# **TraceFinder Shortcut Menus Quick Reference Guide**

This quick reference guide describes the shortcut menus in the Thermo TraceFinder<sup>™</sup> analytical application.

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- Acquisition Mode
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# Acquisition Mode

The following pages in the Acquisition mode include shortcut menus:

- Sample Definition Page
- Finish Page
- Real Time Status Pane

## Sample Definition Page

By right-clicking anywhere on the Sample Definition page, you can use the shortcut menu commands to create a sample list.

| Samples            |                 | Reference Sample   |
|--------------------|-----------------|--|
| ▶ 1<br>2<br>3<br>4 | Status Filename | Insert copy sample<br>Reinject selected samples<br>Remove selected samples |

 Table 1.
 Sample Definition page shortcut menu commands (Sheet 1 of 2)

| Command                   | Description  |  |
|---------------------------|--|--|
| Add Sample                | Adds an empty row to the sample grid.  |  |
| Insert Sample             | Inserts an empty row to the sample grid above the selected row.  |  |
| Insert Copy Sample        | Copies the currently selected row and inserts a copy above the row.  |  |
| Reinject Selected Samples | Creates a copy of the selected sample or samples and appends INJ001 to the end of<br>the file name. Additional reinjections of the same sample are numbered INJ002,<br>INJ003, and so forth. |  |
| Remove Selected Samples   | Removes the selected samples from the sample grid.   |  |
| Import Samples            | Opens the Sample Import Tool where you can import a sample list from a CSV, an XML, or an SLD file.  |  |



| Command  | Description   |
|--|---|
| Copy Down  | Copies the value in the selected row to all rows below it. This command is available only when you have selected a value that can be copied down.   |
| Fill Down  | Enters sequential values in the column, starting with the value in the selected row and<br>ending with the last row in the column. This command is available only when you<br>have selected a value that can be filled down.  |
| Modify Columns   | Opens the Modify Columns dialog box to choose which columns to display and to change their display order.   |
| Enable/Disable Sample<br>Weight Calculation  | Displays or hides the Sample Volume, Dilution Factor, Sample Weight, Calculation Type, and Final Units columns.   |
| Copy Copies the data in the selected rows or columns to the Clipboard. Use this of to copy sample information to a text editor or spreadsheet application. You paste this data back into the Acquisition mode sample list.   |   |
| Copy with Headers<br>Copies the data in the selected rows or columns and the associated colu<br>the Clipboard. Use this command to copy sample information to a tex<br>spreadsheet application. You cannot paste this data back into the meth-<br>development compound list. |   |
| Paste  | Pastes a column of copied data from a text editor or spreadsheet application into the selected column.  |
| Undo Last Paste  | Removes the last pasted item in the Acquisition mode sample list.   |
| Export to CSV File   | Opens the Save As dialog box to save the batch to a CSV file.   |
| Edit Instrument Method   | <ul> <li>Opens the Instrument Setup window where you can edit the parameters of the instrument method.</li> <li>When you edit an external method, the application updates the method in the\Xcalibur\methods folder.</li> <li>When you edit an internal method, the application updates the method in the\TraceFinderData\3.3\Projects\\batch\Methods\method folder.</li> </ul> |
| View Sample in Qual<br>Explorer  | Opens the current sample in either the FreeStyle™ or Qual Browser application.  |

 Table 1.
 Sample Definition page shortcut menu commands (Sheet 2 of 2)

# **Finish Page**

By right-clicking a device name on the Finish page, you can use the shortcut menu commands to specify a device state for your configured instruments.

| Device On      |
|----------------|
| Device Standby |
| Device Off     |
|                |

Table 2. Finish page shortcut menu commands

| Command             | Description  |
|---------------------|--|
| Turn Device On      | Keeps the system in the On state when the current run finishes, so you can begin another<br>run without waiting. All power and flows are maintained at operational levels.<br>Default: On  |
| Turn Device Standby | Places the system in the Standby state when the current run finishes, so you can begin another run with only a short delay between runs.   |
| Turn Device Off     | Places the system in the Off state when the current run finishes. The Off state indicates that all power to the instrument—that the TraceFinder application can control—is turned off. This includes power to all heaters and subassemblies but, in some cases, not all subassemblies. |

## Real Time Status Pane

By right-clicking the name of a queue, batch, or sample on the Queues page in the Real Time Status pane, you can use the shortcut menu commands to control the Acquisition and Processing queues.



Table 3. Queues page shortcut menu commands

| Command                | Description  |
|------------------------|--|
| Queue-level command    |  |
| Pause Queue            | After the current sample is complete, the application pauses the specified queue.<br>This affects only the selected queue. |
| Stop Active Batch      | Removes all pending samples from the specified queue. This does not affect the active sample.                              |
| Stop All Batches       | Removes all pending samples and batches from the specified queue. This does not affect the active sample.                  |
| Reactivate All Batches | Returns all paused batches to active status.   |
| Remove Pending Batches | Removes all pending batches from the specified queue. The active batch is not affected.                                    |
| Batch-level command    |  |
| Stop Batch             | After the current sample is complete, the application removes all samples in the selected batch.                           |
| Remove Pending Batch   | Removes all samples from the selected pending batch.   |
| Remove Pending Samples | Removes all pending samples from the selected batch.   |
| Sample-level command   |  |
| Remove Sample          | After the current sample is complete, the application removes the selected sample from the batch.                          |

# Analysis Mode

The following views in the Analysis mode include shortcut menus:

- Batch View for All Batch Types
- Sample View for Quantitation Batch Types
- Unknown Screening View for Unknown Batch Types

### Batch View for All Batch Types

The Batch View provides a shortcut menu in the sample list. By right-clicking anywhere in the sample list pane, you can use the shortcut menu commands to add, insert, or remove samples.

|       | Status | Filename             | Sample type  | Groups  |        |
|-------|--------|----------------------|--|---|--------|
| 1 2 3 |        | Unknown3<br>Unknown4 | Add sample<br>Insert sample<br>Insert copy sam<br>Reinject selected<br>Remove selected<br>Import samples.<br>Browse in raw fil<br>Browse in r | d samples<br>d samples<br>d samples<br><br>le (Move)<br>le (Copy)<br>samples<br>samples<br>Weight Calcul<br>Weight Calcul<br>ers<br>e<br>method | lation |

 Table 4.
 Sample list pane shortcut menu commands (Sheet 1 of 2)

| Command                   | Description  |  |
|---------------------------|--|--|
| Add Sample                | Adds an empty row to the sample grid.  |  |
| Insert Sample             | Inserts an empty row to the sample grid above the selected row.  |  |
| Insert Copy Sample        | Copies the currently selected row and inserts a copy above the row.  |  |
| Reinject Selected Samples | Creates a copy of the selected sample or samples and appends INJ001 to the end<br>of the file name. Additional reinjections of the same sample are numbered<br>INJ002, INJ003, and so forth.   |  |
| Remove Selected Samples   | Removes the selected samples from the sample grid.   |  |
| Browse in Raw File (Move) | Opens a dialog box where you can select a raw data file to use for the selected<br>sample row. The application removes the raw data file from the source location.<br>You can also select and browse in multiple raw data files to create multiple<br>samples. |  |
| Browse in Raw File (Copy) | Opens a dialog box where you can select a raw data file to use for the selected sample row. The application copies the raw data file from the source location. You can also select and browse in multiple raw data files to create multiple samples.           |  |
| Map Raw Files to Samples  | Opens a dialog box where you can select raw data files to use for the sample rows.   |  |
| Copy Down                 | Copies the value in the selected row to all rows below it. This command is available only when you have selected a value that can be copied down.  |  |

| Command                                     | Description   |  |
|---|---|--|
| Fill Down                                   | Enters sequential values in the column starting with the value in the selected row<br>and ending with the last row in the column. This command is available only when<br>you have selected a value that can be filled down.   |  |
| Modify Columns                              | Opens the Modify Columns dialog box to choose which columns to display and to change their display order.   |  |
| Enable/Disable Sample<br>Weight Calculation | Displays or hides the Sample Volume, Dilution Factor, Sample Weight,<br>Calculation Type, and Final Units columns.  |  |
| Сору  | Copies the data in the selected rows or columns to the Clipboard. Use this command to copy sample information to a text editor or spreadsheet application. You cannot paste this data back into the Acquisition mode sample list.   |  |
| Copy with Headers                           | Copies the data in the selected rows or columns and the associated column headers<br>to the Clipboard. Use this command to a text editor or spreadsheet application.<br>You cannot paste this data back into the method development compound list.  |  |
| Paste                                       | Pastes a column of copied data from a text editor or spreadsheet application into the selected column.  |  |
| Undo Last Paste                             | Removes the last pasted item in the Batch View.   |  |
| Export to CSV File                          | Opens the Save As dialog box where you can save the current sample list to a CSV file.  |  |
| Edit Instrument Method                      | <ul> <li>Opens the Instrument Setup window where you can edit the parameters of the instrument method.</li> <li>When you edit an external method, the application updates the method in the\Xcalibur\methods folder.</li> <li>When you edit an internal method, the application updates the method in the\TraceFinderData\3.3\Projects\\batch\Methods\method folder.</li> </ul> |  |
| View Sample in Qual<br>Explorer             | Opens the current sample in either the FreeStyle or Qual Browser application.   |  |

 Table 4.
 Sample list pane shortcut menu commands (Sheet 2 of 2)

# Sample View for Quantitation Batch Types

The Sample View page in Data Review for a quantitation batch provides the following shortcut menus:

- Quan Peak Page Menu
- Confirming Ions Page Menu

Quan Peak Page Menu

By right-clicking anywhere on the Quan Peak page, you can use the shortcut menu commands to control the display of the quantitative peaks.



Table 5. Quan Peak page shortcut menu commands

| Command  | Description   |
|--|---|
| Method Integration Settings  | <b>Use Local Method Peak Detection Settings</b> : Applies the local method integration settings to the selected compound.   |
|  | <b>Use User Peak Detection Settings</b> : Applies the user-customized method integration settings to the selected compound.   |
| Manual Integration Settings  | Displays the manual integration settings.   |
| Add Quan Peak<br>–or–<br>Remove Quan Peak<br>–or–<br>Cancel Add Peak | Adds a quantitation peak, removes a peak, or cancels an add peak operation that is in progress.   |
| Confirming Ion List  | Lists confirming ions for all quantitative peaks, including any ions with coelution failure. Not available for analog compounds.  |
| Peak Labels  | Displays or hides the peak labels (Label Area, Label Retention Time,<br>Label Height, or Label Signal to Noise).  |
| Show Peak Info   | Displays peak information for the selected compound.  |
| Reset Scaling  | Resets the original scaling after a zoom operation.   |
| Peak Detection Settings  | Edit Local Method Peak Detection Settings: Makes changes to the selected compound for all samples in this batch.  |
|  | <b>Edit User Defined Peak Detection Settings</b> : Makes changes to the selected compound for only the selected sample. The TraceFinder application saves these changes with the batch and stops applying the local method detection settings to the compound for this sample only. |
| Copy to Clipboard  | Copies the graphic display to the Clipboard.  |

**Confirming Ions Page Menu** 

By right-clicking anywhere on the Confirming Ions page, you can use the shortcut menu commands to control the display of the confirming ion peaks.



 Table 6.
 Confirming lons page shortcut menu commands

| Command  | Description   |  |
|--|---|--|
| Method Integration Settings  | Displays the method integration settings.   |  |
| Manual Integration Settings  | Displays the manual integration settings.   |  |
| Add Quan Peak<br>–or–<br>Remove Quan Peak<br>–or–<br>Cancel Add Peak | Adds a quantitation peak, removes a peak, or cancels an add peak operation in progress.                           |  |
| Range Calc Method  | Selects the method used to calculate the ion ratio range windows: Manual,<br>Average, Weighted Average, or Level. |  |
| Range Calc Level   | Displays the range based on the calibration level.  |  |
| Target Ratio   | Specifies the theoretical ratio of the confirming ion's response to the quantification ion's response.            |  |
| Window Type  | Specifies the Absolute or Relative calculation approach for determining the acceptable ion ratio range.           |  |
| Window   | Specifies the acceptable ion ratio range as a percentage.   |  |
| Peak Labels  | Displays or hides the peak labels (Label Area, Label Retention Time,<br>Label Height, or Label Signal to Noise).  |  |
| Show Peak Info   | Displays peak information for the selected compound.  |  |
| Reset Scaling  | Resets the original scaling after a zoom operation.   |  |
| Peak Detection Settings  | Opens the Peak Detection Settings dialog box for the selected compound.   |  |
| Copy to Clipboard  | Copies the graphic display to the Clipboard.  |  |

Unknown Screening View for Unknown Batch Types

The Unknown Screening View page in Data Review provides a shortcut menu in the Chromatogram Peak pane. By right-clicking anywhere in the Chromatogram Peak pane, you can use the shortcut menu commands to control the display of the peaks and to switch between manual integration and method integration displays.

| Peak Chromatogram  | m  |
|--------------------|--|
| Apple_PosHCD4      | _05_01 m/z: 245.0783   |
| Relative Intensity | <ul> <li>Reset Scaling</li> <li>Copy To Clipboard</li> <li>Swipe Manual Integration</li> <li>Toggle Integration Settings [Manual]</li> <li>Delete Peak</li> <li>Peak Display Settings</li> </ul> |

 Table 7.
 Quan Peak page shortcut menu commands

| Command   | Description  |
|---|--|
| Reset Scaling                                     | Resets the original scaling after a zoom operation.                                |
| Copy to Clipboard                                 | Copies the graphic display to the Clipboard.                                       |
| Swipe Manual Integration                          | Switches to manual integration mode, where you can manually define the peak.       |
|   | Also available from the icon in the upper right corner, 🔼 🗙 .                      |
| Toggle Integration Settings<br>(Manual or Method) | Switches the display between manual and method integration modes.                  |
| Delete Peak                                       | Removes the peak and all data for this peak from the Unknown Screening View panes. |
|   | Also available from the icon in the upper right corner, 🔺 🔀 .                      |
| Peak Display Settings                             | Opens the Peak Settings dialog box to customize the display settings.              |

# Method Development Mode

For quantitation methods only, the following pages in the Master Method view of the Method Development mode provide shortcut menus:

- Compounds Page
  - QAQC Page

#### Compounds Page

The Detection page on the Compounds page in the Master Method view provides several shortcut menus.



#### **Compound List**

By right-clicking anywhere in the compound list pane, you can use the shortcut menu commands to manage, copy, and export compounds. The compound list shortcut menu is available for all compound lists on the following Compounds pages: Identification, Detection, Calibration, Calibration Levels, and QC Check Levels.

|   |   | RT   |   | Compound                      |
|---|---|------|---|-------------------------------|
| • | 1 | 3.14 |   | Copy down                     |
|   | 2 | 3.15 | ~ | Display retention time column |
|   | 3 | 3.67 |   | Delete compound from method   |
|   | 4 | 4.70 |   | Сору                          |
|   |   |      |   | Copy with headers             |
|   |   |      |   | Paste                         |
|   |   |      |   | Export to CSV file            |
|   |   |      |   | Sort by Compound Name         |
|   |   |      |   | Sort by Retention Time        |

**Table 8.** Compound list shortcut menu commands

| ties the value in the selected row to all rows below it. This command is<br>lable only when you have selected a value that can be copied down.<br>plays or hides the RT column in the compound list.<br>noves the selected compound from the current master method.<br>ties the data in the selected rows or columns to the Clipboard. Use this<br>mand to copy compound information to a text editor or spreadsheet<br>lication. You cannot paste this data back into the method development<br>pound list, but you can paste this copied data into other areas of the<br>reFinder application.<br>ties the data in the selected rows or columns and the associated column headers<br>ne Clipboard. Use this command to copy sample information to a text editor<br>preadsheet application. You cannot paste this data back into the method |
|--|
| noves the selected compound from the current master method.<br>ies the data in the selected rows or columns to the Clipboard. Use this<br>mand to copy compound information to a text editor or spreadsheet<br>lication. You cannot paste this data back into the method development<br>pound list, but you can paste this copied data into other areas of the<br>reFinder application.<br>ies the data in the selected rows or columns and the associated column headers<br>ne Clipboard. Use this command to copy sample information to a text editor  |
| ties the data in the selected rows or columns to the Clipboard. Use this<br>mand to copy compound information to a text editor or spreadsheet<br>lication. You cannot paste this data back into the method development<br>pound list, but you can paste this copied data into other areas of the<br>reFinder application.<br>wies the data in the selected rows or columns and the associated column headers<br>are Clipboard. Use this command to copy sample information to a text editor  |
| mand to copy compound information to a text editor or spreadsheet<br>lication. You cannot paste this data back into the method development<br>pound list, but you can paste this copied data into other areas of the<br>reFinder application.<br>wies the data in the selected rows or columns and the associated column headers<br>are Clipboard. Use this command to copy sample information to a text editor  |
| ne Clipboard. Use this command to copy sample information to a text editor   |
| elopment compound list.  |
| es a column of copied data from a text editor or spreadsheet application into<br>selected column. The pasted data must be valid data for the selected column.  |
| noves the last pasted item in the method development compound list.  |
| ens the Save As dialog box where you can save the current compound list to a 7 file.   |
| s the compounds alphabetically from A to Z.  |
| s the compounds from shortest retention time to longest retention time.  |
| s the selected compound to the compound database. When the compound<br>ady exists in the compound database, the TraceFinder application updates the<br>pound database with the current compound information.   |
| lable only in the Identification page shortcut menu.   |
| s all compounds in the current method to the compound database. When any<br>nese compounds already exist in the compound database, the TraceFinder<br>lication updates the compound database with the current compound<br>rmation.   |
|  |
|  |

#### **Headers**

By right-clicking the header bar in the quantitative peak and confirming peak panes, you can use the shortcut menu commands to add, swap, or remove peaks. You can also add a quantitative or confirming peak to the Real Time Status pane when you perform an acquisition in the Acquisition mode or when you acquire a development batch in the Method Development mode.



Table 9. Headers shortcut menu commands

| Command                          | Description  |
|----------------------------------|--|
| Display in Real Time Viewer      | Adds the quantitative peak or confirming peak to the Real Time Status pane.  |
| Remove Quan Peak                 | Removes the selected quantitative peak. If there is only one quantitative peak, a message warns that you are removing the entire compound. |
| Swap with Quan Peak              | Replaces the quantitative peak with the confirming ion peak.   |
| Promote to Separate<br>Quan Peak | Sets the confirming peak as an additional quantitative peak.   |
| Cut Confirming Peak              | Removes the selected confirming peak.  |
| Paste Confirming Peak            | Pastes a previously cut confirming peak.   |

#### **Times Page**

By right-clicking anywhere on the Times page, you can use the shortcut menu commands to copy window settings for the selected peak to all peaks in the compound or to all peaks in the method.

| Times Signal Det | tect Suitability 🖾 🕐                               |
|------------------|--|
| Detection type   | Set peak windows settings to all peaks in compound |
| Expected R       | Set peak windows settings to all peaks in method   |

Table 10. Times page shortcut menu commands

| Command   | Description  |  |
|---|--|--|
| Set Peak Windows Settings<br>to All Peaks in Compound | Applies the View Width and Window values to all peaks for the compound and updates the compound. |  |
|   | Available only when a compound has multiple quantitative peaks.                                  |  |
| Set Peak Windows Settings<br>to All Peaks in Method   | Applies the View Width and Window values to all peaks for the method and updates the method.     |  |

## Signal Page

By right-clicking anywhere on the Signal page, you can use the shortcut menu commands to copy filter options for the selected peak to all peaks in the compound or to all peaks in the method.



#### Table 11. Signal page shortcut menu commands

| Command   | Description   |
|---|---|
| Set Filter Options on All<br>Peaks in This Compound | Applies the filter settings for the selected peak to all other peaks in the compound.         |
| Set Filter Options on All<br>Compounds              | Applies the filter settings for the selected peak to all other peaks in the method.           |
| Set Quan Peak Filter Options<br>on All Compounds    | Applies the quan peak filter settings for the selected peak to all other peaks in the method. |

#### **Detect Page**

By right-clicking anywhere on the Detect page, you can use the shortcut menu commands to copy detect settings for the selected peak to all peaks in the compound or to all peaks in the method.

| Times   Sig     | gnal 🛛 Detect 🖉 Suitability 📄 🔛  |
|-----------------|--|
| Sensitivity:    | Genesis 👻  |
| Detect<br>Smoot | Apply to all peaks in method<br>Apply to all peaks with like sensitivity setting<br>Apply to all peaks in compound |

#### Table 12. Detect page shortcut menu commands

| Command   | Description  |
|---|--|
| Apply to All Peaks in<br>Method                     | Updates all compounds in the method with the current settings on the Detect page. These updates apply to both quantitative and confirming ion peaks.   |
| Apply to All Peaks with Like<br>Sensitivity Setting | Uses the current settings on the Detect page to update all compounds in the<br>method that use the Genesis sensitivity mode. These updates apply to both<br>quantitative and confirming ion peaks that use the Genesis sensitivity mode. |
| Apply to All Peaks in<br>Compound                   | Updates all peaks in the current compound with the current settings on the<br>Detect page. These updates apply to both quantitative and confirming ion peaks.  |

#### **Suitability Page**

By right-clicking anywhere on the Suitability page, you can use the shortcut menu commands to copy suitability settings for the selected peak to all peaks in the compound or to all peaks in the method.

| Times Signal | Detect Suitability                                |
|--------------|---|
| Edit         | <u>_</u>  |
| - Resolution | Set suitability settings to all peaks in compound |
| Resoluti     | Set suitability settings to all peaks in method   |

Table 13. Suitability page shortcut menu commands

| Command  | Description  |
|--|--|
| Set Suitability Settings to All<br>Peaks in Compound | Copies the suitability settings to all quantitative peaks for the compound and<br>updates the compound. Available only when a compound has multiple<br>quantitative peaks. |
| Set Suitability Settings to All<br>Peaks in Method   | Copies the suitability settings to all quantitative peaks for the method and updates the method.   |

**Spectrum Page** 

By right-clicking anywhere on the Spectrum page, you can use the shortcut menu commands to add and modify quantitative peaks and confirming ions.



**Table 14.** Spectrum page shortcut menu commands

| Command  | Description   |
|--|---|
| Update Confirming Ion<br>Ratios with This Spectrum | Updates the confirming ion ratios by using the selected peak.   |
| Set This Mass as Quan Mass                         | Adds the quantitation mass of the selected ion to the quantitation mass used for<br>the quantitative peak. You can choose whether to update the ion ratios by using<br>this reference spectrum.     |
| Add This Mass to Existing<br>Quan Mass Range       | Adds the selected mass to your existing quantitation mass range. You can choose to<br>update the ion ratios to adjust the confirming ion comparisons to the new<br>summed quantitative peak signal. |
| Set This Mass as New Quan<br>Peak                  | Adds a new quantitative peak to an existing compound.   |
| Add This Mass as New<br>Confirming Ion             | Adds one or more confirming ions to an existing compound.   |
| Reset Scaling                                      | Returns the chromatogram or spectrum display to its original size.  |
| Copy to Clipboard                                  | Copies the graphic display to the Clipboard.  |

#### **Library Page**

By right-clicking anywhere on the Library page, you can use the shortcut menu commands to apply library settings to other peaks in the compound or method.

| Suitability Spect | rum Library          | 4 >                |               |
|-------------------|----------------------|--------------------|---------------|
| Enable            |                      |                    |               |
|                   | Set peak library set | ttings to all peak | s in compound |
| Library search    | Set peak library set | ttings to all peak | s in method   |

#### Table 15. Library page shortcut menu commands

| Command   | Description   |
|---|---|
| Set Peak Library Settings to<br>All Peaks in Compound | Copies the Library Search Type, Score Threshold, and Reverse Library Search values to all peaks in the compound and updates the compound. |
| Set Peak Library Settings to<br>All Peaks in Method   | Copies the Library Search Type, Score Threshold, and Reverse Library Search values to all peaks in the method and updates the method.     |

#### **Isotopes Page**

By right-clicking anywhere on the Isotopes page, you can use the shortcut menu commands to apply isotope settings to other peaks in the compound or method.

| Fit Threshol | Set peak isotope settings to all | l peaks in method |
|--------------|----------------------------------|-------------------|
| Chable [     | Set peak isotope settings to al  | peaks in compound |
| The state    |                                  |                   |
| Spectrum     | Library Isotopes Fragments       |                   |

#### Table 16. Isotopes page shortcut menu commands

| Command   | Description  |
|---|--|
| Set Peak Isotope Settings to<br>All Peaks in Compound | Copies the Fit Threshold, Allowed Mass Deviation, Allowed Intensity Deviation,<br>and Internal Mass Calibration values to all peaks in the compound and updates<br>the compound. |
| Set Peak Isotope Settings to<br>All Peaks in Method   | Copies the Fit Threshold, Allowed Mass Deviation, Allowed Intensity Deviation,<br>and Internal Mass Calibration values to all peaks in the method and updates the<br>method.     |

#### **Fragments Page**

By right-clicking anywhere on the Fragments page, you can use the shortcut menu commands to apply fragment settings to other peaks in the compound or method.

| Spectru | m Library Isotopes <b>Fragments</b>                 |  |  |  |
|---------|---|--|--|--|
| 🔽 Ena   | ble   |  |  |  |
| Ignore  | Set peak fragment settings to all peaks in compound |  |  |  |
| Ignor   | Set peak fragment settings to all peaks in method   |  |  |  |

Table 17. Fragments page shortcut menu commands

| Command  | Description  |
|--|--|
| Set Peak Fragment Settings to<br>All Peaks in Compound | Copies the Ignore if Not Defined, Min # of Fragments, Intensity Threshold, and<br>Mass Tolerance values to all peaks in the compound and updates the compound. |
| Set Peak Fragment Settings to<br>All Peaks in Method   | Copies the Ignore if Not Defined, Min # of Fragments, Intensity Threshold, and Mass Tolerance values to all peaks in the method and updates the method.        |

#### **Ratios Page**

By right-clicking anywhere on the Ratios page, you can use the shortcut menu commands to apply ion ratio settings to other confirming peaks in the compound or method.



Table 18. Ratios page shortcut menu commands

| Command   | Description   |
|---|---|
| Set Ion Ratio to All<br>Confirming Peaks in<br>Compound | Copies the Window Type, Window, and Ion Coelution values to all confirming ion peaks for the compound and updates the compound. |
|   | Available only when a compound has multiple confirming ion peaks.   |
| Set Ion Ratio to All<br>Confirming Peaks in Method      | Copies the Window Type, Window, and Ion Coelution values to all quantitative peaks for the method and updates the method.       |

**Chromatogram Pane** 

By right-clicking anywhere in the Chromatogram pane, you can use the shortcut menu commands to add a compound or quantitative peak to a method.



Table 19. Chromatogram pane shortcut menu commands

| Command                           | Description  |
|-----------------------------------|--|
| Add This Peak as New Quan<br>Peak | Adds the selected peak to the selected compound and displays the quantitation peak information for the compound. |
| Add This Peak as New<br>Compound  | Opens the Add New Compound dialog box to choose the compound to add to the method.                               |
| Reset Scaling                     | Returns the chromatogram display to its original size.   |
| Copy to Clipboard                 | Copies the graphic display to the Clipboard.   |
| Show Graphics Side by Side        | Displays the Chromatogram and Spectra panes side by side.  |
| -or-                              | -07-   |
| Stack Graphics                    | Stacks the Chromatogram pane above the Spectra pane.   |

#### **Spectra Pane**

By right-clicking anywhere in the Spectra pane, you can use the shortcut menu commands to add compounds and quantitative peaks to a method.



**Table 20.** Spectra pane shortcut menu commands

| Command  | Description  |
|--|--|
| Use This Spectrum for<br>Compound Reference Spectrum | Sets this spectrum as the reference spectrum for the compound.   |
| Set this Spectral Peak as Quan<br>Value              | Prompts you to update the ion ratios or not update the ion ratios, and then adds this peak as a quantitative peak.                           |
| Add This Spectral Peak to<br>Existing Quan Ranges    | Prompts you to update the ion ratios or not update the ion ratios, and then adds the selected peak to the existing quantitation mass ranges. |
| Add This Spectral Peak as New<br>Quan Peak           | Adds the selected peak as a new quantitative peak for the selected compound.   |
| Add This Spectral Peak as New<br>Compound            | Opens the Add New Compound dialog box so that you can choose the compound to add to the method.  |
| Set This Spectral Peak as<br>Confirming              | Sets the selected peak as the confirming peak.   |
| Add This Spectral Peak as New<br>Confirming          | Adds the confirming ion to the selected quantitative peak.   |
| Reset Scaling  | Returns the spectrum display to its original size.   |
| Copy to Clipboard                                    | Copies the graphic display to the Clipboard.   |
| Show Graphics Side by Side                           | Displays the Chromatogram and Spectra panes side by side.  |
| -or-   | -no-   |
| Stack Graphics                                       | Stacks the Chromatogram pane above the Spectra pane.   |

# QAQC Page

By right-clicking on any page on the QAQC page, you can use the shortcut menu commands to manage, copy, and export compounds.

| Limits Calil | bration Chk Std Matrix Blank ISTD Sc |
|--------------|--------------------------------------|
|              | Copy down                            |
| ► 1 ✓        | Display retention time column        |
| 2            | Delete compound from method          |
| 3            | Сору                                 |
| 4            | Copy with headers                    |
|              | Paste                                |
|              | Export to CSV file                   |
|              | Sort by Compound Name                |
|              | Sort by Retention Time               |

**Table 21.** QAQC page shortcut menu commands

| Command                          | Description   |
|----------------------------------|---|
| Copy Down                        | Copies the value in the selected row to all rows below it. This command is available<br>only when you have selected a value that can be copied down.  |
| Display Retention Time<br>Column | Displays or hides the RT column in the compound list.   |
| Delete Compound from<br>Method   | Removes the selected compound from the current master method.   |
| Сору                             | Copies the data in the selected rows or columns to the Clipboard. Use this command<br>to copy compound information to a text editor or spreadsheet application. You cannot<br>paste this data back into the method development compound list, but you can paste<br>this data into other areas of the TraceFinder application. |
| Copy with Headers                | Copies the data in the selected rows or columns and the associated column headers to<br>the Clipboard. Use this command to copy sample information to a text editor or<br>spreadsheet application. You cannot paste this data back into the method<br>development compound list.  |
| Paste                            | Pastes a column of copied data from a text editor or spreadsheet application into the selected column. The pasted data must be valid data for the selected column.  |
| Undo Last Paste                  | Removes the last pasted item in the method development compound list.   |
| Export to CSV File               | Opens the Save As dialog box where you can save the current compound list to a CSV file.  |
| Sort by Compound Name            | Sorts the compounds alphabetically from A to Z.   |
| Sort by Retention Time           | Sorts the compounds from shortest retention time to longest retention time.   |

# Quick Acquisition

By right-clicking anywhere in the Quick Acquisition window, you can use the shortcut menu commands to create a sample list.

|     |   | Filename | Sample ID                   | Sample name | C |
|-----|---|----------|-----------------------------|-------------|---|
| ▶ 1 | 1 | Unknown  | Add sample<br>Insert sample |             |   |
|     |   |          | Insert copy sample          |             |   |
|     |   |          | Remove selected sam         | nples       |   |
|     |   |          | Import samples              |             |   |
|     |   |          | Fill down                   |             |   |
|     |   |          | Copy down                   |             |   |
|     |   |          | Сору                        |             |   |
|     |   |          | Copy with headers           |             |   |
|     |   |          | Paste                       |             |   |
|     |   |          | Export to CSV file          |             |   |
|     |   |          | Edit instrument meth        | od          |   |
|     |   |          | View sample in Qual         | Explorer F7 |   |

Table 22. Quick Acquisition window shortcut menu commands

| Command                         | Description   |
|---------------------------------|---|
| Add Sample                      | Adds an empty row to the sample grid.   |
| Insert Sample                   | Inserts an empty row to the sample grid above the selected row.   |
| Insert Copy Sample              | Copies the currently selected row and inserts a copy above the row.   |
| Remove Selected Samples         | Removes the selected samples from the sample grid.  |
| Import Samples                  | Opens the Sample Import Tool to import samples from a CSV, an XML, or an SLD file.  |
| Fill Down                       | Enters sequential values in the column starting with the value in the selected row and<br>ending with the last row in the column. This command is available only when you<br>have selected a value that can be filled down.   |
| Copy Down                       | Copies the value in the selected row to all rows below it. This command is available only when you have selected a value that can be copied down.   |
| Сору                            | Copies the data in the selected rows or columns to the Clipboard. Use this command<br>to copy sample information to a text editor or spreadsheet application. You cannot<br>paste this data back into the Acquisition mode sample list.   |
| Copy with Headers               | Copies the data in the selected rows or columns and the associated column headers to<br>the Clipboard. Use this command to copy sample information to a text editor or<br>spreadsheet application. You cannot paste this data back into the method<br>development compound list.  |
| Paste                           | Pastes a column of copied data from a text editor or spreadsheet application into the selected column.  |
| Undo Last Paste                 | Removes the last pasted item in the Acquisition mode sample list.   |
| Export to CSV File              | Opens the Save As dialog box to save the batch to a CSV file.   |
| Edit Instrument Method          | <ul> <li>Opens the Instrument Setup window where you can edit the parameters of the instrument method.</li> <li>When you edit an external method, the application updates the method in the\Xcalibur\methods folder.</li> <li>When you edit an internal method, the application updates the method in the\TraceFinderData\3.3\Projects\\batch\Methods\method folder.</li> </ul> |
| View Sample in Qual<br>Explorer | Opens the current sample in either the FreeStyle or Qual Browser application.   |

# **Trademarks**

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