

TraceFinder Analysis Quick Reference Guide

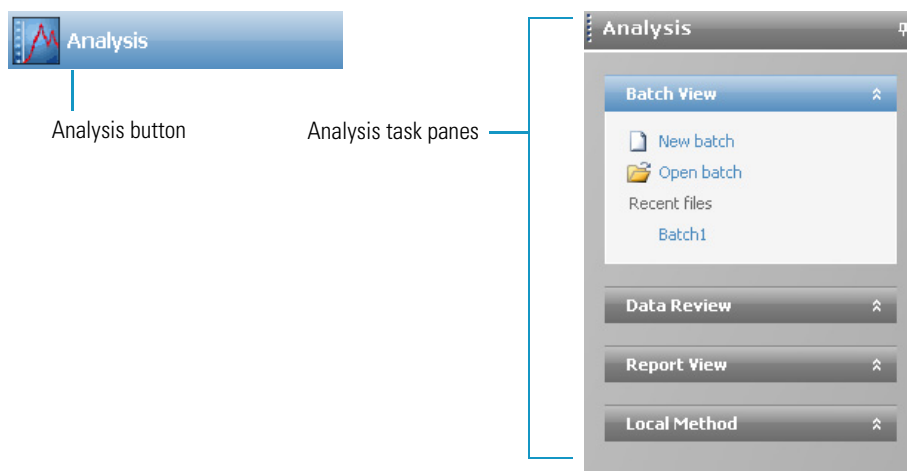
This quick reference describes the Analysis mode tasks assigned to the Technician role in Thermo TraceFinder analytical software.

Contents

- [Batch View](#)
- [Data Review View](#)
- [Report View](#)
- [Local Method View](#)
- [Quick Acquisition](#)

❖ To open the Analysis mode

Click the **Analysis** button on the dashboard or from any mode.



Batch View

In the Batch view of the Analysis mode, you can manually create and edit a new batch or open and edit a previously saved batch. When you submit a batch, you can acquire, process, or create reports for the submitted samples.

- [To open the Batch View](#)
- [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 Batch View

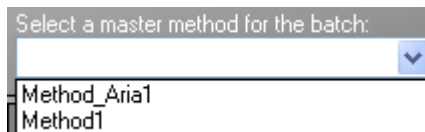
Click **Batch View** in the navigation pane, or select a batch from the Recent Files list in the Batch View task pane.

❖ To create a batch

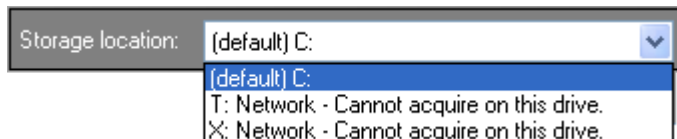
1. Click **New Batch** in the Batch View taskpane, or choose **File > New > Batch**.

The Create a New Batch dialog box opens.

2. Select a master method from the Method list.



3. Select a drive from the Storage Location list.



The Project list displays all projects, subprojects, and batches on the selected drive. The application does not display drives that do not have a project and subproject.

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


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

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

5. Click **Save**.

A new, unnamed batch opens with one Unknown sample.


❖ To add samples to the list

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

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

The application adds the specified number of new, empty samples to the end of the Sample list.

❖ To insert samples into the list

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

The application inserts the Unknown samples above the selected sample.

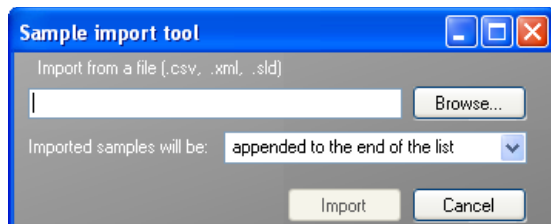
	Status	Filename	Sample type	Level	Sample ID
1		cal_std_5	Cal Std	10	cal std = 5 ng/uL
2		Unknown2	Unknown		
3		Unknown1	Unknown		
4		cal_std_10	Cal Std	10	cal std = 10 ng/uL

Inserted samples

❖ To import samples into the list

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

The Sample Import Tool dialog box opens.



2. Click **Browse** and select a .csv, .xml, or .sld file that contains the sample definitions you want to import.

Note The .csv, .xml, or .sld file format must match the TraceFinder file format.

3. From the Imported Samples Will Be list, select either **Appended to the End of the List** or **Inserted at the Selected Row**.
4. Click **Import**.

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

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

Xcalibur column	TraceFinder column	Xcalibur sample type	TraceFinder sample type
Position	Vial Position	Blank	Matrix Blank
Inj Vol	Injection Volume	Std Bracket	Cal Std
Dil Factor	Conversion Factor	QC	QC Std

❖ To remove samples from the list

1. Select the samples you want to remove.

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

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

❖ To copy a sample

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

The TraceFinder application inserts the copy above the selected sample.

❖ To reinject a sample

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

The TraceFinder application creates a copy of the selected sample and appends INJ001 to the end of 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:
Highlight the current file name and type a new 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

Matrix Blank	Solvent	Unknown
Cal Std	QC Std	Unknown/Qual

3. For each Cal Std or QC Std sample, select a level from the Level list.
The sample levels are defined in the master method. If there are no levels to select from the Level list, do the following:
 - a. Return to the Method Development mode.
 - b. Open the method.
 - c. Click the **Compounds** tab.
 - d. Click the **Calibration Levels** tab.
 - e. Add the levels.
 - f. Save the method.
 - g. Return to the Analysis mode, and then click **Update**.



Local Method:  

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

4. Enter or edit the values for the remaining columns.

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

❖ To submit samples

1. To submit all samples in the batch, do the following:
 - a. Click the **Submit Batch** button, .
 - The Submit Options dialog box opens.
 - b. (Optional) In the Submit Options dialog box, select the **Create Reports** check box.
2. To submit only selected samples, do the following:
 - a. Select the samples you want to submit.
 - b. Click the **Submit Selected Samples** button, .
 - The Submit Options dialog box opens.
 - c. (Optional) In the Submit Options dialog box, select the **Create Reports** check box.

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

3. Click **OK**.

Data Review View

In the Data Review view of the Analysis mode, you can view the data generated by the master method. Use the Data Review view to verify the data for a sample-specific compound before you generate reports. Use the functions in the Data Review view to investigate and edit the quantification values in a batch.

The Data Review view uses a [Samples List](#) and one of two modes: [Quan Mode](#) or [Qual Mode](#). The Qual Mode is available only for Unknown/Qual sample types. When you view the data for an Unknown/Qual sample type, you can switch between Qual Mode and Quan Mode.

❖ To open the Data Review view

Click **Data Review** in the navigation pane, or select a batch from the Recent Files list in the Data Review task pane.

Samples List

The samples list displays all the quantitative data for the samples of a batch. The application displays a list of compounds that are available for a specific method. The Flags column in the samples list displays a caution symbol if there is a problem with the results of the sample.

Method: Method1

	Status	Flags	Filename	Sample type	Level	Sample ID	Compounds
1			cal_std_10	Cal Std	10	cal std = 10 ng/uL	Peak@0.67 + c Full ms2 363.300
2			cal_std_20	Cal Std	20	cal std = 20 ng/uL	Peak@1.39 + c Full ms2 331.300
3			level1	Unknown		level 1 = 5 ng/uL	Peak@1.99 + c Full ms2 303.300 Peak@3.18 + c Full ms2 315.300

Status indicators
 Sample caution flags
 Compound flags

The samples list is the same in both Quan Mode and Qual Mode and displays all the quantitative data for the samples of a batch.

- In [Quan Mode](#), the samples list works with the Compounds pane to select a unique sample and compound combination, which then has its textual and graphical values displayed in the Quan Mode pane. The Compounds pane lists the compounds that are available for a specific method.

From the samples list, you can make a compound active or inactive. Switching a compound to inactive status does not remove its data and calculated values from the result set. Instead, the TraceFinder application masks off the appearance of that compound for that particular sample and grays the compound in the Compounds list. For a calibration standard, the application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. It is no longer part of the result set.

- In [Qual Mode](#), the samples list works with the Peaks pane to select a unique sample and peak combination, which then has its textual and graphical values displayed in the Qual Mode pane.

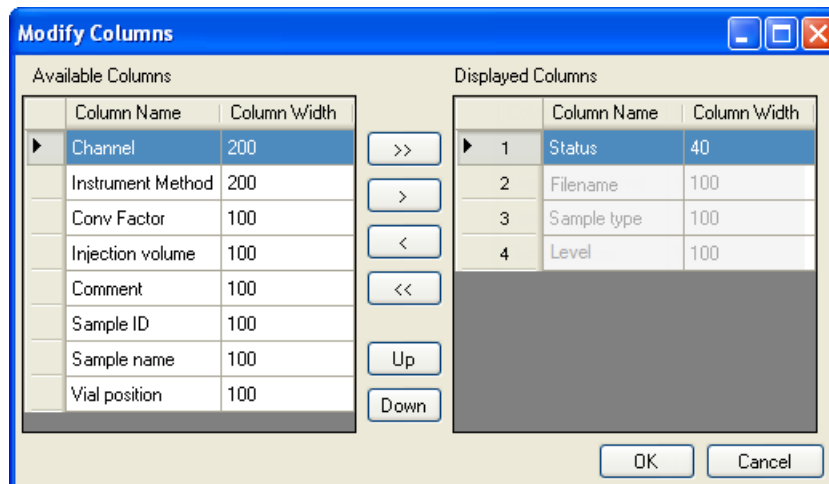
Column Display

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

❖ To customize the column display

1. Right-click the Data Review sample list and choose **Modify Columns** from the shortcut menu.

The Modify Columns dialog box opens.



Parameter	Description
>>	Moves all columns to the Displayed Columns pane.
>	Moves the selected column to the Displayed Columns pane.
<	Moves the selected column to the Available Columns pane. You cannot move the Status, Filename, Sample Type, or Level columns.
<<	Moves all columns except Status, Filename, Sample Type, or Level to the Available Columns pane.
Up	Moves the selected column name in the Displayed Columns pane one row up in the column order. You cannot move the Status, Filename, Sample Type, or Level columns.
Down	Moves the selected column name in the Displayed Columns pane one row down in the column order. You cannot move the Status, Filename, Sample Type, or Level columns.

2. Use the arrow buttons to move all the columns that you want to display to the Displayed Columns pane.

The selected columns display after the Status, Filename, Sample Type, and Level columns.

3. To arrange the order of the columns, do the following:


- a. In the Displayed Columns pane, select a column name.

- b. Use the **Up** and **Down** buttons to move the selected column up or down in the list.

The first column in the list represents the leftmost column in the Batch View sample list. The last column in the list represents the rightmost column in the Batch View sample list.

Note You cannot move the Status, Filename, Sample Type, or Level columns.

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

	Sample ID	100
	Injection volume	100
	Vial position	100





- b. Type a new value for the width.
5. After completing your changes, click **OK**.

The columns in the sample list immediately reflect your changes. The application uses these settings for all sample lists in the Data Review view.

You can use the drag-and-drop method to temporarily reorder the columns in your sample list, but you cannot save this order. When you restart the TraceFinder application, the Data Review view displays your columns in the order specified in the Modify Columns dialog box.

Status Indicators









Status indicators show the current status of each sample during the acquisition and processing:

-  Sample is not acquired.
-  Sample is acquired but not processed.
-  Sample is acquired and processed.
-  Sample is currently acquiring.

Caution Flags

Sample flags indicate when compounds within the samples contain an error.

- Sample flags remain static when you switch between compounds for chromatogram review until the completion of a change, for example, when a compound is manually integrated and no longer falls outside the accepted criteria.
- Click the caution flag to list a summary of all compound indicator messages within the sample.

	Status	Flags	Filename	Sample type	Level	Sample ID	Vial position
1							
2							
3							
4							

cal_10 Flag Details




15-acetyldeoxynivalenol*
Rsquared 0 < R2Threshold 0.99

15-acetyldeoxynivalenol+NH4*
Rsquared 0 < R2Threshold 0.99

17beta-estradiol_neg*
Rsquared 0 < R2Threshold 0.99

1-Naphthylacetic_acid_neg*

Compound Flags

Compounds	
	1,2-Benzenedicarboxylic acid, 4-methyl-
	2-Propyn-1-amine, N-methyl-
	9,10-Anthracenedione

Hold your cursor over a flag to display a Tooltip with the specific problems with the compound.

The TraceFinder application displays compound flags in these situations:

- When a compound has violated (or is activated by) any of the values set in the method
- When compounds are not found
- When compounds are not found in the Cal Std or QC Std sample types
- When compounds are outside the specified ion ratio range

These criteria do not apply to Matrix Blank sample types when the compound is an internal standard.

The TraceFinder application sorts the compounds list first by flag indicators and then by compound names. Compound flags indicate the following:

- Red flags for compounds that have ion ratio failures or method validation failures
- Orange flags for compounds that are below the LOQ, below the LOD, or between the LOD and LOQ values specified in the method
- Green flags for compounds that are over the LOR amount specified in the method
- Yellow flags for compounds that are below the LOR amount specified in the method
- No flag for compounds that have no errors or compounds that have no report options selected.

Inactive and Excluded Compounds

Use the Active and Excluded columns to control which compounds are used for calculating the calibration curve and for reporting.

❖ To make a sample active or inactive

1. Select the sample in the samples list.

The Compounds pane displays all compounds in the selected sample. The default status of a specific compound in a batch is determined by the Compounds Active Status pane in the Batch View for the batch. Inactive compounds are dimmed.

2. In the Compounds pane, select the compound whose active/inactive status you want to change.
3. In the samples list, select or clear the **Active** check box.

Use the horizontal scroll bar at the bottom of the table to scroll to the Active column.

❖ To exclude a calibration point

In the samples list, select the **Excluded** check box for the sample.

Use the horizontal scroll bar at the bottom of the table to scroll to the Excluded column.

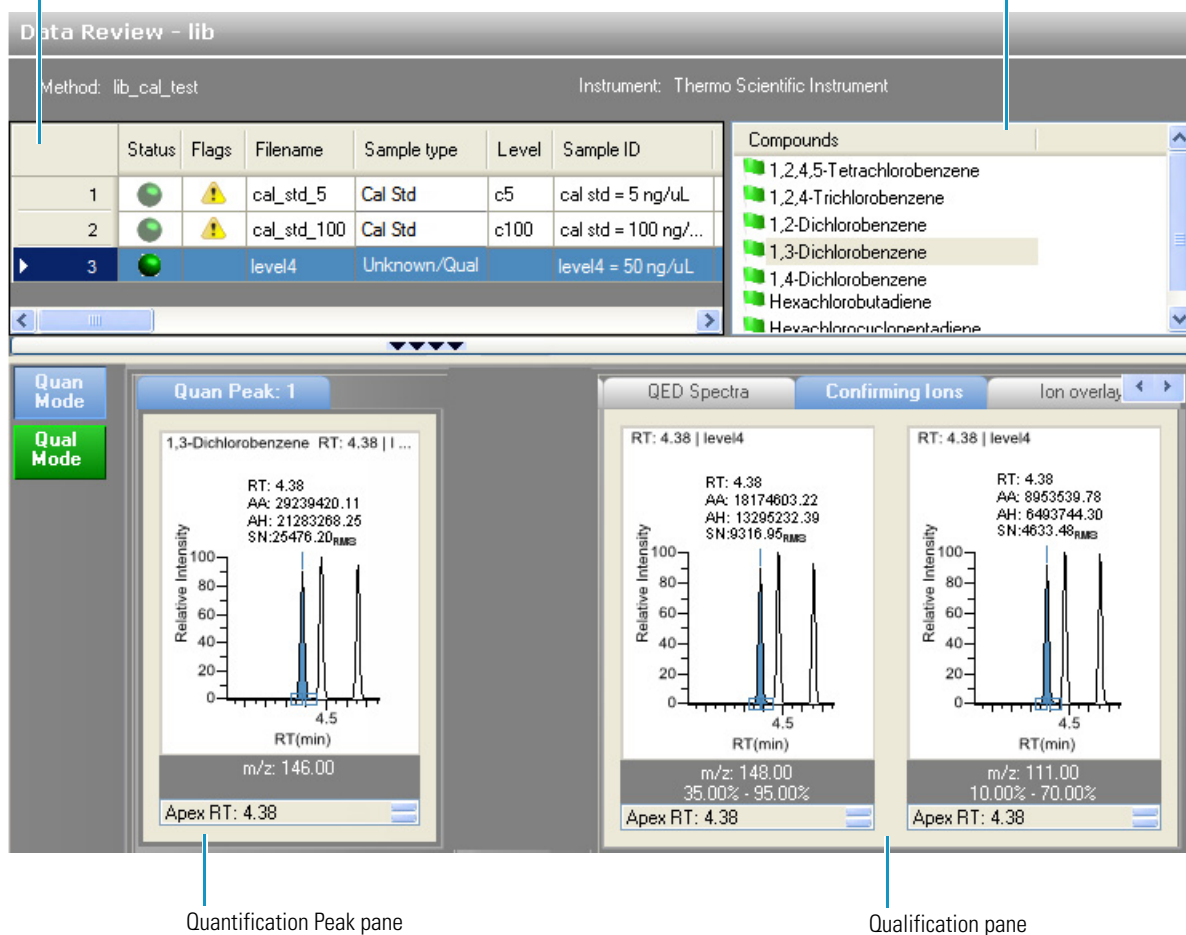
When a value is no longer used for calibration, it is displayed as an empty box in the graphical view of the calibration curve.

Quan Mode

Use the Quan Mode and the associated Compounds pane to view quantitative information to complement the textual information for the selected sample. The Quan Mode displays quantitative peak and confirming ion information for selected compounds that are found in the processed samples.

Samples list

Compounds pane



In addition to the [Samples List](#), the Quan Mode view uses a [Compounds](#) pane, a [Quantification Peak](#) pane, and a [Qualification](#) pane.

Compounds

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

❖ To display peaks for a specific compound

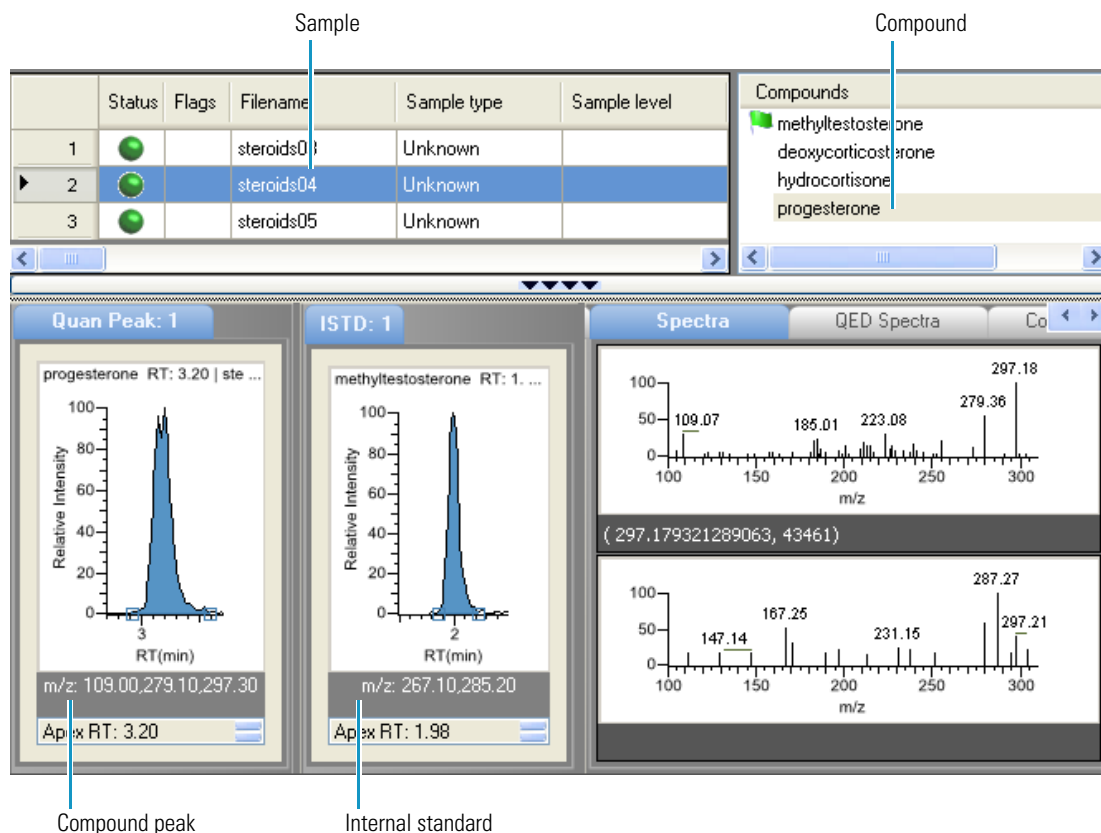
1. In the samples list, select the sample.

The Compounds pane lists all compounds specified in the method.

2. In the Compounds pane, select the compound in the sample.

The Quantification Peak pane displays the peaks for the selected compound and its internal standard.

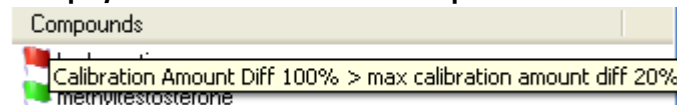
Figure 1. Peak information for progesterone



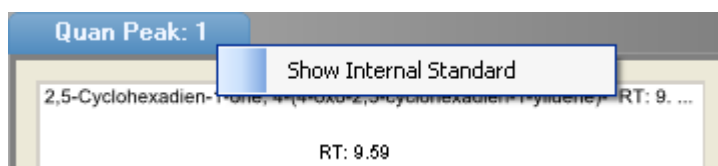
❖ To display specific problems with a compound

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

❖ To display the internal standard for a compound



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



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

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

Quantification Peak

The Quantification Peak pane displays the compound selected in the Quantitative Data and Compounds panes. You can store two peak value sets (method and manual integration settings) with each compound in each file. These settings can result in a different set of stored values. The method values were originally calculated according to the processing method parameters. The manual values are a result of what you have viewed or altered.

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

❖ To manually integrate a quantification or qualification ion

1. Hold your cursor over one of the two peak delimiter tags in the Quantification Peak pane.

If the tag can be selected, the cursor changes to a crosshair style cursor. You can zoom in on the baseline to make it easier to select the tag.

2. Drag the tag to another location to place the peak delimiter tag and automatically update the peak values (area, height, and so forth) into the result set.

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

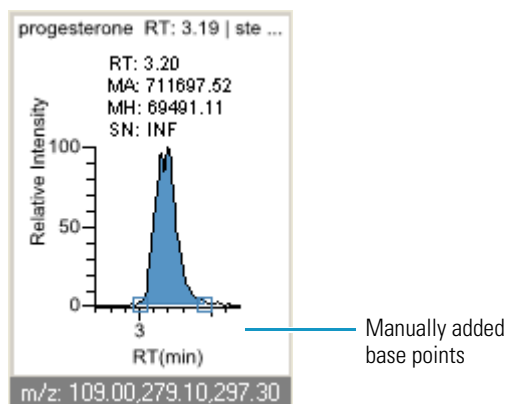
❖ To manually add a peak

1. Right-click anywhere in the Quantification Peak pane and choose **Add Peak** from the shortcut menu.

If a peak is already detected, the Add Peak command is not enabled.

2. Click to indicate the left and right base points for the peak.

The application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



❖ To remove a manually created peak

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

The application removes the manually added peak.

❖ To switch between method and manual integration modes

Right-click the chromatogram view and choose **Method Integration Settings** or **Manual Integration Settings** from the shortcut menu.

Initially, the method and manual integration settings stored for a compound and file are identical and when you select one mode it does not affect the saved result set. However, when manual data are available, the chromatogram plots and the result set update as you switch between method and manual modes.

As you switch between modes, each pane reflects the changes. The generated reports for these data identify the manual modifications.

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

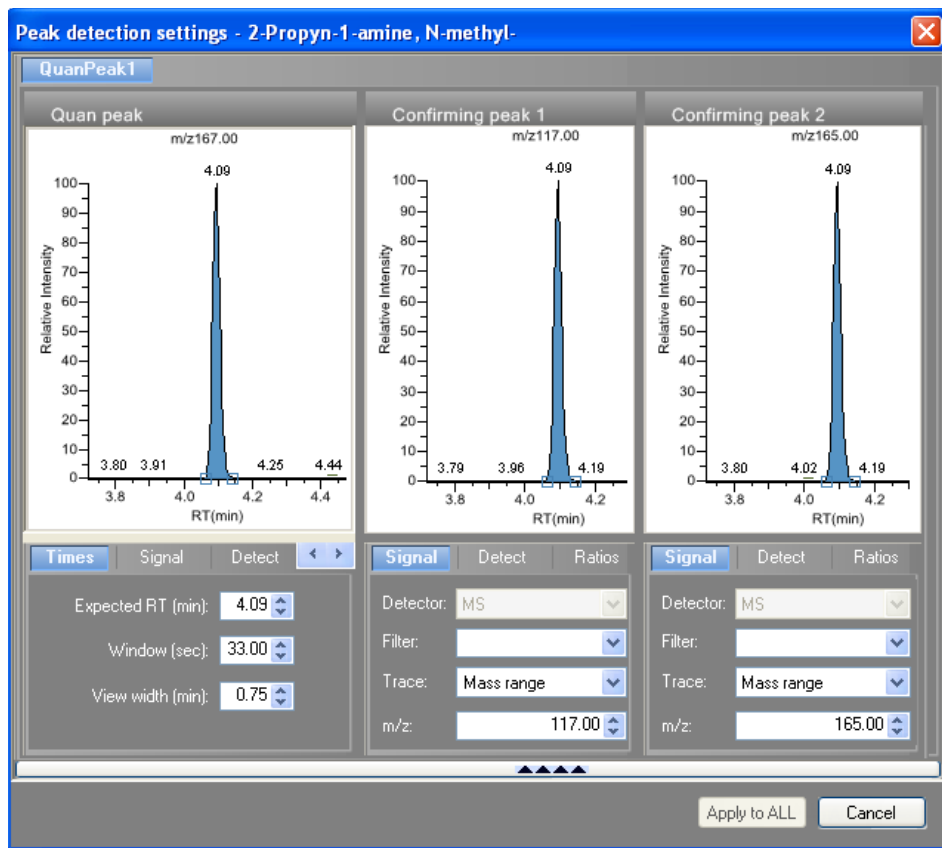
1. Right-click the quantification chromatogram plot and hold the cursor over **Peak Labels**.
2. Choose to display labels for the peak retention time, peak height, peak area, or signal-to-noise ratio.
The label types in the list are selected for the displayed labels and cleared for the labels that are not displayed.
3. To remove a label, select the label type again and clear it.

Label settings are globally applied to quan peaks, confirming peaks, and internal standard peaks.

Tip The labels do not always update on all peak displays. To update all labels, select a different compound, and then select the compound whose labels you changed.

❖ **To modify the peak detection settings**

1. Right-click the chromatogram view and choose **Peak Detection Settings** from the shortcut menu.
The Peak detection setting dialog box opens. This dialog box contains the detection settings defined in the method.



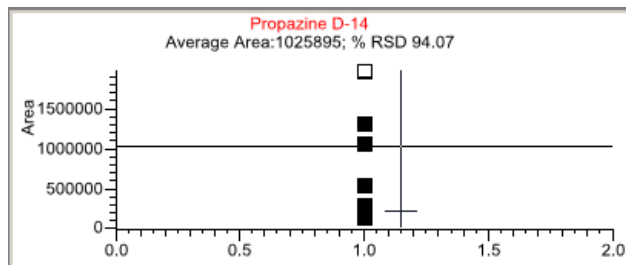
2. Edit any of the detection settings.
For detailed descriptions of all detection settings, refer to the “Using the Analysis Mode” chapter in the *TraceFinder User Guide*.
3. To save your changes to this compound in all samples in this batch, click **Apply to ALL**.

Qualification

The Qualification pane displays the compound selected in the Quantification Peak and Compounds panes and has five pages: [Calibration Curve](#), [Spectra](#), [QED Spectra](#), [Confirming Ions](#), and [Ion Overlay](#).

- Calibration Curve

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



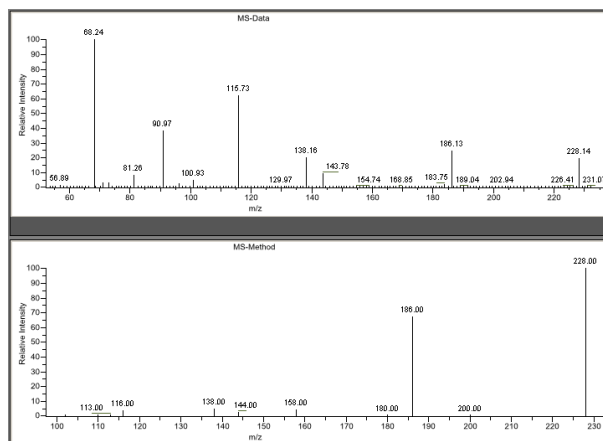
- Spectra

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



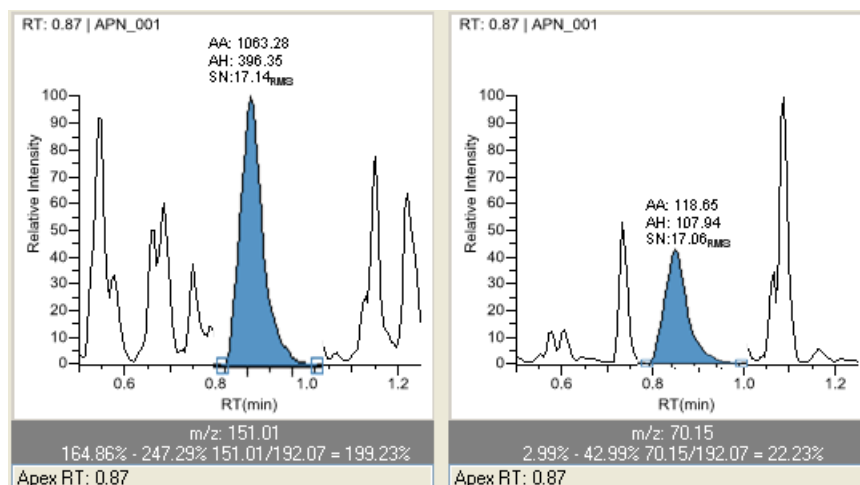
- QED Spectra

The QED Spectra page displays the averaged QED spectra from the raw file and the data-store match. If the sample contains no QED data, the page is blank.



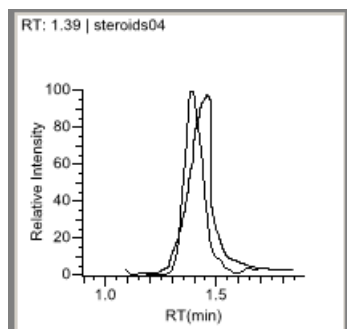
- Confirming Ions

The Confirming Ions page displays a graphical view of all qualifying or confirming ions for the selected sample and compound and displays the calculated ion ratios and ion ratio acceptance windows.



- Ion Overlay

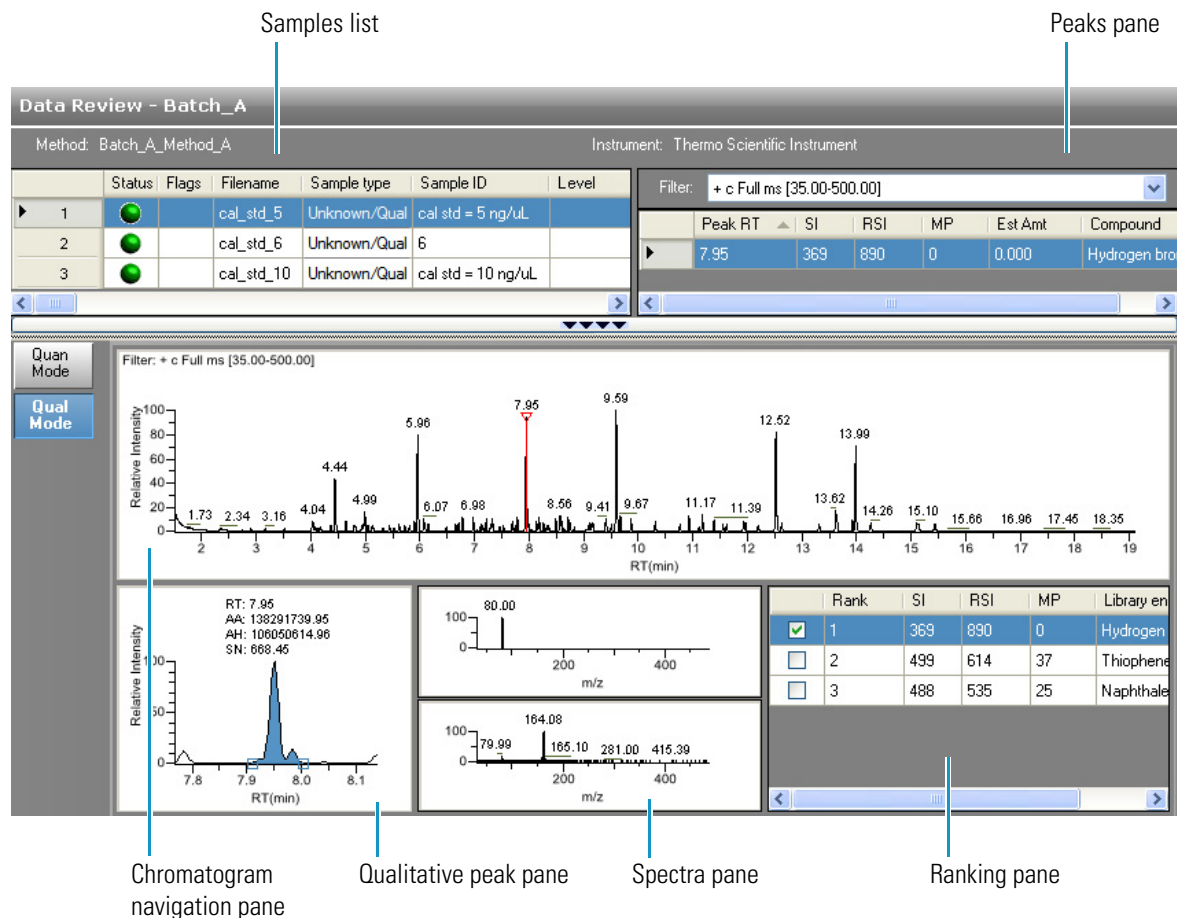
The Ion Overlay page displays an overlay of the entire ion set—quantification and qualifying or confirming—for the selected sample and compound. Use this page to graphically review the peak apex alignment and co-eluting peak profiles.



Qual Mode

Use the Qual Mode and the associated peaks pane to view qualitative information that complements the textual information for the selected Unknown/Qual sample. The Qual Mode view displays the detected peaks for the selected sample and lets you manually add peaks. The Qual Mode view is available only for Unknown/Qual sample types.

In addition to the [Samples List](#), the Qual Mode view displays data in the [Peaks pane](#), [Chromatogram Navigation Pane](#), [Qualitative Peak Pane](#), [Spectra Pane \(Reference and Selected\)](#), and [Ranking Pane](#).



Tip To resize the panes, drag the separators that divide the panes.

Peaks Pane

The peaks pane works with the samples list to display graphical values for a unique sample and peak combination.

Filter: + c Full ms [35.00-500.00]					
	Peak RT (min)	SI	RSI	MP	Library entry
	8.00	937	937	80	Acenaphthene
▶	8.84	259	549	0	Naphthalene, 1-methyl-

❖ To display peaks for a specific compound

1. In the samples list, select a sample.

Note If you choose a sample other than an Unknown/Qual sample, the TraceFinder application returns to Quan Mode. The peaks pane is not displayed in Quan Mode.

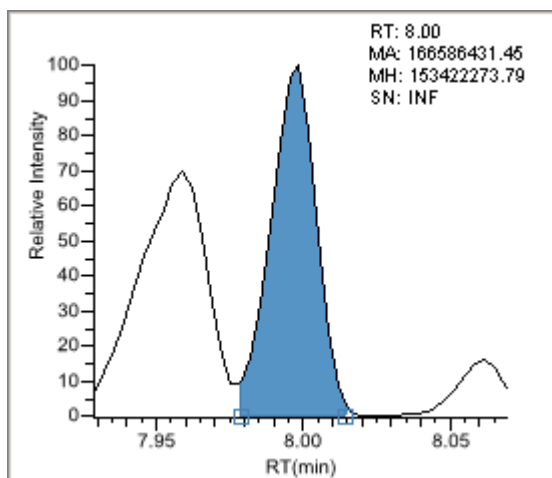
The peaks pane lists the retention time for peaks identified in the selected sample, the values for the best match methods for each peak, and the compound match.

The number of listed peaks is specified in the method. You can change the number of identified peaks in the Method Template Editor.

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

	Peak RT (min)	SI	RSI	MP	Library entry
	5.01	844	847	33	o-Toluidine
	5.46	892	894	98	2-Cyclohexen-1-one, 3,5,5-trimethyl-
▶	8.00	937	937	80	Acenaphthene
	8.84	259	549	0	Naphthalene, 1-methyl-
	10.94	942	943	53	Fluoranthene

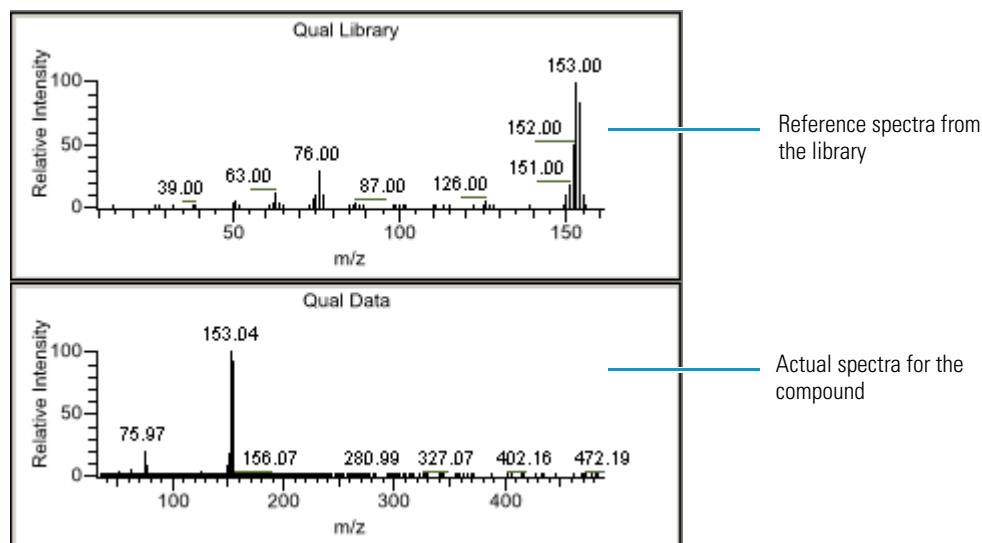
The TraceFinder application displays the selected peak in the qualitative peak pane.



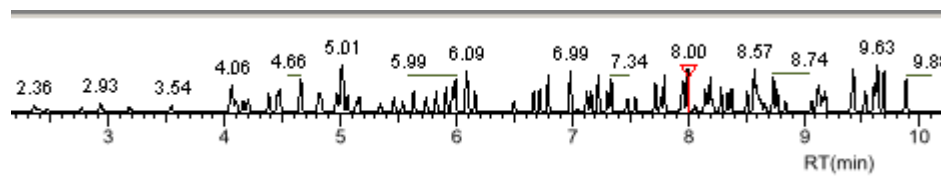
When you select a data-dependent sample, the peak can be from either a full scan or a QED spectrum of an SRM-filtered chromatogram.

The TraceFinder application displays the Spectra pane with two sections:

- The Qual Data pane that shows spectra data for the peak in the raw data file
- The Qual Library pane that shows actual spectra for the identified library compound



The TraceFinder application locates the selected peak in the navigation chromatogram.



❖ To remove a peak

1. Select a peak in the peaks pane.
2. Right-click and choose **Remove Selected Peak** from the shortcut menu.

The TraceFinder application removes the selected peak from the peaks list.

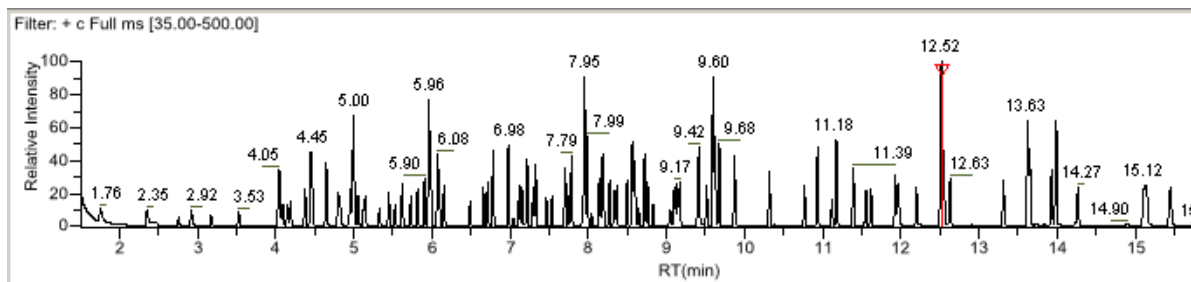
Note There is no undo for this action, but you can manually add a peak to redefine a removed peak. See [“To manually add a peak” on page 11](#).

Table 1. Peaks pane parameters

Command	Description
Filter	Filter used to identify the peaks. Specified in the raw data file or the master method. When your raw data file is data-dependent, the filter indicates this with a “d”: <div style="border: 1px solid black; padding: 2px; display: inline-block;">Filter: + c d Full ms2 179.15@cid35.00 [35.00-370.00] ▼</div> <div style="margin-left: 20px;">Data-dependent filter</div>
Peak RT (min)	Peak retention time. The time after injection when the compound elutes. The total time that the compound is retained on the column.
SI	Search index method used to search the NIST library.
RSI	Reverse search index method used to search the NIST library.
MP	Match probability.
Library entry	Library compound that matches the identified peak.
Remove selected peak	Shortcut menu command that removes the selected peak from the peaks list.

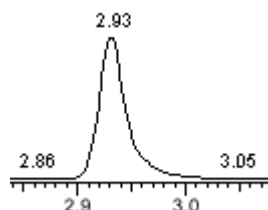
Chromatogram Navigation Pane

The chromatogram navigation pane displays all of the peaks in the selected sample. The application indicates the selected peak in the peaks pane with a red marker.



❖ To manually add a peak

1. Zoom in to make it easier to identify the peak you want to add to the results set.

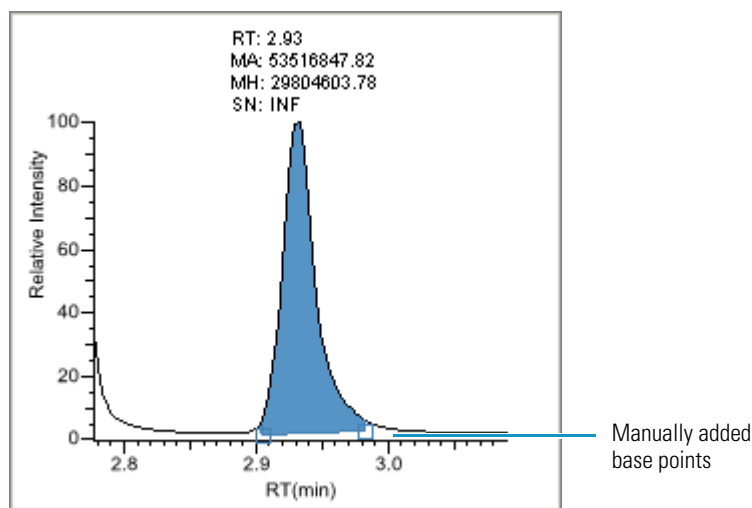


2. Right-click the chromatogram navigation pane and choose **Add Peak** from the shortcut menu.
3. Click to indicate the left and right base points for the peak.

The TraceFinder application marks the peak in the chromatogram navigation pane.

The TraceFinder application places the peak delimiter tags at the base point locations and automatically updates the peak values in the peaks pane and qualitative peak pane.

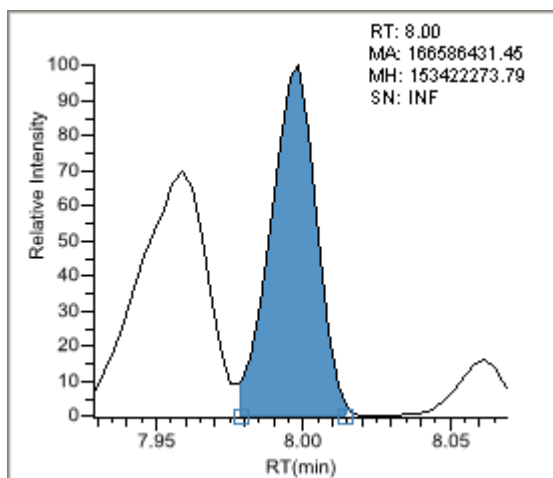
Figure 2. Qualitative peak pane with a manually added peak



	Peak RT (min)	SI	RSI	MP	Library entry
▶	2.93	930	933	94	Phenol, 2-fluoro-
	3.18	834	845	96	Ethanamine, N-ethyl-N-nitroso-
	5.01	800	903	5	Phenol, 3-methyl-

Qualitative Peak Pane

The qualitative peak pane displays the selected peak.



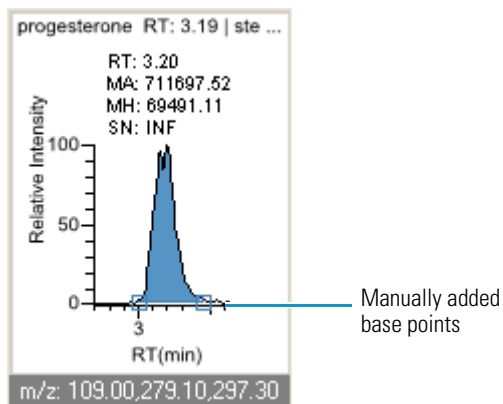
❖ To zoom in on a peak

1. In the chromatogram plot, drag the cursor to delineate a rectangle around the peak.
The delineated area expands to fill the view.
2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

❖ To manually add a peak

1. Right-click anywhere in the qualitative peak pane and choose **Add Peak** from the shortcut menu.
If a peak is already detected, the Add Peak command is not enabled.
2. Click to indicate the left and right base points for the peak.

The TraceFinder application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



❖ To remove a peak

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

The TraceFinder application removes the peak displayed in the qualitative peak pane. It removes all data for this peak from the Qual Mode panes.

❖ To switch between method and manual integration modes

Right-click the chromatogram view and choose **Method Integration** or **Manual Integration** from the shortcut menu.

Initially, the method and manual integration settings stored for a compound and file are identical and selecting one mode does not affect the saved result set. However, when manual data are available, the chromatogram plots and the result set update as you switch between method and manual modes.

As you switch between modes, each pane reflects the changes. The generated reports for these data identify the manual modifications.

❖ To change the displayed information for the detected peaks

1. Right-click the chromatogram plot and hold the cursor over **Peak Labels**.
2. Choose to display labels for the peak retention time, peak height, peak area, or signal-to-noise ratio.

The label types in the list are selected for the displayed labels and cleared for labels that are not displayed.

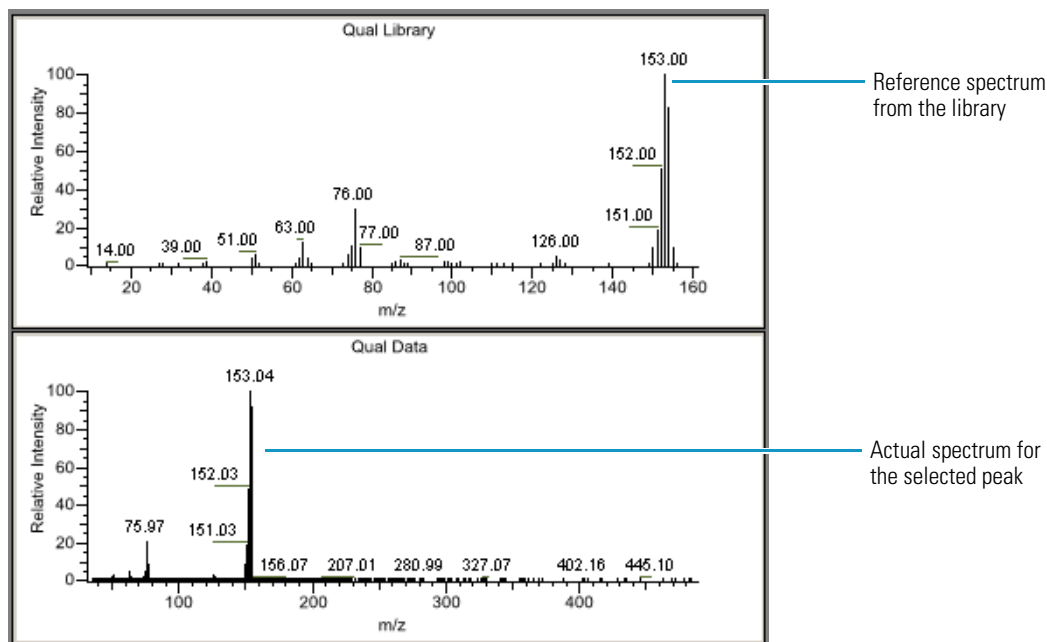
3. To remove a label, select the label type again and clear it.

The TraceFinder application globally applies label settings to qualitative peaks, confirming peaks, and internal standard peaks.

Spectra Pane (Reference and Selected)

Tip The labels do not always update on all peak displays. To update all labels, select a different compound, and then select the compound whose labels you changed.

The spectra pane displays the reference spectra and the spectra for the selected sample. The top pane displays the reference spectra for the identified compound from the library. The bottom pane displays the spectra for the selected peak.



Ranking Pane

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

	Rank	SI	RSI	MP	Library entry
<input checked="" type="checkbox"/>	1	937	937	80	Acenaphthene
<input type="checkbox"/>	2	865	868	11	Biphenyl
<input type="checkbox"/>	3	856	856	8	Naphthalene, 2-ethenyl-

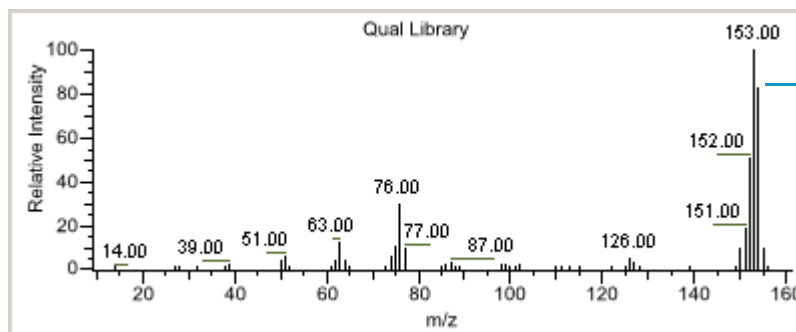
❖ To change the library entry for a selected peak

In the ranking pane, select the check box for the library entry you want to use to identify the selected peak.

- In the spectra pane, the reference spectra change to show the spectrum for the selected library entry.
- In the peaks pane, the SI, RSI, MP, and Library Entry values update to reflect the selected library entry.

	Rank	SI	RSI	MP	Library entry
<input checked="" type="checkbox"/>	1	937	937	80	Acenaphthene
<input type="checkbox"/>	2	865	868	11	Biphenyl
<input type="checkbox"/>	3	856	856	8	Naphthalene, 2-ethenyl-

Selected library entry
in Ranking pane



Reference spectrum
for Acenaphthene

	Peak RT (min)	SI	RSI	MP	Library entry
	5.01	844	847	33	o-Toluidine
	5.46	892	894	98	2-Cyclohexen-1-one, 3,5,5-trimethyl-
▶	8.00	937	937	80	Acenaphthene

Peaks pane for Acenaphthene

Table 2. Ranking pane parameters

Command	Description
<Check box column>	Indicates the selected library entries for the selected peak.
Rank	Indicates the order of best matches between the selected peak and library entries.
SI	Search index method used to search the NIST library.
RSI	Reverse search index method used to search the NIST library.
MP	Match probability.
Library Entry	Library compound that matches the identified peak.

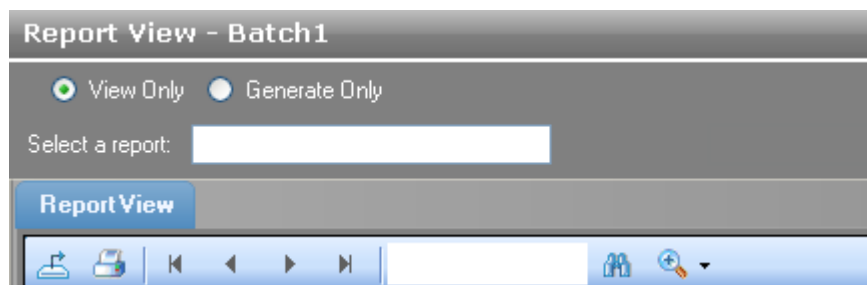
Report View

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”](#) on page 22.

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 25.

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. Click the Select a Report box.

The report list opens, displaying all configured report types.

Report Name	Type	Requires
Alternate BatchReport	Custom	Batch
Alternate ConfirmationReport	Custom	Sample
Batch Report	Standard	Batch
Blank Report	Standard	Sample

Filter Reports

☐ Only show automated batch reports

☒ Standard reports ☒ Custom reports ☒ Target Screening reports

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

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

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

- To limit the types of reports you want to display in the report list, select any combination of options in the Filter Reports area.

Table 3. Filter Reports parameters

Parameter	Description
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.
Target Screening Reports	Displays the Target Screening report types.

- Double-click the name of the report.

The report list closes.

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

Select a report: Sample file:

Follow the procedure “To select a sample” on page 23.

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

Select a report: Compound:

Follow the procedure “To select a compound” on page 24.

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

Select a report: Sample file: Compound:

Follow the procedure “To select a sample and a compound” on page 24.

❖ To select a sample

- Click the Sample File list.

The sample list displays all samples in the batch.

Sample Name	Sample ID	Sample Type
level2	level 2 = 10 ng/uL	Unknown
level3	level 3 = 20 ng/uL	Unknown

Filter Samples
☐ Only show samples relevant to the selected report.

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

For example, if you selected the QC Standard Report, the sample list displays only QC Std 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.


- Double-click the name of the sample.

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

❖ **To select a compound**

1. Click the Compound list.

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

Compound: <input type="text"/> 	
RT	Compound Name
	All Compounds
6.00,6.00,6.00,6.00	Acetamiprid
6.00,6.00	Amitraz
6.00	Atrazine D6
6.00,6.00	Beflubutamid

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. Click the Sample File list.

The sample list displays all samples in the batch.

Sample Name	Sample ID	Sample Type
level2	level 2 = 10 ng/uL	Unknown
level3	level 3 = 20 ng/uL	Unknown

Filter Samples
☐ Only show samples relevant to the selected report.

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

For example, if you selected the QC Standard Report, the sample list displays only QC Std 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. Click the Compound list.

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

Compound: <input type="text"/> 	
RT	Compound Name
	All Compounds
6.00,6.00,6.00,6.00	Acetamiprid
6.00,6.00	Amitraz
6.00	Atrazine D6
6.00,6.00	Beflubutamid

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. Click the Select a Report list.

The report list opens.

Report Name	Type	Requires
Blank Report	Standard	Sample
BlankReport	Custom	Sample
Alternate ConfirmationReport	Custom	Sample
Chromatogram Report	Standard	Sample
Filter Reports		
<input type="checkbox"/> Only show automated batch reports		
<input checked="" type="checkbox"/> Standard reports <input checked="" type="checkbox"/> Custom reports <input checked="" type="checkbox"/> Target Screening reports		

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

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

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

For a description of the Filter Reports options, see [“Filter Reports parameters”](#) on [page 23](#).

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 in the Report View page.
- When the selected report includes separate reports for each sample, you must select a sample file.

Select a report:	<input type="text" value="TIC Summary Report"/>	Sample file:	<input type="text"/>
------------------	-------------------------------------------------	--------------	----------------------

❖ **To select a sample**

1. Click the **Sample File** list.

The sample list displays all samples in the batch.

Select	Sample Name	Sample ID	Sample Type
<input type="checkbox"/>	Unknown1	unknown sample 1	Unknown
<input type="checkbox"/>	cal_std_5	cal std = 5 ng/uL	CalStd
<input type="checkbox"/>	chk_std_50	chk std = 50 ng/uL	ChkStd
<input type="checkbox"/>	matrix_blank	matrix blank	Blank
<input type="checkbox"/>	sample1	unknown sample 1	UnknownTIC

Filter Samples:
☐ Only show samples relevant to the selected report.

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

For example, when you select the QC Standard Report, the sample list displays only QC Std 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 you want to include in the report.
4. Click **Generate**.

The Report Selection Confirmation dialog box opens.

Report Selection Confirmation

You have selected the following report for generation: ConfirmationReport

Sample Name	Sample ID	Sample Type
level1	level 1 = 5 ng/uL	Unknown

What action would you like to perform?

☐ Print to default printer
☒ Generate PDF
☒ Generate XLSM
☐ Generate XML

Cancel
Continue

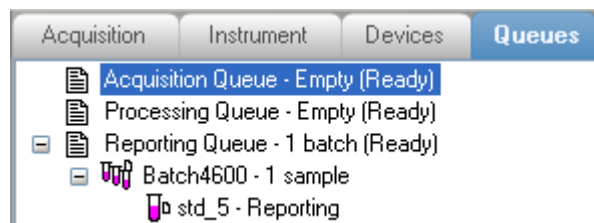
5. In the What Action Would You Like to Perform area, select the types of reports to create.

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 new report is time-stamped 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.

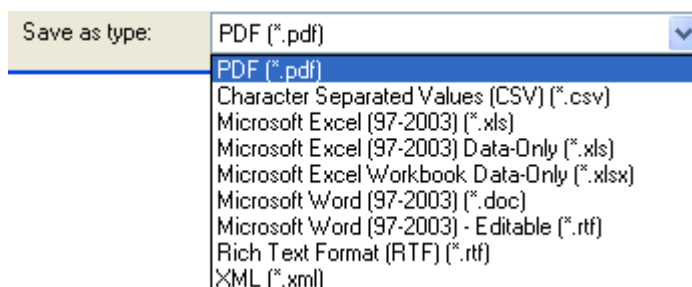
- A PDF file report view is available for all Standard and Target Screening report types.
- An Excel Macro-Enabled Workbook report view is available for any Custom report types generated with the Generate XLSM option selected.

❖ 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** button, .
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 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** button, .
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.


Sample ID

APN001

APN002

APN003

❖ To enlarge the report text

1. Select a report from the Select a Report list.
2. Click the **Zoom** button, , 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.

☒ View Only
 ☐ Generate Only

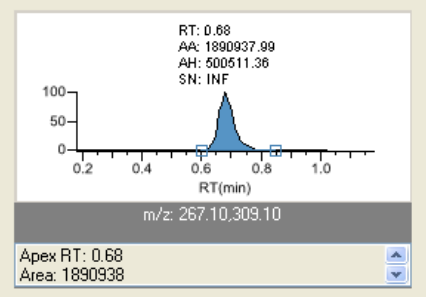
Select a report: **High Density Calibration Report**
 Sample file: **steroids01_110504155226**

Report View **Active View**


Total Rows: 4 Showing: **All Compounds**

	Status	Compound Name	Compound Type	QAQC Flags	Quan Flags	Manual Flags	Quan Peak m/z	Total Response
▶	✓	hydrocortisone	Target Compound				267.10,309.10	1890938
	✓	deoxycorticosterone	Target Compound				109.10,277.30,295.30	1040194
		methylestosterone	Internal Standard	Out of range			267.10,285.20	684395
	✓	progesterone	Target Compound				109.00,279.10,297.30	2995894

Quan Peak: 1



Calibration curve



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.

Select a report: **Blank Report**
 Sample file: **APN_001**

❖ To filter which compounds to display

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

Showing: **All Compounds**
 Showing: **Flagged Compounds Only**

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 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.

Local Method View - BatchA_MethodA

Master method: MethodA

General Compounds QAQC Groups Reports

Lab name:

Assay type:

Injection volume:

Ion range calc method:

Instrument method:

Qualitative peak processing template:

Background subtraction range option:

Number of scans to subtract:

Stepoff value:

Set chromatogram reference sample:

Set Reference sample:

Mass Tolerance: ☒ MMU ☐ PPM

Quick Acquisition

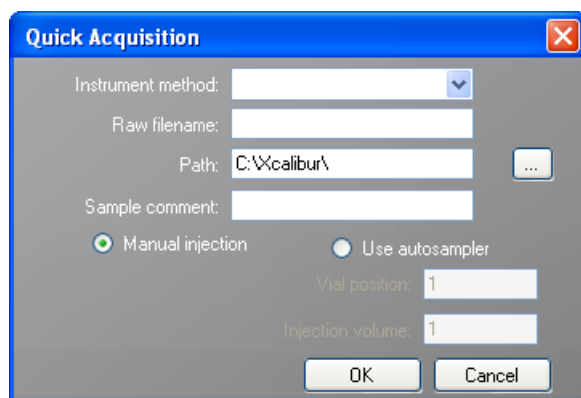
With the quick acquisition feature, you can quickly submit a single sample from any view of the Analysis mode.

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

❖ To run a quick acquisition

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

The Quick Acquisition dialog box opens.



2. Select an instrument method.
3. Type a name for the raw data file that you acquire.
4. Click the browse button and locate a folder where you want to save the acquired raw data file.
5. Select either the manual injection or the autosampler option:

- To perform manual injection, do the following:
 - a. Select the **Manual Injection** option.
 - b. Click **OK**.

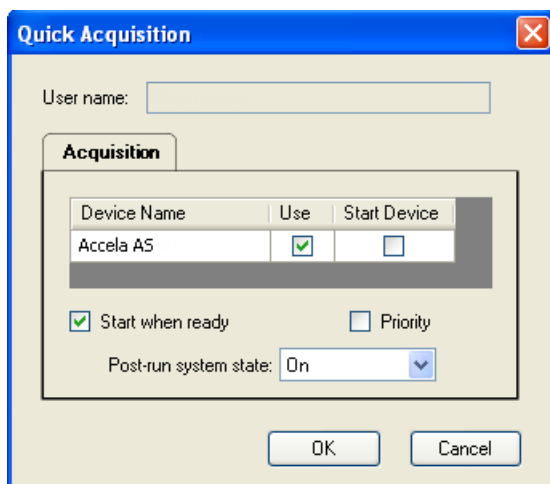
The application submits the sample to the Acquisition queue.

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

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

- d. Click **OK**.

The Quick Acquisition dialog box opens.



Device Name	Use	Start Device
Accela AS	<input checked="" type="checkbox"/>	<input type="checkbox"/>

- e. Select the **Use** check box for the device that you want to use for this acquisition.
- f. (Optional) Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

This is usually the autosampler.

- g. (Optional) Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

When this is cleared, individual instruments can start at different times and then have to wait for the last instrument to be ready.

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

- i. (Optional) Select a value for the Post-run System State: **Unknown**, **On** (default), **Off**, or **Standby**.

The application sets the system to this state after it acquires the last sample.

- j. Click **OK**.

The application submits the sample to the Acquisition queue.