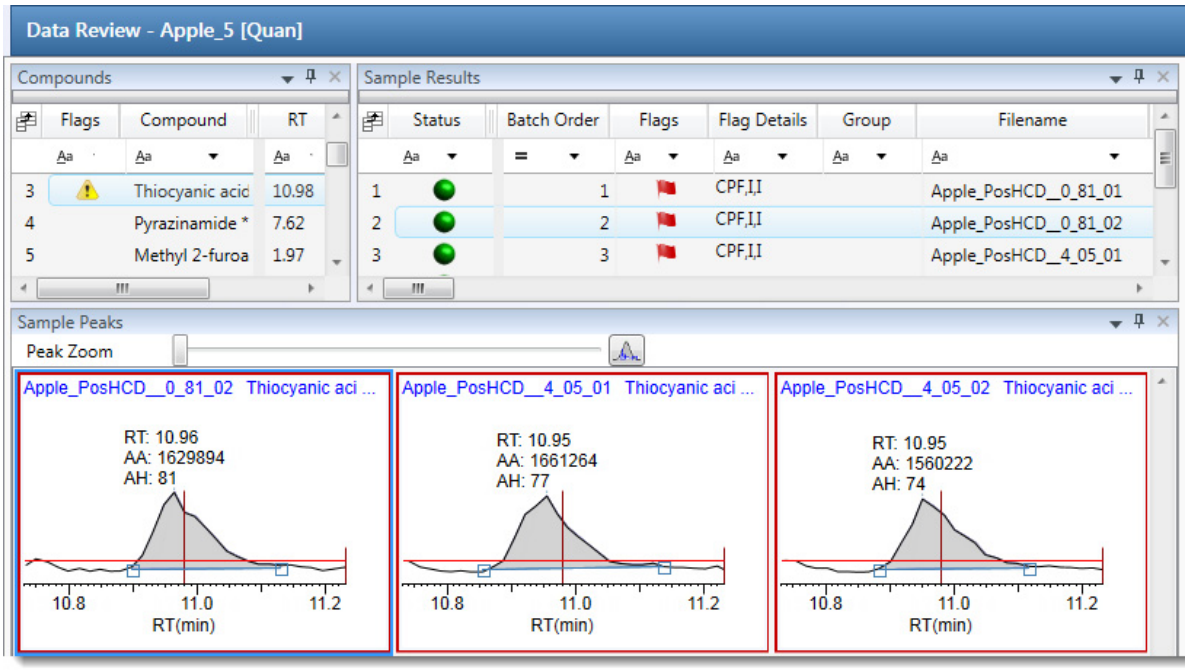
- **Retention Time Summary pane**

  Use the Retention Time Summary pane to view variations of the retention times for a compound across all samples in a batch. The Retention Time Summary pane displays each color-coded compound for each sample in the batch.

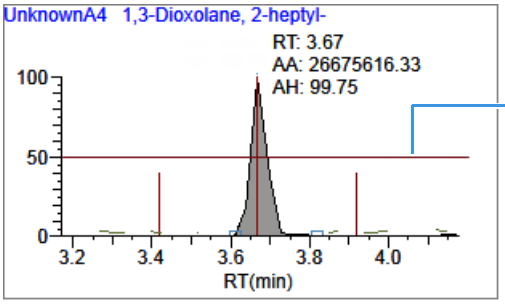


Tip (Animation) To view "Using the Comparative View," choose **Help > Animations**.

The Comparative View uses three panes to display a list of all compounds available in the method (Compounds pane), all samples in the current batch (Sample Results pane), and the sample peak plots for all compounds found in the samples (Sample-centric Plot pane) with the horizontal threshold guide.



The Comparative View uses the threshold method and amount that you specified in the method, the group that you created on the Samples page, and the threshold sample that you selected on the Threshold Samples page to define the threshold guide that it displays on the sample peak plots.



Horizontal guide indicates the threshold value as specified in the method.

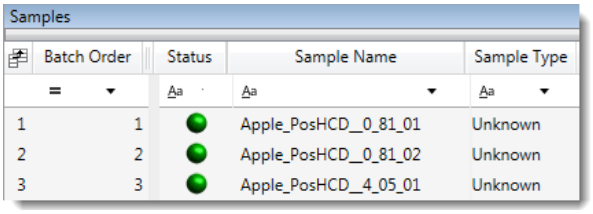
Qualitative View

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

The Qualitative View displays a list of all samples in the batch (**Samples pane**), a list of all peaks in the selected sample (**Peaks pane**), the chromatogram for the selected sample (**Sample Chromatogram pane**), the chromatogram for the selected peak (**Peak Chromatogram pane**), the reference spectrum and spectrum data for the selected sample (**Spectrum pane**), and the best library matches for the selected peak (**Library Hits pane**).

- **Samples pane**

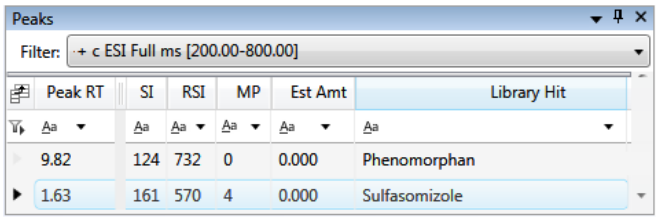
  Use the Samples pane to select a specific sample.



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

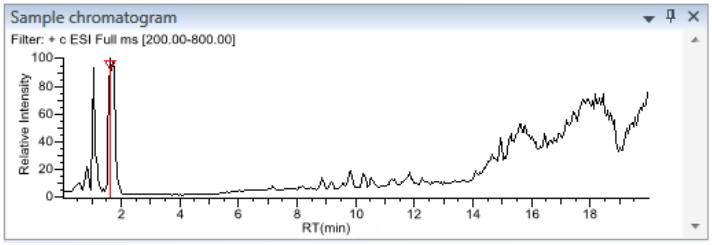
- **Peaks pane**

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



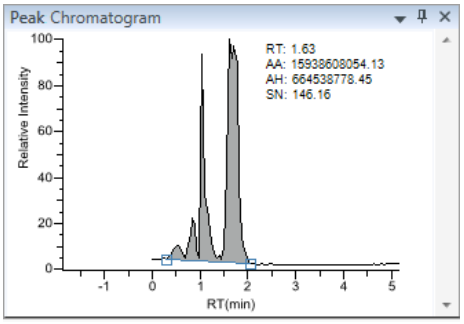
- **Sample Chromatogram pane**

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



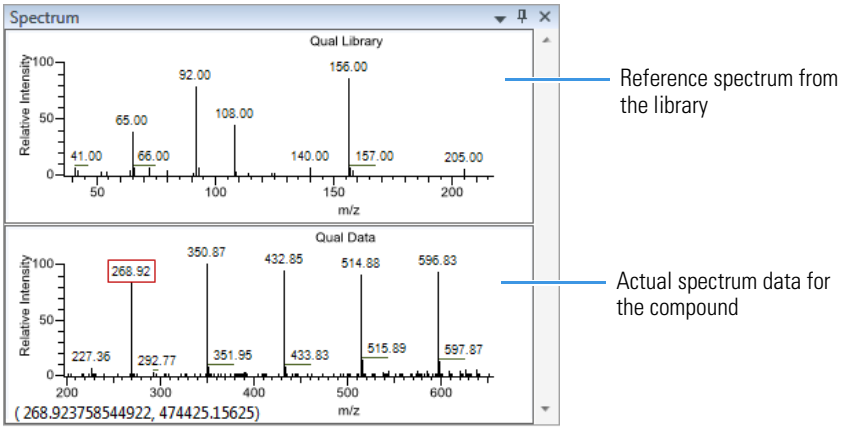
- **Peak Chromatogram pane**

  The Peak Chromatogram pane displays the selected peak.



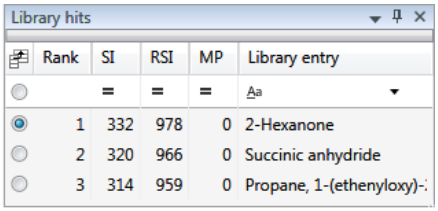
- **Spectrum pane**

  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.



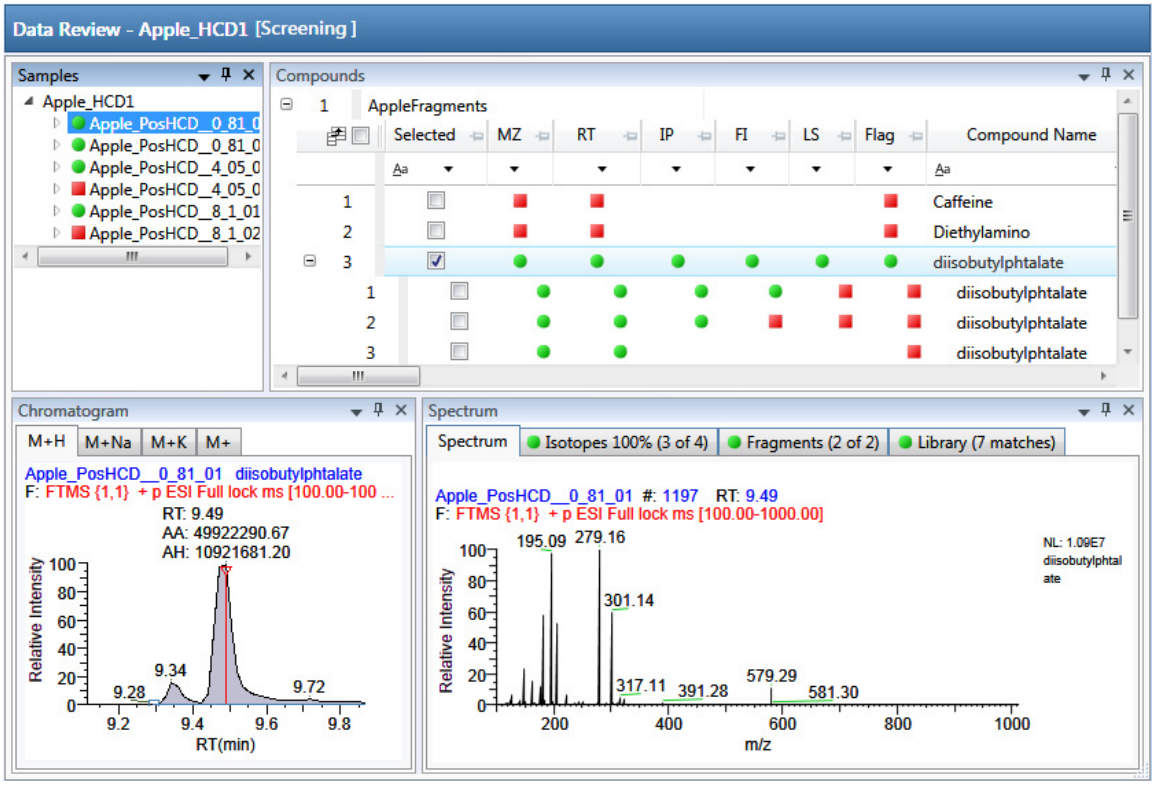
- **Library Hits pane**

  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 Batches

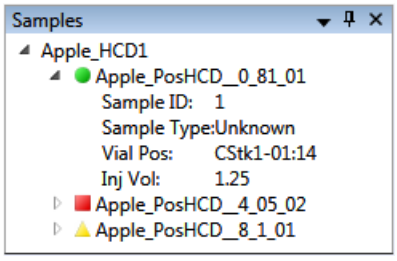
In the target screening display, the application displays a list of all samples in the current batch, the compound results for all compounds in the method, and chromatogram and spectrum plots for all compounds found in the currently selected sample.



The Target Screening View displays a list of all samples in the batch (Samples Pane), a list of all compounds in the selected sample (Compounds Pane), the chromatogram for the selected peak (Chromatogram Pane), and the reference spectrum and spectrum data for the selected sample (Spectrum Pane).

Samples Pane

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



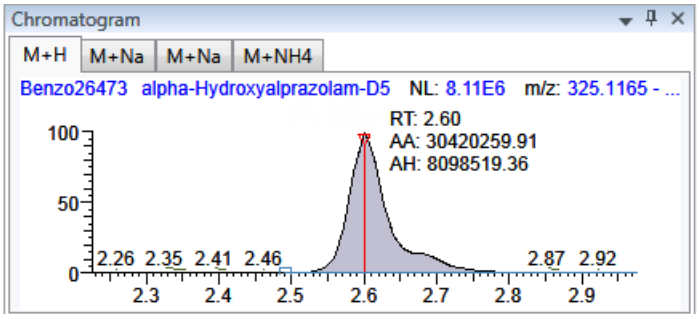
Flags in the Samples pane indicate the following:

- (green circle): The sample/compound/peak combination is identified and fully confirmed.
- (yellow triangle): The sample/compound/peak combination is identified but not fully confirmed.
- (red square): The sample/compound/peak combination is not identified.

Chromatogram Pane

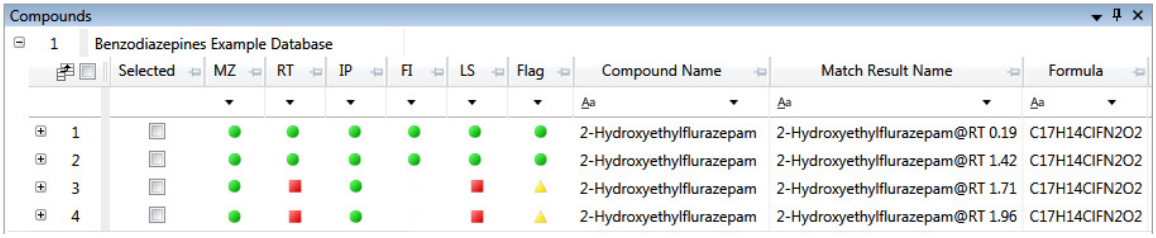
Use the Chromatogram pane to display all extracted chromatograms of all adducts of the selected compound.

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, the first tab 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.



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.



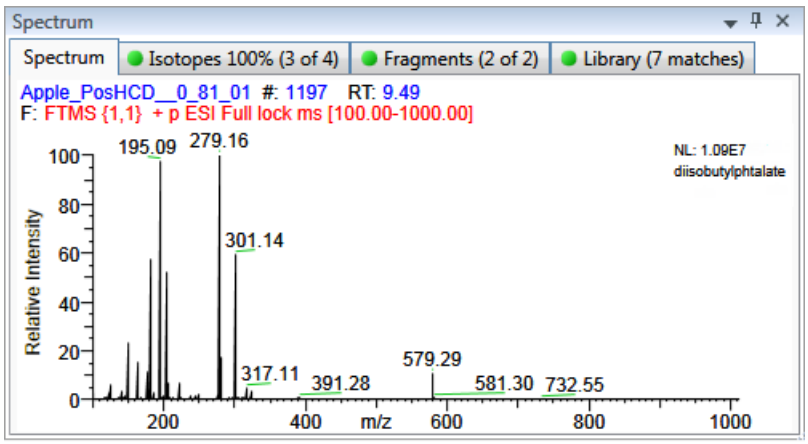
Spectrum Pane

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:

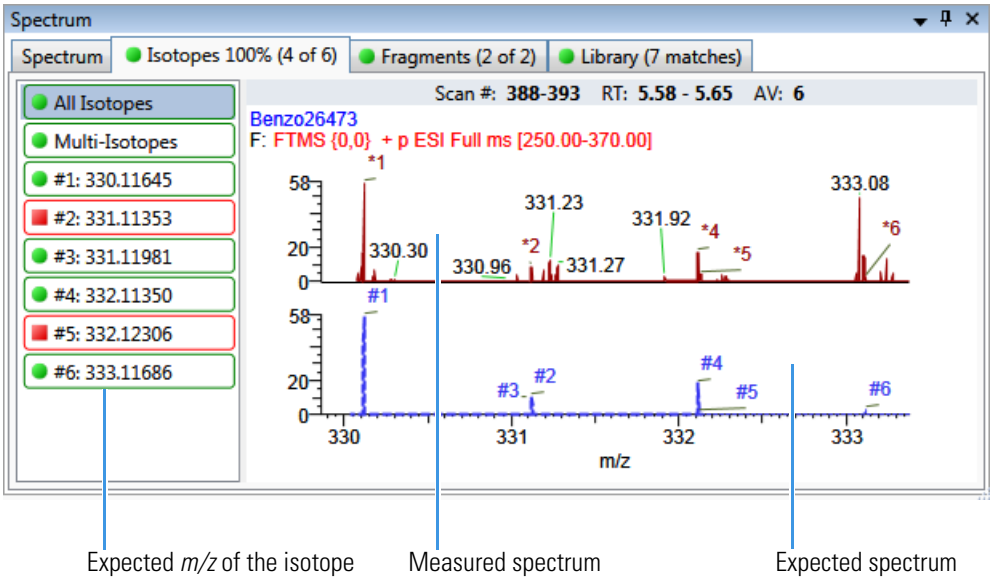
- **Spectrum**

  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.



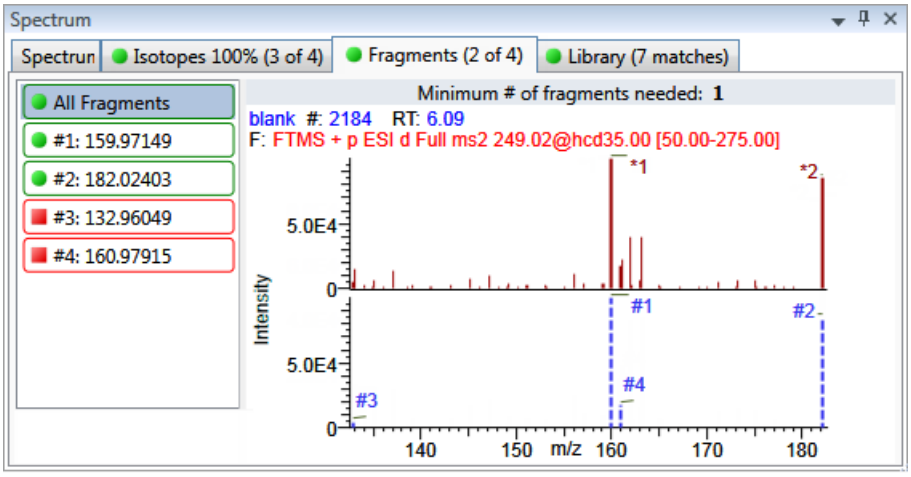
- **Isotopes**

  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**

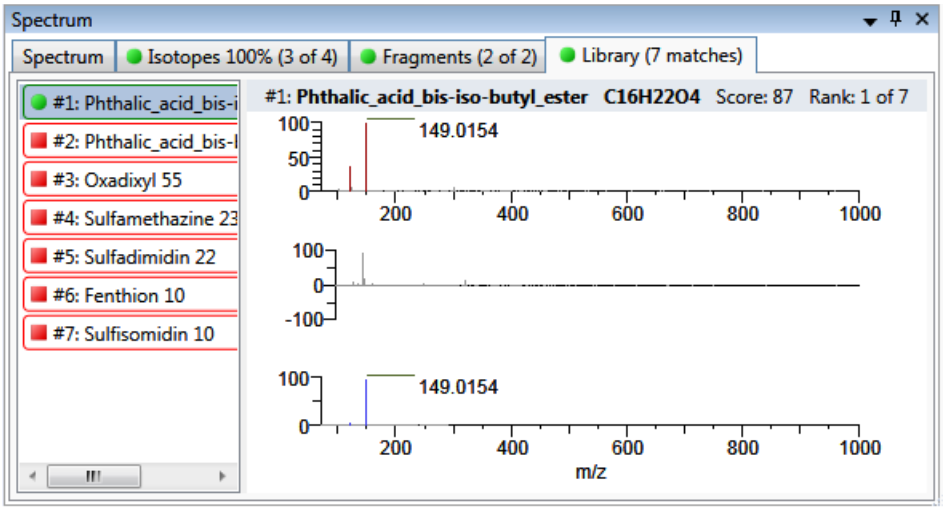
  The Fragments page displays the maximum number of fragments as specified in the screening method. You must define fragments in the screening library.



- **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 measured spectra at 100 percent intensity and displays the resulting neutral loss (NL) value for the matched library entry name to the right of the plot.



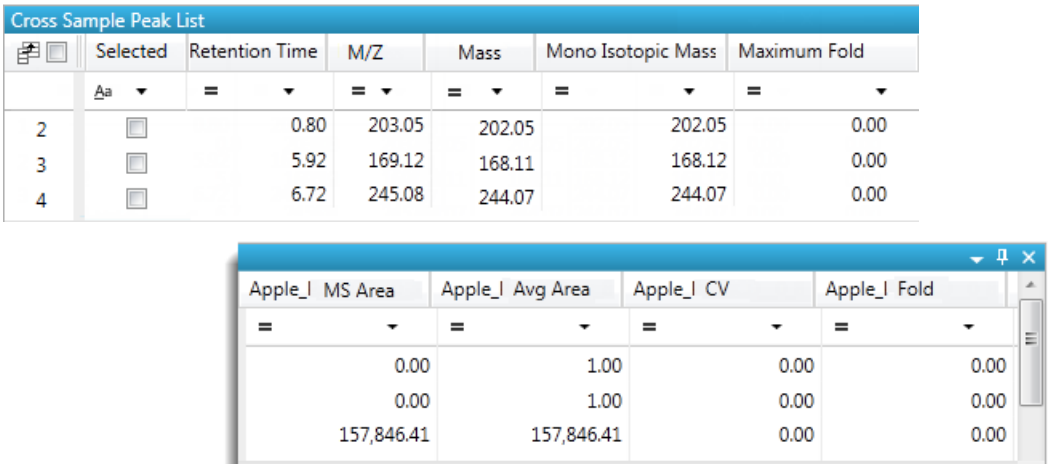
Data Review for Unknown Screening Batches

In the unknown screening view, the application displays the following panes:

- Cross Sample Peak List Pane
- Heat Map Pane
- Sample List Pane
- Spectrum Pane
- Peak List Pane
- Peak Identifications Pane
- TIC Chromatogram Pane
- XIC
- Peak Chromatogram Pane
- Chemical Structure Pane
- XIC Overlay Pane
- Group Averages Pane
- Cross Sample Peak Overlay Pane
- Library Search Pane
- Fragments Pane
- Isotopes Pane

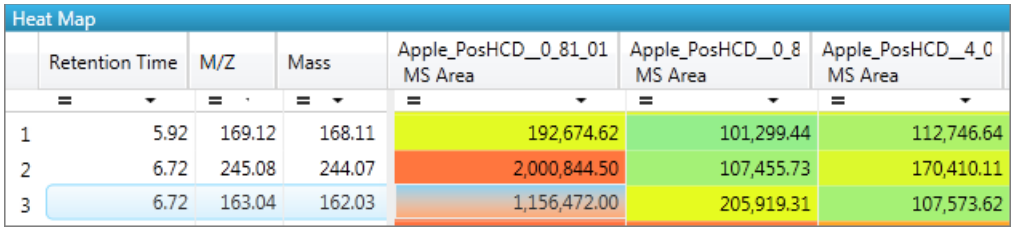
Cross Sample Peak List Pane

Use the Cross Sample Peak List pane to compare peak values across all samples in a batch.



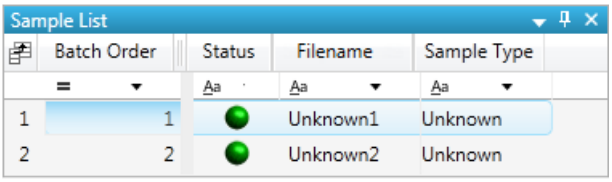
Heat Map Pane

Use the Heat Map pane to display the response of each peak occurrence in the batch. The Heat Map pane displays all MS Area values for all peaks in all samples in the batch that are above the peak threshold value specified in the method. When you select a peak in the Heat Map pane, the application displays the associated results for the selected peak in all panes of the Unknown Screening view.



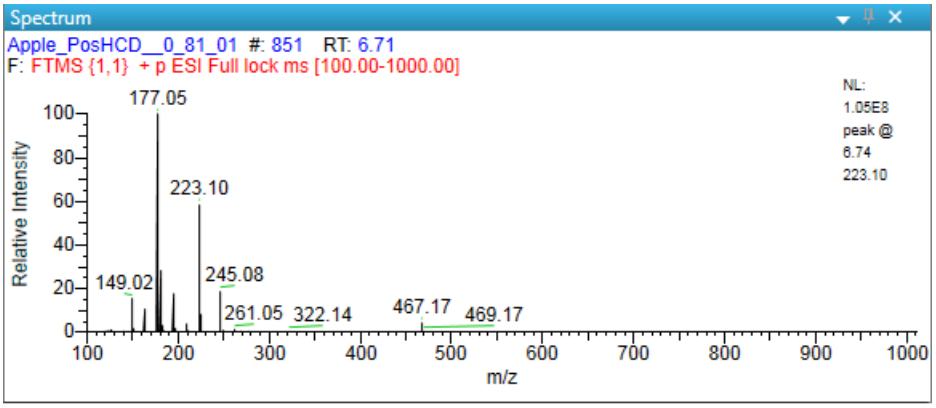
Sample List Pane

Use the Sample List pane to select a sample of interest. The application displays the associated results for the selected sample in all panes of the Unknown Screening view.



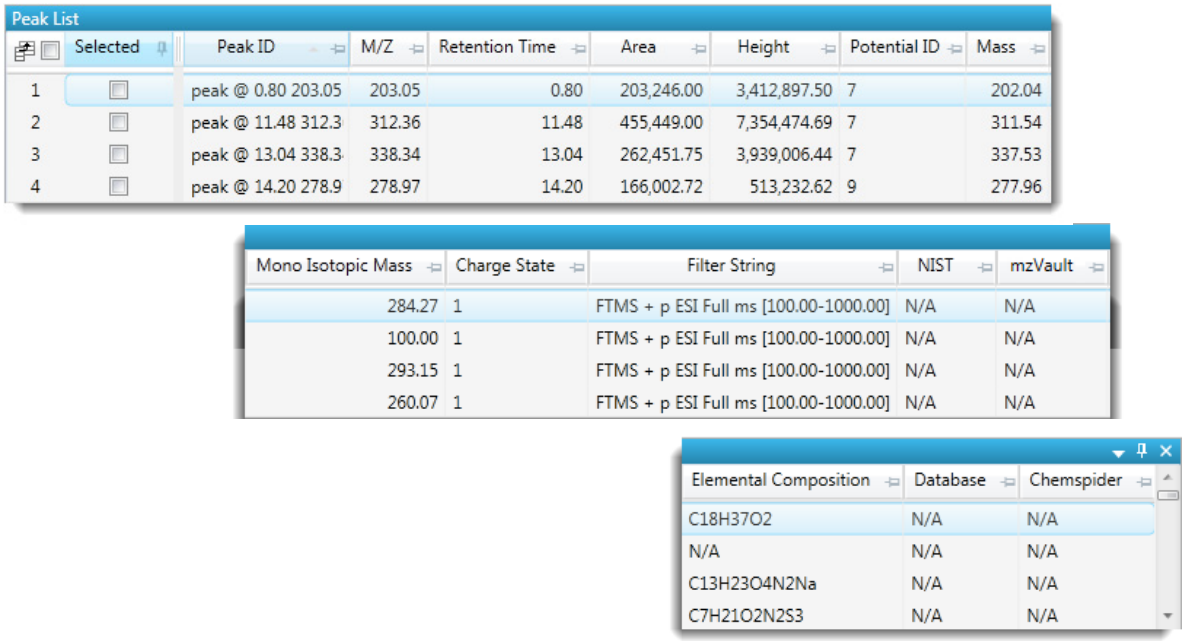
Spectrum Pane

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.



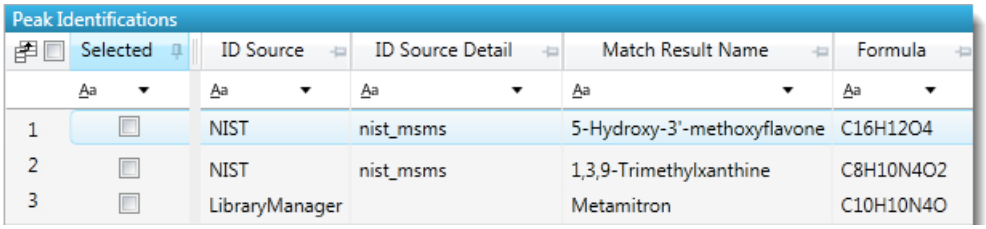
Peak List Pane

Use the Peak List pane to select a specific peak found in the selected sample. The Peak List displays each peak that the application identified in the sample.



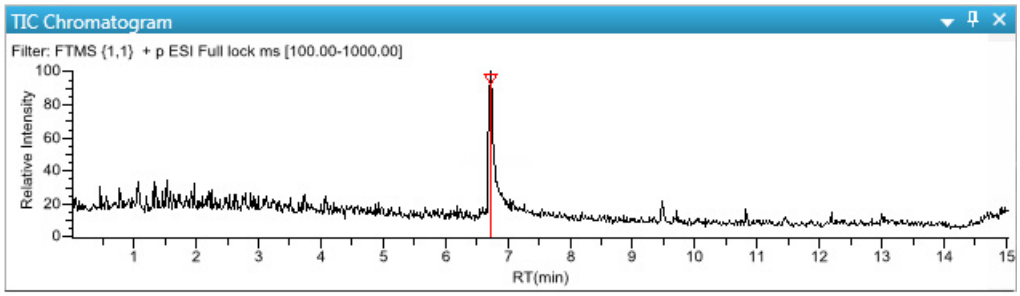
Peak Identifications Pane

Use the Peak Identifications pane to display the name and formula for identified peaks and the source of the identification.



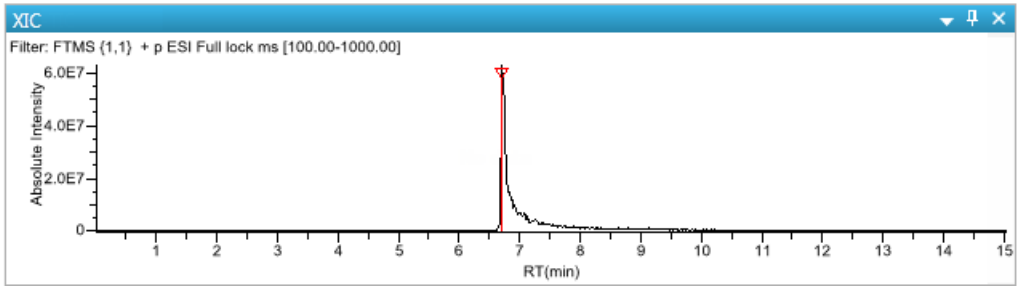
TIC Chromatogram Pane

Use the TIC Chromatogram pane to display the relative intensity of a trace along the length of the sample data retention window.



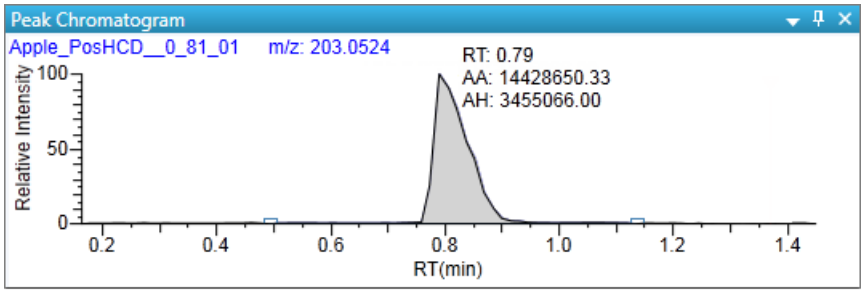
XIC

Use the XIC pane to display the absolute intensity of an extracted trace along the length of the sample data retention window.



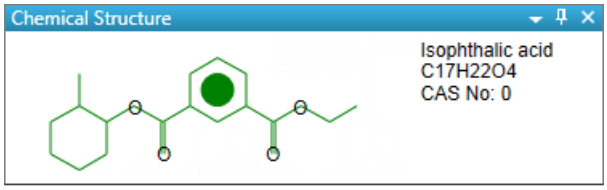
Peak Chromatogram Pane

Use the Peak Chromatogram pane to display the selected chromatogram peak. Initially this Peak Chromatogram pane displays the apex scan for the detected peak. You can manually integrate the peak and use the updated peak to generate reports.



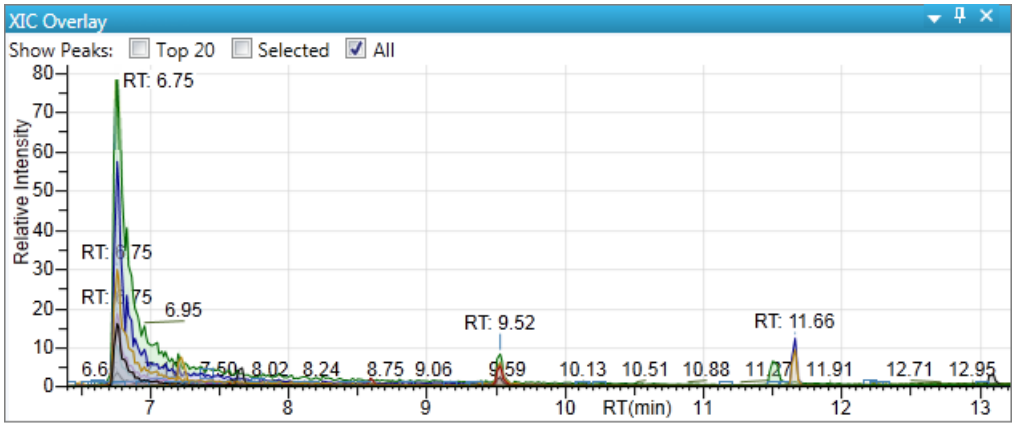
Chemical Structure Pane

Use the Chemical Structure pane to view the chemical formula and structure for the peak that is currently selected in the Peak List pane. The application displays the chemical formula (and CAS number when available) from the search database that you specified in the method.



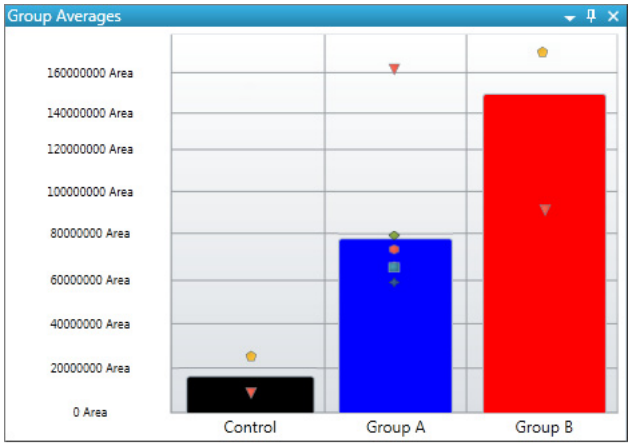
XIC Overlay Pane

Use the XIC Overlay pane to view specific groups of peaks. You can choose to view all peaks, selected peaks only, or the top twenty most intense peaks (by area). The XIC Overlay plot is a collection of overlaid, extracted *m/z* ion plots that use a different color for each peak.



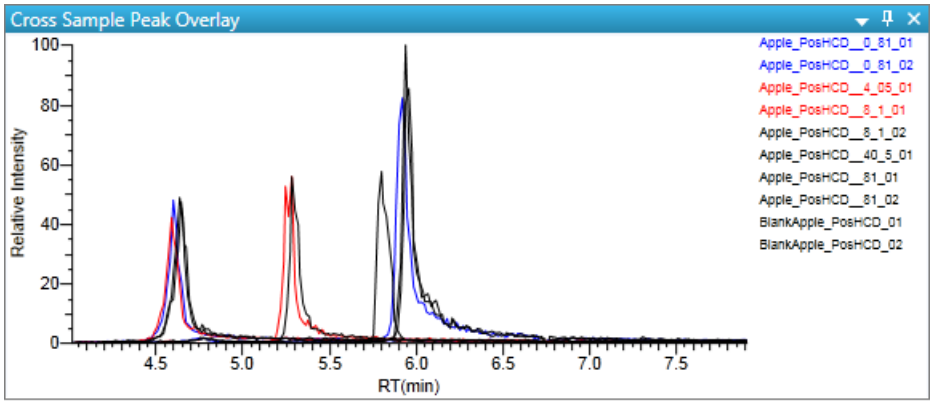
Group Averages Pane

Use the Group Averages pane to compare the peak areas of different samples to a control group of samples.



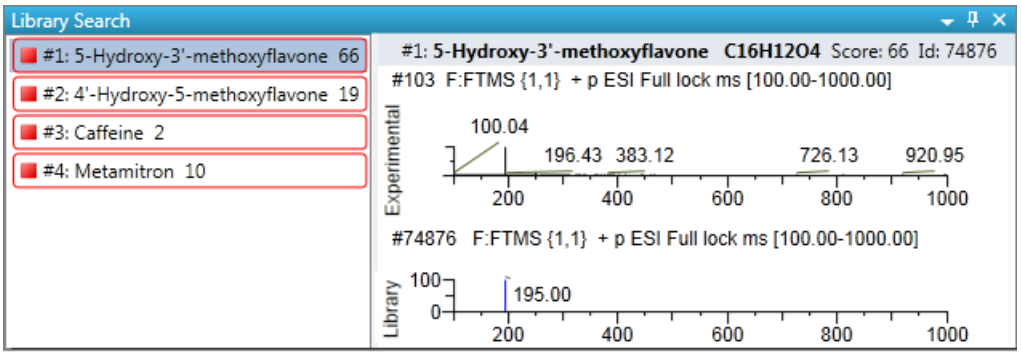
Cross Sample Peak Overlay Pane

Use the Cross Sample Peak Overlay pane to compare instances of a selected peak across all samples in the batch. The application overlays all occurrences of the peak in the batch. The application displays the names of all samples in the batch where the selected peak is found. Samples that are assigned to groups are color coded, and the peaks found in those samples are color coded in the plot.



Library Search Pane

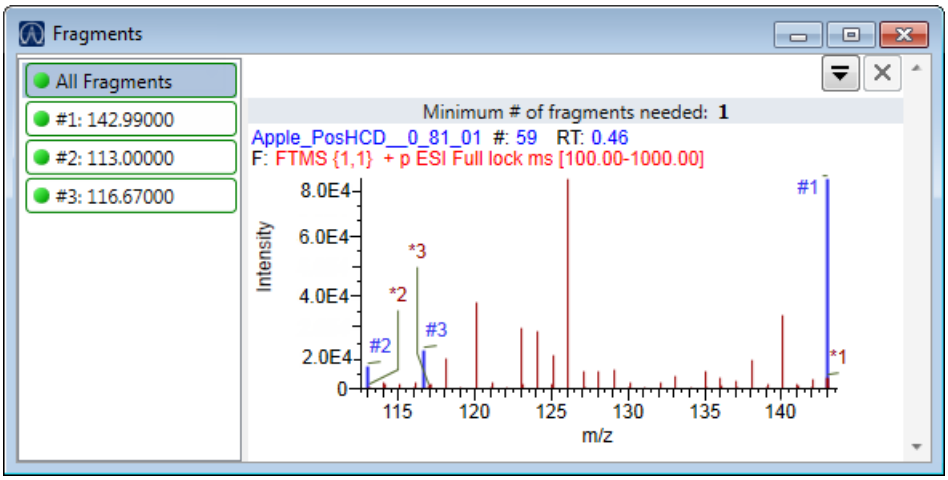
The Library Search pane displays the best library matches for the selected peak, with the highest score listed first.



Fragments Pane

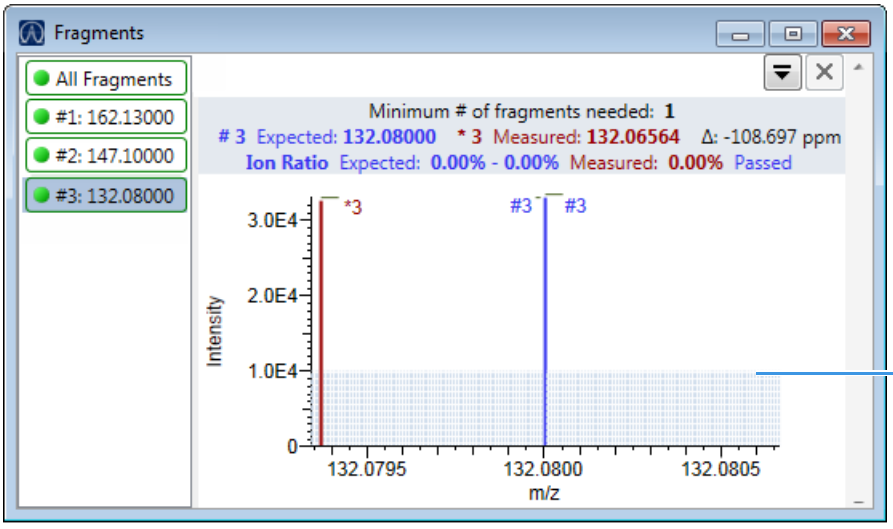
The Fragments pane displays the maximum number of fragments as specified in the unknown screening method. When a compound database search returns a match for a peak that has fragments, the Fragments pane displays the theoretical fragments. When the data has an MS/MS element that is identified as belonging to the chromatographic peak, the Fragments pane displays the fragments found in the MS/MS scan.

Figure 11. All fragments



Expected spectrum in blue Measured spectrum in red

Figure 12. Individual fragment



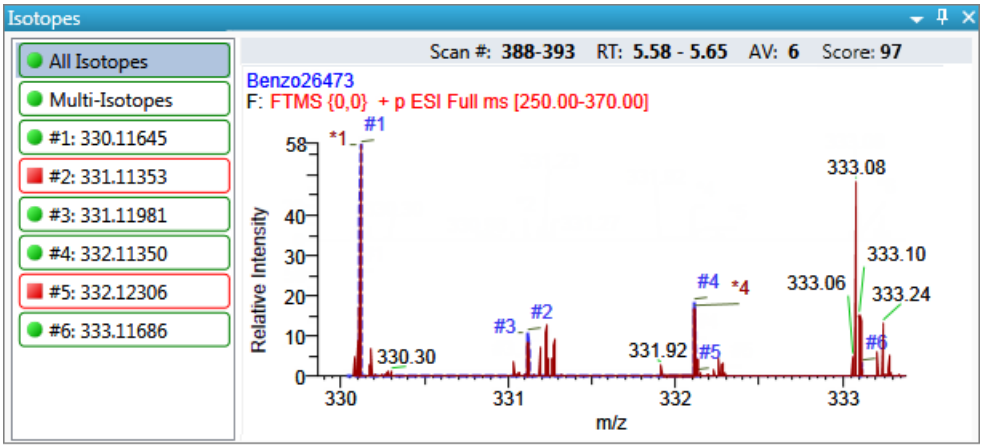
Intensity threshold specified in the method

Expected spectrum in blue Measured spectrum in red

Isotopes Pane

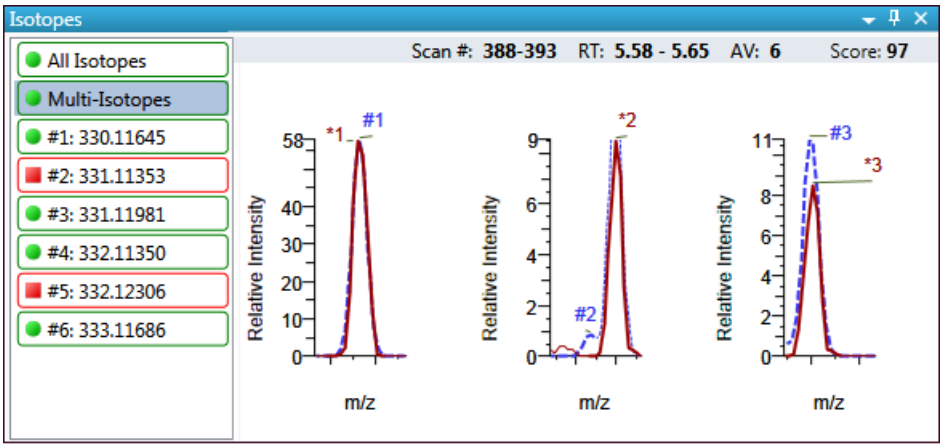
The isotopes pane displays isotopic pattern results for all adducts of a compound according to the threshold and deviation parameters defined in the unknown method. To identify or confirm the presence of a compound, the resulting score percentage from isotopic pattern matching must be higher than the specified fit threshold percentage.

Figure 13. Isotopes pane with overlaid spectra for all isotopes



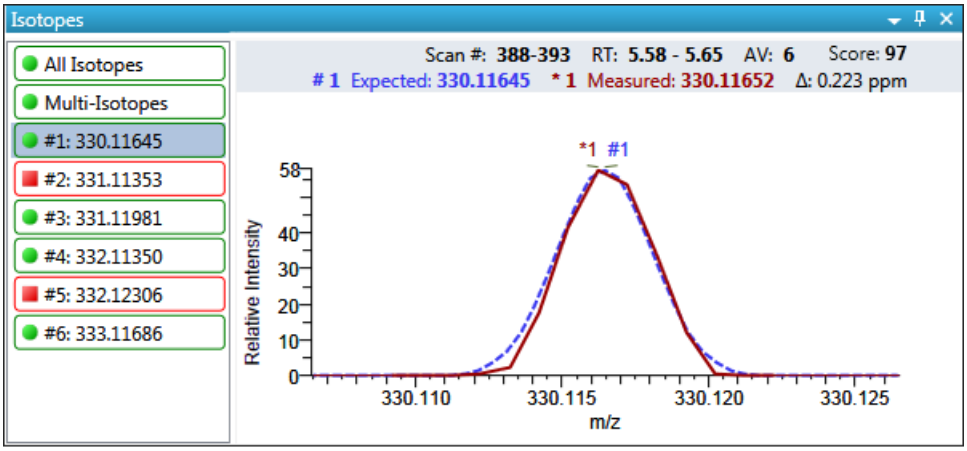
Expected spectrum in blue Measured spectrum in red

Figure 14. Isotopes pane with overlaid spectra for multi-isotopes



Expected spectrum in blue Measured spectrum in red

Figure 15. Isotopes pane with overlaid spectra for a single isotope



Expected spectrum in blue Measured spectrum in red

Report View

The Report View displays example reports for the current batch. You must have an open batch to use the features in the Report View. Follow these procedures:

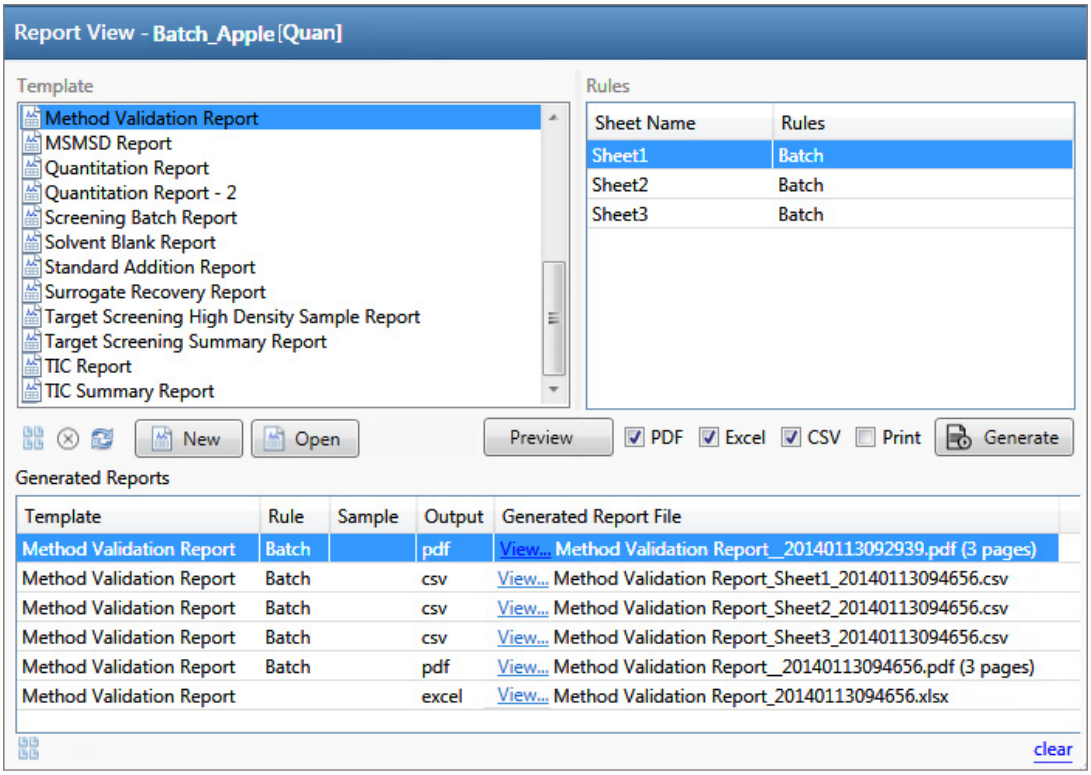
- To open the Report View
- To preview a report
- To generate a report as a PDF, an Excel™, or a CSV file
- To print a report
- To display a generated report
- To edit a report template
- To create a new report template

❖ To open the Report View

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

The application opens the Report View.

Figure 16. Report View

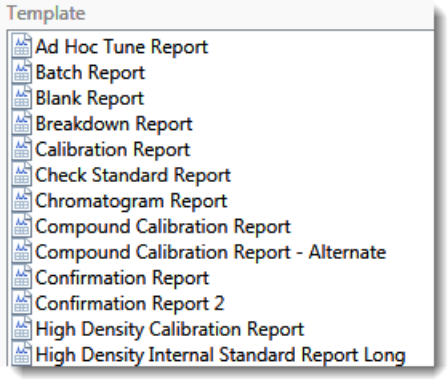


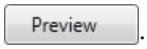
The Open and New buttons open the Report Designer. For details about using the Report Designer, refer to "Working in the Report Designer" in the *TraceFinder User Guide*.

❖ To preview a report

1. In the Template pane, select a report template.

   The template list shows all the report templates that you configured in the Configuration console.



2. Click **Preview**, 

.

   The application opens the Report Designer, showing the report information for the current batch in the selected report template format.

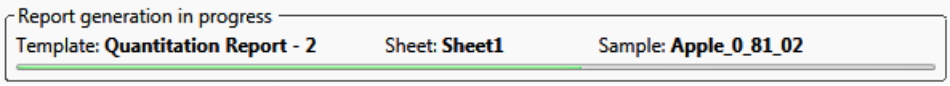
❖ To generate a report as a PDF, an Excel™, or a CSV file

1. In the Template pane, select a report template.
2. Select the check box for each of the file types that you want to create: **PDF**, **Excel**, or **CSV**.
3. Click **Generate**, 

.

   The application does the following:

   - Displays a green progress bar as it generates the reports.



   - Creates a report with the selected report template as a PDF, an Excel, or a CSV file.
   - Adds information about the generated report to the Generated Reports pane.
   - Saves the report files to the …\TraceFinderData\Projects\…*batchname*\ReportOutput folder.

❖ To print a report

1. In the Template pane, select a report template.
2. Select the check box for the **Print** file format.
3. Click 

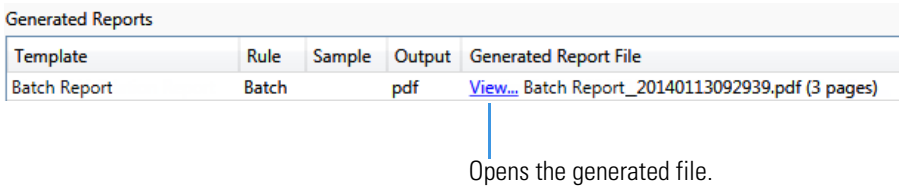
.

   The application does the following:

   - Creates a report for the current batch using the selected report template format.
   - Prints the report to your default printer.
   - Adds information about the generated report to the Generated Reports pane.
   - Saves the report files to the …\TraceFinderData\Projects\…*batchname*\ReportOutput folder.

❖ To display a generated report

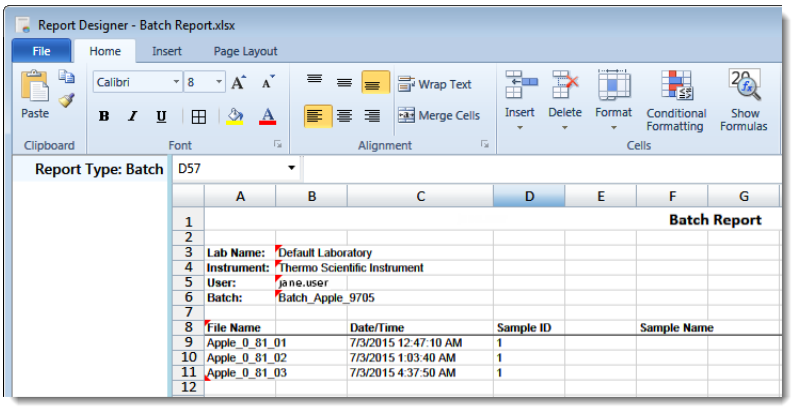
In the Generated Reports pane, click **View** for the report that you want to see.



❖ To edit a report template

1. In the Template pane, select a report template.
2. Click **Open**, Open.

   The application opens the Report Designer showing the template in an Excel spreadsheet.



3. Use the features in the Report Designer to edit the template.

❖ To create a new report template

1. Click New.

   The application opens the Report Designer showing an empty template in an Excel spreadsheet.
2. Use the features in the Report Designer to create the template.

Local Method View

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 Acquisition page of the Local Method View opens. The Acquisition pages are different for quantitation methods, target screening, and unknown screening methods. See Local Method View for a quantitation method, Local Method View for a target screening method, or Local Method View for an unknown screening method.

From the Local Method view, access the method parameters just as you would for a master method.

Local methods are named *BatchName_MasterMethodName*.

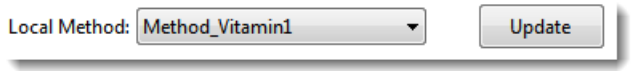
❖ To edit a local method

1. Enter any changes to the local method.

   To edit a method, refer to the method development chapters in the *TraceFinder Lab Director 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.

Figure 17. Local Method View for a quantitation method

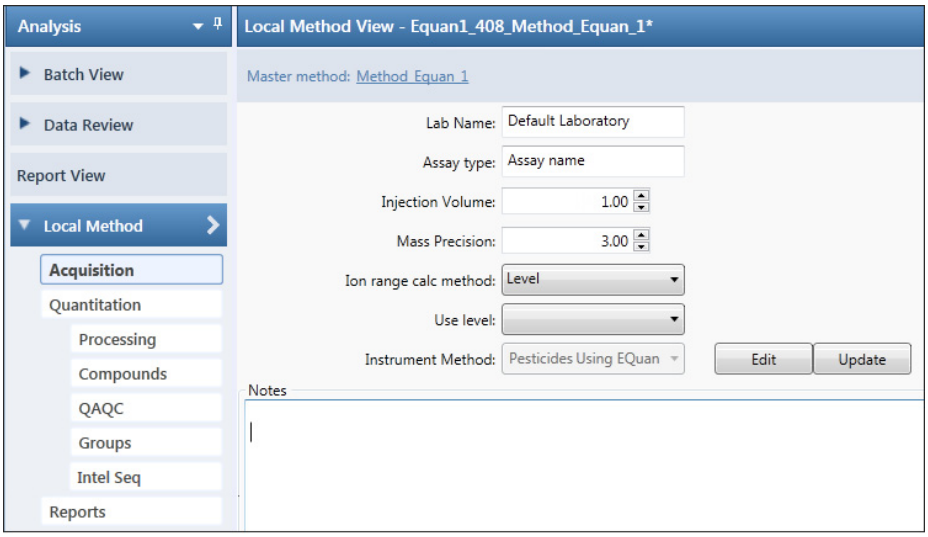


Figure 18. Local Method View for a target screening method

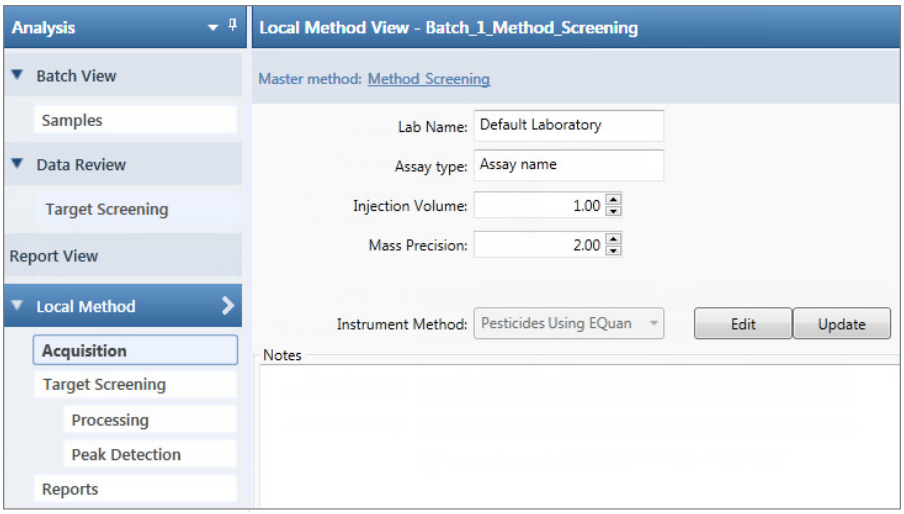
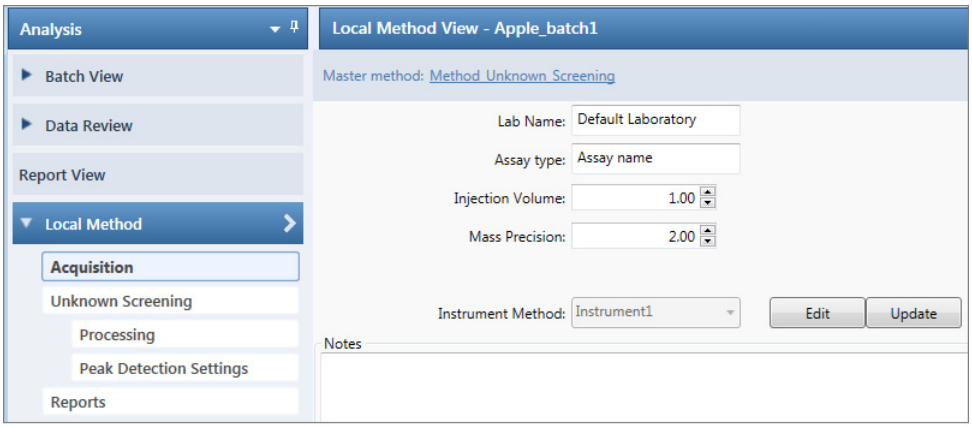


Figure 19. Local Method View for an unknown screening method



Trademarks