TraceFinder Analysis Quick Reference Guide

This quick reference guide describes tasks using the Analysis mode in Thermo TraceFinder™ analytical software.

For detailed descriptions of all procedures described in this quick reference guide, refer to Chapter 8, "Using the Analysis Mode," in the *TraceFinder User Guide*.

Contents

- Batch View
- Data Review
- Report View
- Local Method View
- Trademarks

* To open the Analysis mode

Click Analysis in the navigation pane.

| Analysis | |
|----------|--|
| | |

The Analysis navigation pane opens.

| Analysis | → ‡ |
|--------------|------------|
| Batch View | |
| Data Review | |
| Report View | |
| Local Method | |

Batch View

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

To open the Batch View

Click Batch View in the navigation pane.

The Batch View navigation pane opens.

| • | Batch View | > |
|---|-------------------|---|
| | Samples | > |
| | Auto Samples | _ |
| | Reference Sample | _ |
| | Threshold Samples | _ |



The Batch View includes the following pages:

- Samples Page
- Auto Samples Page
- Reference Sample Page
- Threshold Samples Page

Samples Page

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

- To open the Samples page
- To create a batch
- To add samples to the list
- To insert samples into the list
- To import samples into the list
- To remove samples from the list
- To copy a sample
- To reinject a sample
- To edit sample values
- To create a group
- To submit samples

To open the Samples page

Click Samples in the Batch View navigation pane.

To create a batch

1. Choose File > New > Batch.

The Create New Batch dialog box opens.

2. Select a drive from the list.



Tip The application displays all configured and enabled repositories.

The project list displays all projects, subprojects, and batches in the selected repository.

3. Select the folder where you want to store your batch.

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

- 4. Select either Quan or Screening from the Type list.
- 5. Select a master method from the Method list.

The application displays all available quantitative or screening methods.



6. Click Create.

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

To add samples to the list

Select the number of sample rows to add and click the **Add Sample** icon, $1 = \mathbb{H}$.

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

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

To insert samples into the list

- 1. Select the sample above which you will insert new samples.
- 2. Select the number of samples to insert and click the **Insert Sample** icon, $1 \ge 10^{\circ}$.

The application inserts the Specimen samples above the selected sample.

| Inserted | | Status | Filename | Sample type | Groups | Qual Processing | Level |
|----------|---|--------|------------|-------------|--------|--------------------|-------|
| samples | 1 | 6 | cal_std_5 | Calibrator | | | 5 |
| | 2 | - 😮 | Unknown2 | Specimen | | | |
| | 3 | - 🕒 | Unknown1 | Specimen | | | |
| | 4 | | cal_std_10 | Calibrator | | | 10 |

To import samples into the list

1. Click the Import Samples icon, 🐻.

The Sample Import Tool dialog box opens.

| Sample import tool | |
|---|--------|
| Import from a file (.csv, xml, .sld) | |
| | Browse |
| Imported samples will be: appended to the end of the list | • |
| Import | Cancel |

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

The Sample Import Tool dialog box closes, and the application adds the specified samples to the sample list. When you import samples from an Xcalibur[™] sequence file, the TraceFinder application makes the following column name and sample type substitutions.

| Xcalibur column | TraceFinder column | Xcalibur sample type | TraceFinder sample type |
|-----------------|--------------------|----------------------|-------------------------|
| Position | Vial Position | Blank | Negative |
| Inj Vol | Injection Volume | Std Bracket | Calibrator |
| Dil Factor | Conversion Factor | | |

To remove samples from the list

1. Select the samples that you want to remove.

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

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

To copy a sample

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

The TraceFinder application inserts the copy above the selected sample.

To reinject a sample

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

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

To edit sample values

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

Type a new file name over the current file name.

-or-

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

-or-

Right-click and choose **Browse in Raw File** from the shortcut menu, and then locate a raw data file to use for the sample.

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

| Available sample types | | | |
|------------------------|------------|----------|----|
| Specimen | Hydrolysis | Solvent | QC |
| Unextracted | Calibrator | Negative | |

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

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

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

| Local Method: | Method_Benzos 🔹 | Update | 1 | Ì |
|---------------|-----------------|--------|---|---|
| | | | _ | |

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

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

Note When you use the scroll bar at the bottom of the sample list, the Status, Filename, Sample Type, Groups, Qual Processing, Level, Sample ID, and Sample Name columns stay fixed while the other columns scroll right and left.

To create a group

1. For each sample, click the Groups column and type the name of a group.

Note Group names are not case sensitive and are always interpreted as lowercase. For example, if you assign one sample to "GroupA" and another sample to "groupa", both samples are assigned to "groupa" on the Threshold Samples page.

- 2. Repeat step 1 for each sample that you want to include in a group.
- 3. Create as many groups as you want.

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

To submit samples

- 1. Do one of the following:
 - To submit all samples in the batch, click the **Submit Batch** icon, **•**.
 - To submit specific samples, select the samples and click the Submit Selected Samples icon, 4.

The Submit Options dialog box opens.

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

Note The Acquire Data and Process Data with Peak Detection options are selected by default when you submit a batch.

3. To start the selected processes, click OK.

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

To open the Auto Samples page

Click Auto Samples in the Batch View navigation pane.

The Auto Samples page opens.

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

To add an auto sample type

1. Right-click and choose Add Auto Sample from the menu, or click the Add New Auto Sample icon, 1 📄 📭. The application adds a Solvent sample to the sample list.

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

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

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

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

After auto sample injections have occurred, you can return to this page to view the number of injections used in each vial.

5. In the Vial Position column, type the vial position for the Solvent or Negative sample.

Auto Samples

Reference Sample Page

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

* To specify a chromatogram reference sample

- 1. Click Reference Sample in the Batch View navigation pane.
 - An empty reference sample table opens.

| Batch V | /iew - Bat | ch_13 [Qua | an] | | | |
|---------|------------|-------------|-------------|---------|---------------|------------------|
| Local M | ethod: Me | thod_Benzo: | 5 | • | Update | |
| Status | Filename | Sample ID | Sample name | Comment | Vial position | Barcod Actual |

Right-click the table and choose Add Reference Sample from the shortcut menu, or click the Add Reference Sample icon, 1 - 14.

The Open Chromatogram Reference Sample dialog box opens.

| Open Chromatogram Reference Sample | | × |
|--|--|--------|
| C:\TraceFinderData\32\Projects | UnknownA2 UnknownA3 UnknownA4 UnknownA1 | ۸ ۳ |
| Select a reference sample from the right panel | and click "Open". Oper | Cancel |

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

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

The application displays only batches that were created using the current master method.

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

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

7. Click Open.

Threshold Samples Page

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

To specify a threshold sample

- 1. Click Threshold Samples in the Batch View navigation pane.
- 2. Click the Sample list for each group and choose a sample in the group to be the threshold sample.

| | Group | Sample |
|---|--------|--------------|
| • | groupb | Benzo26473 🔹 |
| | | Benzo26473 |
| | | Benzo25557 |
| | | Benzo26154 |

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

See also "To create a group" on page 4 and "Comparative View" on page 13.

Data Review

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

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

To open the Data Review view

Click Data Review in the navigation pane.

The Data Review navigation pane opens.

Data Review for quantitative methods

| T | Data Review | > |
|---|------------------|---|
| | Sample View | > |
| | Compound View | |
| | Comparative View | |
| | Qualitative View | |

Data Review for target screening methods

| T | Data Review | > |
|---|------------------|---|
| | Target Screening | > |

Data Review for Quantitative Methods

The Data Review for quantitative methods includes these views:

- Sample View
- Compound View
- Comparative View
- Qualitative View

Sample View

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

These are the default panes and their locations.



You can display, hide, or move any of these panes. For procedures about creating docked, floating, or tabbed panes, see "Data Review Pane Display Features" in Chapter 8 of the *TraceFinder User Guide*.

• Samples pane

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

| Sa | mples | | | | | | Ψ× | Compound Results | | | | | | |
|----|-------|-------|--------|--------|-------|-----|--------|------------------|---------------------|-------------------|----------------------|---------|-------|-------|
| P | | Flags | St | tatus | Filen | ame | Sampl | e Type | Flags | Flag | g Details | Com | pound | ype |
| 7, | A | a 🔻 | Aa | • | Aa | • | Aa | • | <u>A</u> a · | Aa | • | Aa | • | |
| Þ. | 1 | | | • | B_255 | 57 | Specim | en | | _ | | FENTH | HON-C | lund |
| ۲ | 2 | | . 0 | • | B_261 | .54 | Specim | en | | - | | Sulfiso | midin | e und |
| × | 3 | | | • | B_264 | 73 | Specim | en | | | | | | |
| þ. | 4 | | 0 | • | B_269 | 84 | Specim | en | | | | | | |
| Þ. | 5 | | | • | B_271 | .26 | Specim | en | | | | | | |
| | | | | | | | | | | | | | | |
| | | S | electe | ed sar | nple | | | | C s | ompour elected | nd error i sample | n the | | |
| | | | | | | | | | No comp selected | ound er sample | ror in the | 9 | | |

• Compound Results pane

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



• Sample Peaks pane

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



To display details for a compound

Double-click the chromatogram in the Sample Peaks pane.

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

Quan Peak

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



Confirming Ions

Quantitative peak with multiple confirming ions.



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

Reference Peak

Quantitative peak with a reference peak.



ISTD

Quantitative peak with an internal standard.



Ion Overlay

Quantitative peak with a confirming ion overlay.



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

Calibration Curve

Quantitative peak with a calibration curve plot.



Spectra

Quantitative peak with data and reference spectra.



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

Compound View

The Compound View displays a list of all compounds available in the method, all samples in the current batch, and the peak plots for all compounds found in each sample. These are the default panes and their locations:



• Compounds pane

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



• Sample Results pane

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



Comparative View

The Comparative View uses three panes to display a list of all compounds available in the method, all samples in the current batch, and the sample peak plots for all compounds found in the samples with the horizontal threshold guide.

These are the default panes and their locations.



The panes in the Comparative View are identical to the Compound View with the addition of the Group column. This column identifies any groups that a sample belongs to, as specified in the Batch View.

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



Qualitative View

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

These are the default panes and their locations.



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

• Samples pane

Use the Samples pane to select a specific sample.

| Sar | mples | | | | | | • | μ× |
|-----|-------|---|-------|------------|-------------|---|------------|------|
| P | | l | Flags | Status | Filename | | Sample | Туре |
| Tp | = | | | <u>A</u> a | <u>A</u> a | • | <u>A</u> a | • |
| Þ | 1 | | | • | Benzo_26474 | | Specime | n |
| • | 2 | | | • | Benzo_27126 | | Specime | n |

• Peaks pane

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

| Pea | aks | | | | | | • ₽ | × | | | | | | |
|------------------|---|------------|--------------|--------------|--------------|---------------|------------|---|--|--|--|--|--|--|
| Fi | Filter: + c ESI Full ms [200.00-800.00] | | | | | | | | | | | | | |
| F | Peak RT | SI | RSI | MP | Est Amt | Library Hit | | - | | | | | | |
| \mathbb{T}_{P} | <u>A</u> a 🔻 | <u>A</u> a | <u>A</u> a 🔻 | <u>A</u> a 🔻 | <u>A</u> a 🔻 | Aa | • | | | | | | | |
| Þ | 9.82 | 124 | 732 | 0 | 0.000 | Phenomorphan | | | | | | | | |
| ۲ | 1.63 | 161 | 570 | 4 | 0.000 | Sulfasomizole | | Ŧ | | | | | | |

• Sample Chromatogram pane

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



• Peak Details pane

The Peak Details pane displays the selected peak.



• Spectrum pane

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



• Library Hits pane

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

| Lib | Library hits 🗸 🗸 🗸 | | | | | | | | | | | | |
|------------|--------------------|-----|-----|----|---------------------------|--|--|--|--|--|--|--|--|
| F | Rank | SI | RSI | MP | Library entry | | | | | | | | |
| \bigcirc | | = | = | = | <u>A</u> a • | | | | | | | | |
| ۲ | 1 | 332 | 978 | 0 | 2-Hexanone | | | | | | | | |
| \bigcirc | 2 | 320 | 966 | 0 | Succinic anhydride | | | | | | | | |
| \bigcirc | 3 | 314 | 959 | 0 | Propane, 1-(ethenyloxy)-: | | | | | | | | |

Data Review for Target Screening Methods

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

These are the default panes and their locations.

Chromatogram pane



You can display, hide, or move any of these panes. For procedures about creating docked, floating, or tabbed panes, see "Data Review Pane Display Features" in Chapter 8 of the *TraceFinder User Guide*.

Samples Pane

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



Flags in the Samples pane indicate one of the following:

A green circle when the sample/compound/peak combination is identified and fully confirmed.

A yellow triangle when the sample/compound/peak combination is identified but not fully confirmed.

A red square when the sample/compound/peak combination is not identified.

Chromatogram Pane

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

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



Compounds Pane

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

| Con | про | unds | | | | | | | | | | → ╄ × |
|-----|-----|------------|--------------|-----------|----------|------|------|------|--------|--------------------------|----------------------------------|---------------|
| Ξ | 1 | Be | nzodiazepine | s Example | Database | 2 | | | | | | |
| | Ē | # 🗆 | Selected + | MZ 👳 | RT 👳 | IP 👳 | FI 👳 | LS 👳 | Flag 👳 | Compound Name += | Match Result Name 👍 | Formula 👍 |
| | | | | • | • | • | • | • | • | <u>A</u> a • | <u>A</u> a • | <u>A</u> a ▼ |
| | ÷ | 1 | | • | • | • | • | • | • | 2-Hydroxyethylflurazepam | 2-Hydroxyethylflurazepam@RT 0.19 | C17H14CIFN2O2 |
| - | ÷ | 2 | | • | • | • | • | • | • | 2-Hydroxyethylflurazepam | 2-Hydroxyethylflurazepam@RT 1.42 | C17H14CIFN2O2 |
| | ÷ | 3 | | ٠ | | ٠ | | | - | 2-Hydroxyethylflurazepam | 2-Hydroxyethylflurazepam@RT 1.71 | C17H14CIFN2O2 |
| | ÷ | 4 | | ٠ | | • | | | - | 2-Hydroxyethylflurazepam | 2-Hydroxyethylflurazepam@RT 1.96 | C17H14CIFN2O2 |
| | ÷ | 5 | | ٠ | • | • | • | • | ٠ | 2-Hydroxyethylflurazepam | 2-Hydroxyethylflurazepam@RT 2.35 | C17H14CIFN2O2 |

Spectrum Pane

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

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

• Spectrum

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

• Isotopes

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

• Fragments

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

• Library

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

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

Report View

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

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

To open the Report View

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

Report View

The application opens the Reporting view.

| Reporting - Batch_Apple | _9705 | | | | | |
|----------------------------|------------|-------------|--------|----------|--------------------|--|
| Template | | | | | Rules | |
| Method Validation Report | t | | | * | Sheet Name | Rules |
| MSMSD Report | | | | | Shoot1 | Patch |
| Quantitation Report | | | | | Sheet2 | Batch |
| Quantitation Report - 2 | | | | | Sheet2 | Batch |
| Screening Batch Report | | | | | Sheet3 | Batch |
| SGS Report | | | | | | |
| Solvent Blank Report | | | | | | |
| Surrogate Recovery Report | rt. | | | | | |
| Target Screening High De | ensity Sar | nole Report | | = | | |
| Target Screening Summa | rv Report | ipic nepore | | | | |
| TIC Report | | | | | | |
| TIC Summary Report | | | | - | | |
| BB | | | | | | |
| BB | | Design | New | Preview | | excel V CSV Print Generate |
| Report generation in progr | ACC | | | | | |
| Template: | 233 | Sheet: | | | | |
| | | | | | | |
| Generated Reports | | | | | | |
| Template | Rule | Sample | Output | Generate | d Report File | |
| Method Validation Report | Batch | | pdf | Method \ | alidation Report_ | 20140113092939.pdf (3 pages) <u>View</u> |
| Method Validation Report | Batch | | CSV | Method \ | alidation Report_S | heet1_20140113094656.csv View |
| Method Validation Report | Batch | | CSV | Method \ | alidation Report_S | heet2_20140113094656.csv View |
| Method Validation Report | Batch | | CSV | Method \ | alidation Report_S | heet3_20140113094656.csv View |
| Method Validation Report | Batch | | pdf | Method \ | alidation Report_ | 20140113094656.pdf (3 pages) View |
| Method Validation Report | | | excel | Method \ | alidation Report_2 | 0140113094656.xlsx <u>View</u> |
| 13/13 | | | | | | 100 g.C |
| 66 | | | | | | clear |

The Design, New, and Preview buttons open the Report Designer. For details about using the Report Designer, see "Working in the Report Designer" in Chapter 8 of the *TraceFinder User Guide*.

To preview a report

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

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

| Template |
|--|
| Ad Hoc Tune Report |
| Batch Report |
| Blank Report |
| Breakdown Report |
| Calibration Report |
| Check Standard Report |
| Chromatogram Report |
| Compound Calibration Report |
| Compound Calibration Report - Alternate |
| Confirmation Report |
| Confirmation Report 2 |
| High Density Calibration Report |
| High Density Internal Standard Report Long |

2. Click **Preview**, Preview

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

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

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

The application does the following:

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

| Report generation in progress | | | |
|-----------------------------------|---------------|-----------------------|--|
| Template: Quantitation Report - 2 | Sheet: Sheet1 | Sample: Apple_0_81_02 | |

- Creates a report with the selected report template as a PDF, an Excel, or a CSV file.
- Adds information about the generated report to the Generated Reports pane.
- Saves the report files to the ...\TraceFinderData\32\Projects\batch\ReportOutput folder.

To print a report

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

The application does the following:

- Creates a report for the current batch using the selected report template format.
- Prints the report to your default printer.
- Adds information about the generated report to the Generated Reports pane.
- Saves the report files to the ...\TraceFinderData\32\Projects\batch\ReportOutput folder.

To display a generated report

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

| Generated Reports | | | | | |
|--------------------------|-------|--------|--------|---|------|
| Template | Rule | Sample | Output | Generated Report File | |
| Method Validation Report | Batch | | pdf | Method Validation Report_20140113092939.pdf (3 pages) | View |
| | | | | | |

Opens the generated file.

To edit a report template

- 1. In the Template pane, select a report template.
- 2. Click **Design**, Bosign

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

| 🔓 Report 🛙 | Report Designer - Batch Report.xlsx | | | | | | | | | | | | | |
|------------|-------------------------------------|--------|-----|-------------|------|-----------|----------------------|-------------|-------------|-------------|---------------------------|------------------|--|--|
| File | Home | Insert | | Page Layou | ıt | | | | | | | | | |
| B 🖢 | Calibri 8 | | 8 | т А́ А | • | = . | 🗉 💼 📑 Wrap Text | ÷ | × | | 1 | 2 | | |
| Paste | B Z | Π | Ħ | 3 🔕 🔺 | | E | Merge Cells | Insert * | Delete • | Format * | Conditional Formatting | Show Formulas | | |
| Clipboard | Clipboard Font | | | | | | Alignment 5 | | | C | ells | | | |
| Report | Type: Ba | tch [| 057 | | • | | | | | | | | | |
| | | | | Α | В | | с | D | | E | F | G | | |
| | | | 1 | | | | | _ | | | Batch | Report | | |
| | | | 2 | | | | | | | | | | | |
| | | | 3 | Lab Name: | Defa | ault Labo | ratory | | | | | | | |
| | | | 4 | Instrument: | The | rmo Scie | ntific Instrument | | | | | | | |
| | | | 5 | User: | dana | a.powers | | | | | | | | |
| | | | 5 | Batch: | Bate | h_Apple | _9705 | | | | | | | |
| | | | 2 | File Name | - | | Date/Time | Comple II | | | Sample Name | | | |
| | | | ŏ | Apple 0 81 | 01 | | 7/3/2010 12:47:10 AM | 1 | | | Sumple Name | , | | |
| | | | 10 | Apple 0 81 | 02 | | 7/3/2010 1:03:40 AM | 1 | | | | | | |
| | | | | | | | | | | | | | | |
| | | | 11 | Apple_0_81 | 03 | | 7/3/2010 4:37:50 AM | 1 | | | | | | |

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

To create a new report template

1. Click New, New

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

2. Use the features in the Report Designer to create the template.

Local Method View

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

To open the Local Method view

Click Local Method in the Analysis navigation pane.

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

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

Local methods are named *BatchName_MasterMethodName*.

To edit a local method

1. Enter any changes to the local method.

To edit a method, refer to the method development chapters in the TraceFinder User Guide.

- 2. Choose File > Save.
- 3. To process the batch or create new reports with the edited local method, return to the Batch View and submit the batch.
- To overwrite the local method with the master method in the Batch View

In the Batch View, click Update.

| Local Method: | Method_Vitamin1 | - | Update |
|---------------|-----------------|---|--------|
| | | | |

The application overwrites the local method with the master method of the same name. You can use this feature to overwrite an edited local method with the original master method or to overwrite the local method with an updated master method.

| Analysis 👻 🖣 | Local Method View - Equan1_408 | 3_Method_Equan_1* | |
|--------------|--------------------------------|--------------------------|-------------|
| Batch View | Master method: Method Equan 1 | | |
| Data Review | Lab Name: | Default Laboratory | |
| Report View | Assay type: | Assay name | |
| | Injection Volume: | 1,100.00 | |
| Local Method | Mass Precision: | 3.00 | |
| Acquisition | Ion range calc method: | Level 🔹 | |
| Quantitation | Use level: | | |
| Processing | | | |
| Compounds | Instrument Method: | Pesticides Using EQuan * | Edit Update |
| QAQC | Notes | | |
| Groups | | | |
| Intel Seq | | | |
| Reports | | | |

Figure 1. Local Method View of a quantitation method

Figure 2. Local Method View of a screening method

| Analysis | | Local Method View - Batch_1_Method_Screening_Alprazolam | | | | | |
|---------------------------------|-----------------------|---|---------------------|------|--------|--|--|
| Batch View | Master method: Method | Master method: <u>Method Screening Alprazolam</u> | | | | | |
| Samples | Lat | Name: Defa | ult Laboratory | | | | |
| Data Review | Ass | ay type: Assay | / name | | | | |
| Target Screening | Injection | Volume: | 1.00 | | | | |
| Report View | Mass Pr | recision: | 2.00 | | | | |
| Local Method | > Instrument I | Method: Pesti | cides Using EQuan 🔹 | Edit | Update | | |
| Acquisition | Notes | | | | | | |
| Screening | | | | | | | |
| Processing | | | | | | | |
| Peak Detection | | | | | | | |
| Reports | | | | | | | |

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