TraceFinder Acquisition Quick Reference Guide

This quick reference guide describes the Acquisition mode tasks of the Thermo TraceFinder™ 5.1 application.

> **Tip (Animation)** To view "Quick Acquisition," choose **Help > Animations**.
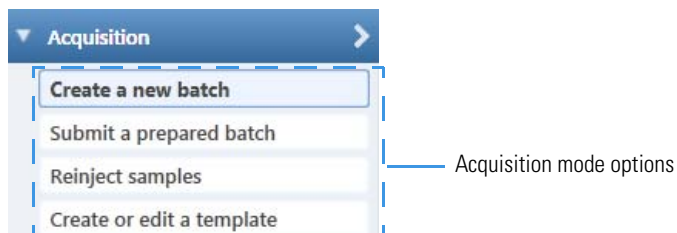
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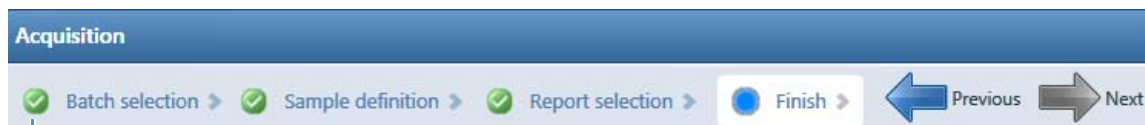- Using Quick Acquisition
- Trademarks

Opening the Acquisition Mode

❖ **To open the Acquisition mode**

Click **Acquisition** in the navigation pane.

The navigation pane for the Acquisition mode opens.

Acquisition mode options

The task pane for the Acquisition mode tracks your actions.

Example of the task pane as you complete each task

Selecting a Batch

Use the Batch Selection page of the Acquisition mode to create a new batch in any of your current projects, or use a batch template to start a new batch.
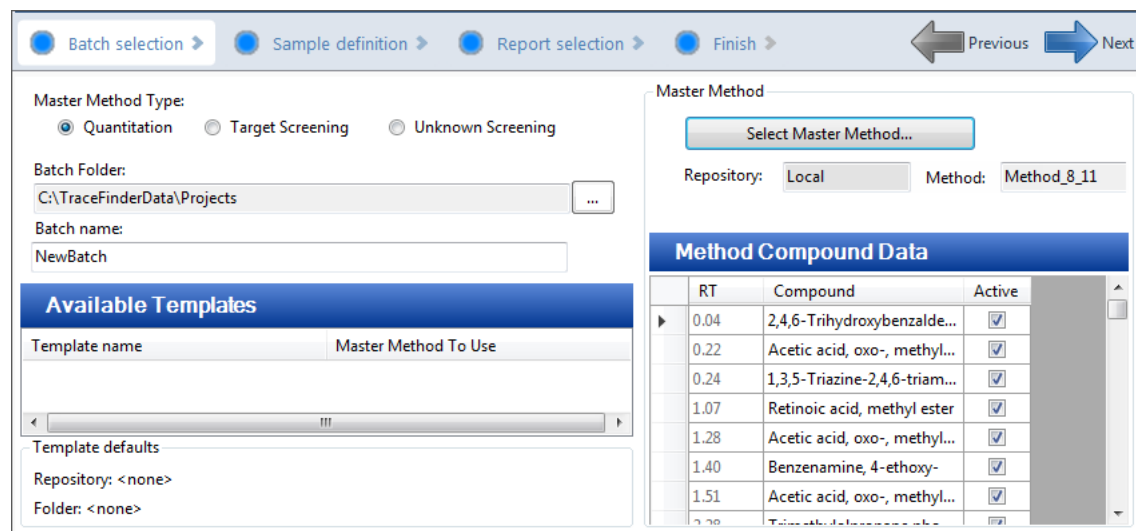
❖ **To start a new batch**

1. In the navigation pane, click **Create a New Batch**.
2. Select one of these options: **Quantitation**, **Target Screening**, or **Unknown Screening**.
3. Select the batch folder where you want to create a new batch.
4. Type a unique name for the new batch in the Batch Name box.
5. Click **Select Master Method**.

   The Select a Master Method dialog box opens.

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6. Select repository and a method from the list, and then click **Select**.

The Method Compound Data pane displays the compounds in the method. You cannot edit the compounds list in the Acquisition mode.

7. To continue to the next page, click **Next**.

The Sample Definition page opens. See Defining the Sample List.

❖ **To start a new batch from a template**

1. In the navigation pane, click **Create a New Batch**.
2. Select one of these options: **Quantitation**, **Target Screening**, or **Unknown Screening**.
3. In the Available Templates pane, select the template and method combination that you want to use.

The system creates a batch name with the selected template name and appends the date and time stamp. The application selects the default project, subproject, and method associated with this template.

4. (Optional) Select a different batch folder where you want to create the new batch.
5. (Optional) Select a different method to use for the new batch.
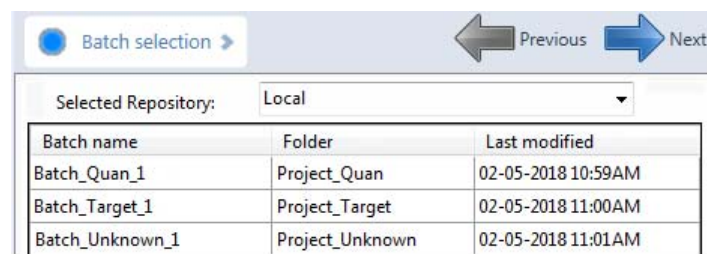6. To continue to the next page, click **Next**.

The Sample Definition page opens. See Defining the Sample List.

❖ **To select a prepared batch**

1. In the navigation pane, click **Submit a Prepared Batch**.
2. Select a repository.

The application displays all the unacquired, saved batches in the selected repository.

3. Select the batch that you want to acquire.

4. To continue to the next page, click **Next**.

The Finish page of the Acquisition mode opens. From the Finish page, you can save the batch, submit the batch for acquisition, or go back to the Sample Definition page to edit the sample list for this batch.

5. Do one of the following:
   - To prepare the batch for acquisition, click [Submit icon] **Submit**.

     For detailed instructions, see Submitting the Batch.

- To edit the samples list, click **Previous**.

  For detailed instructions, see Defining the Sample List.

–or–

- To save the batch to be acquired later, click [🖫 Save] .

  The application saves your batch, closes the Acquisition mode, and returns you to the mode you were last using.

  The application saves batches to the …\TraceFinderData\Projects\… folder.

❖ **To reinject samples in a previously acquired batch**

1. In the navigation pane, click **Reinject Samples**.
2. Browse to and select a batch folder and batch.

   The Select a Batch dialog box displays all previously acquired quantitation, target screening, and unknown screening batches.

3. Select a batch and click **Select**.
4. To continue to the next page, click **Next**.

   The Sample Definition page opens. See Defining the Sample List.

❖ **To create a quantitation batch template**

1. In the navigation pane, click **Create or Edit a Template**.
2. Select the **Quantitation** option.
3. Browse to the folder where you want to create the new batch template.
4. Type a name for the new batch template in the Template Name box.
5. Select a method from the Method Selection list.

   The Method Compound Data pane displays the compounds in the method. You cannot edit the compounds list from the Acquisition mode.

	RT	Compound	Active
▶	0.00	9(10H)-Acridinone	☑
	0.01	Pyrazinamide	☑
	1.07	Methyl 2-furoate	☑

   Method Compound Data

6. To continue to the next page, click **Next**.

   The Sample Definition page opens. See Defining the Sample List.

❖ **To create a target screening batch template**

1. In the navigation pane, click **Create or Edit a Template**.
2. Select the **Target Screening** option.
3. Browse to the folder where you want to create the new batch template.
4. Type a name for the new batch template in the Template Name box.
5. Select a method from the Method Selection list.

   The Method Compound Databases pane displays the screening databases available for the selected method.

   Method Compound Databases

	Enabled	Database File
▶	☑	Default Database
	☑	Database 1

6. Select the check box for each database that you want to use for screening.
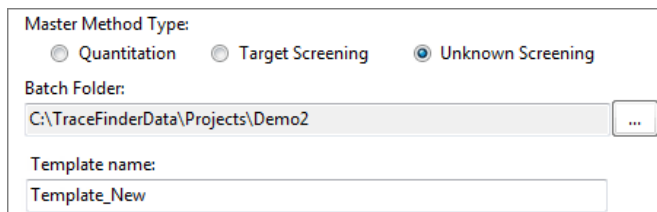7. To continue to the next page, click **Next**.

   The Sample Definition page opens. See Defining the Sample List.

❖ **To create an unknown screening batch template**

1. In the navigation pane, click **Create or Edit a Template**.

> **Note** When user security is activated, you must have Acquisition Wizard – Template Editing permission to create a batch template.

2. Select the **Unknown Screening** option.

3. Browse to the folder where you want to create the new batch template.

4. Type a name for the new batch template in the Template Name box.

5. Select a method from the Method Selection list.

The Method Compound Databases pane displays the unknown screening databases available for the selected method.

6. Select the check box for each database that you want to use for unknown screening.

7. To continue to the next page, click **Next**.

The Sample Definition page of the Acquisition mode opens. See Defining the Sample List.

Defining the Sample List

Use the Sample Definition Page of the Acquisition mode to create a list of samples for the batch. You can add or insert samples to the list, import a sample list, or remove samples from the list.

As you enter sample values, you can use the Copy Down and Fill Down commands to quickly enter column values. For detailed instructions, refer to the "Using Copy Down and Fill Down" appendix in the *TraceFinder User Guide*.

After defining the list of samples, click **Next.**

- If you are creating a batch from scratch, creating a batch from a template, or editing a batch template, the Report Selection page opens. See Selecting and Reviewing Reports.

- If you are editing a previously acquired batch or a prepared batch, the Finish page opens. See Submitting the Batch.

❖ **To add samples to the list**

1. Select the number of sample rows to add and then click **Add** .

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

2. For each sample, type a unique file name in the Filename column.

3. For each sample, select a sample type from the Sample Type list.

Available sample types				
Matrix Blank	Solvent	QC	Unknown	Cal Std

For a detailed description of sample types, refer to "Using the Acquisition Mode" in the *TraceFinder User Guide*.

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

The sample levels are defined in the master method. If there are no levels to select from the Level list, ask a user with Supervisor or LabDirector permissions to edit the method and specify the levels.

For detailed instructions about defining sample levels, refer to the method development chapters in the *TraceFinder Lab Director User Guide*.
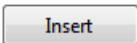
5. For each sample, type a vial position in the Vial Position column.

> **Tip** Use the Fill Down command to make entering vial positions easier.

6. For each sample, type a volume in the Injection Volume column.

7. (Optional) Type or edit the values for the remaining columns.

> **Note** When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening) Level, Sample ID, and Sample Name, while the other columns scroll right and left.

❖ **To 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 ⬚ Insert ⬚.

The application inserts the Unknown samples above the selected sample.

	Status	Filename	Sample type	Groups
1	🟡	cal_std_5	Cal Std	
2	🔵	Unknown2	Unknown	
3	🔵	Unknown1	Unknown	
4	🟡	cal_std_10	Cal Std	

Inserted samples (labels pointing to rows 2 and 3)

3. For each sample, type a unique file name in the Filename column.

4. For each sample, select a sample type from the Sample Type list.

5. 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, ask a user with Supervisor or Lab Director permissions to edit the method and specify the levels.

For detailed instructions about defining sample levels, refer to the method development chapters in the *TraceFinder Lab Director User Guide*.

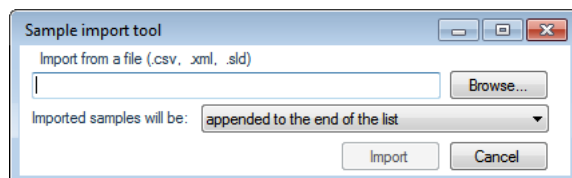6. Type a vial position in the Vial Position column for each sample.

> **Tip** Use the Fill Down command to make entering vial positions easier.

7. For each sample, type a volume in the Injection Volume column.

8. (Optional) Type or edit the values for the remaining columns.

❖ **To import samples into the list**

1. Click ⬚ Import ⬚.

The Sample Import Tool dialog box opens where you can import a sample list from a CSV, an XML, or an SLD file.

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. Browse to and select a CSV, an XML, or an SLD file with the sample definitions that you want to import.

> **Note** The .csv, .xml, or .sld data format must match the TraceFinder data 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, 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		

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

   The sample levels are defined in the master method. If there are no levels to select from the Level list, ask a user with Method Development permission to edit the method and specify the levels.

   For detailed instructions about defining sample levels, refer to the method development chapters in the *TraceFinder Lab Director User Guide*.

6. For each sample, type a vial position in the Vial Position column.

   > **Tip** Use the Fill Down command to make entering vial positions easier.

7. For each sample, type a volume in the Injection Volume column.

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

   > **Note** When you use the scroll bar at the bottom of the sample list, the following columns remain fixed: Status, Filename, Sample Type, Groups, Qual Processing (quantitation) or Blank Subtraction (target screening) Level, Sample ID, and Sample Name, while the other columns scroll right and left.

9. (Optional) When using the Multi-Channel LC feature, select a channel for each imported sample.

   Imported samples default to Auto.

❖ **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**.

❖ **To reinject a sample from a previously acquired batch**

1. In the sample list, select the sample to reinject.

2. Right-click and choose **Reinject Selected Samples**.

   The 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 application copies all parameter values from the original sample. A green status icon indicates previously acquired samples (acquired and processed), and the sample name is grayed out. A blue status icon indicates samples created for reinjection (not acquired).

   When you submit this batch, the application acquires only the reinjection samples.

Sample Definition Page

Table 1. Sample Definition page parameters

Parameter	Definition
Previous	Returns you to the previous Acquisition page.
Next	Takes you to the next Acquisition page.
Sample Controls	
Add	Adds the specified number of empty rows to the sample grid.
Insert	Inserts the specified number of empty rows above the selected row.
Import	Opens the Sample Import Tool to import samples from a CSV, an XML, or an SLD file.
Shortcut menu	
Add Sample	Adds one empty row to the sample grid.
Insert Sample	Inserts one 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 samples and appends INJ001 to the end of the file name. Additional reinjections of the same sample are numbered INJ002, INJ003, and so forth.
Remove Selected Samples	Removes the selected samples from the sample grid.
Import Samples	
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 ending with the last row in the column.
Modify Columns	Opens the Modify Columns dialog box to customize the column display. Refer to "Using the Analysis Mode" in the *TraceFinder User Guide*.
Show Sample 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 command to copy sample information to a text editor or a 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 to the Clipboard. Use this command to copy sample information to a text editor or a spreadsheet application. You cannot paste this data back into the method development compound list.
Paste	Pastes one column of copied data from a text editor or a spreadsheet application into the selected column.
Undo Last Paste	Removes the last pasted item in the sample list.
Export to CSV File	Opens the Save As dialog box to save the batch to a CSV file.
Edit Instrument Method	Opens the Xcalibur Instrument Setup window where you can edit the parameters of the instrument method.
View Sample in Qual Explorer	Displays the selected sample in the configured qualitative explorer application.

Selecting and Reviewing Reports

Use the Report Selection page of the Acquisition mode to specify the types of reports that you want to create.

The Report Selection page lists all the available reports and displays the report name, report title, and the options to create printed, PDF, CSV, or Microsoft™ Excel™ output.

After specifying your report options, click **Next** to go to the Finish page and submit your batch. See Submitting the Batch.

The application saves the resulting output files for your reports in the following folder:

…\TraceFinderData\Projects\…*batchname*\ReportOutput

❖ **To edit a report title**

Select the report name (the default text) in the Report Title column and edit it.

The default text in this column is the same as the report name.

❖ **To specify a report in print format or as a PDF, a CSV, or an Excel file**

1. For each report that you want to create, select the check box in the Print, Create PDF, Create CSV, or Create Excel column.

2. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.
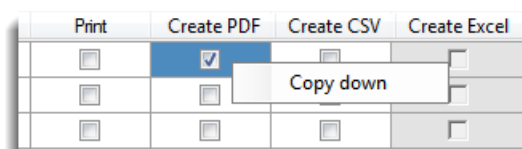
All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell.

Report Selection Page

Parameter	Description
Report Name	The name of a report.
Report Title	User-editable description of the report.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files.
Create CSV	Reports to be exported as CSV files.
Create Excel	Reports to be exported as Excel files.
Shortcut menu: Copy Down	Copies the selected or cleared state to all subsequent reports in the column. This action applies only to report types that make this output format available.

Submitting the Batch

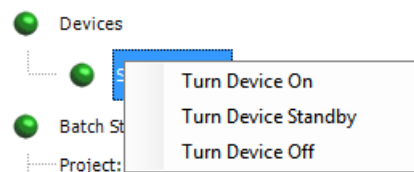Use the Finish Page of the Acquisition mode to specify a startup method, a shutdown method, or a calibration file. You can save the batch to be acquired later, or you can submit the batch and acquire data, process data, or create reports.

Note If you are working with a batch template, the only available function is Save.

❖ **To specify device states**

In the System Status area of the Finish page, right-click the name of the device, and then choose a device state.

Instrument state	
Turn Device On	(Default) Keeps the system in the On state when the current run finishes, so you can begin another run without waiting. All power and flows are maintained at operational levels.
Turn Device Standby	Keeps 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	Keeps the system in the Off state when the current run finishes. The Off state indicates that all power to the instrument, which the TraceFinder application can control, is turned off. Power to the instrument includes power to all heaters and most subassemblies, but in some cases not all subassemblies.

Instrument status indicators	
🟢	Green indicates that the device is turned on.
🟡	Yellow indicates that the device is in standby mode.
🔴	Red indicates a device error.

❖ **To specify startup or shutdown methods**

1. (Optional) Select a method from the System Startup Method list on the Finish page.

   The application runs this method before running the batch. No autosampler injection takes place. This feature is not available for all instruments.

2. (Optional) Select a method from the System Shutdown Method list.

   The application runs this method after running the batch. No autosampler injection takes place. This feature is not available for all instruments.

❖ **To automatically update the timed selected reaction monitoring information**

On the Finish page, select the **Auto TSRM Update** check box.

When you submit the batch, the application updates the TSQ™ method with mass transitions, collision energy, and other appropriate data for TSRM functionality.

❖ **To specify a calibration file**

1. In the Calibration area of the Finish page, select a calibration (.calx) file from the list.

> **Note** You must acquire at least one batch with the current method to create a calibration (.calx) file.

2. To add calibration data from the current batch to the selected calibration file, select the **Extend Calibration** check box.

❖ **To save a batch for later acquisition or processing**

From the Finish page, click 🖫 Save.

The application saves your batch as a prepared file.

❖ **To start an acquisition or processing**

1. From the Finish page, click 📚➡ Submit.

   The Submit Options Dialog Box opens.

2. To acquire (or reacquire) the submitted samples, select the **Acquire Data** check box.

   • When all submitted samples have been previously acquired, this option is (by default) not selected.

   • When there are any samples in the batch that have not been acquired, this option is (by default) selected.

   > **Tip** You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.

3. To process the submitted samples, select the **Process Data** check box.

   The application displays options for each type of method that the batch uses: Quantitation, Target Screening, Unknown Screening, or a combination of methods.

4. For each method type, select the check box for the options that you want to use.

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

   Quantitate: Performs quantitation for quantitation methods.

   Identify: Performs identification for unknown screening methods.

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

   With RT Alignment: Performs retention time alignment for unknown screening methods. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.

5. (Optional) Select the **Create Reports** check box.

6. (Optional with the Multi-Channel LC feature activated) Select the **Priority Sequence** check box.

   The application acquires the priority batch on the next available channel or the assigned channel.

7. (Optional without the Multi-Channel LC feature activated) Select the **Priority Sequence** check box and then select one of the following priority options to place the batch in the queue:

   • **Next Available Batch** places the batch immediately after the currently acquiring batch.

   • **Next Available Sample** places the batch immediately after the currently acquiring sample.

   > **Note** When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.

8. To specify the following optional parameters, click **Show Details**.

   a. Select the **Use** check box for the device that you want to use for this acquisition.

   b. Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.

      This is usually the autosampler.

   c. Select the **Start When Ready** check box, which starts all instruments together when they are all ready.

      When you clear this check box, individual instruments can start at different times and then must wait for the last instrument to be ready.

   d. Select the system state after it acquires the last batch: **On**, **Standby**, or **Off**.

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

   The selected processes begin, and the application shows the real-time display at the bottom of the current window. You can begin another batch in the Acquisition mode while you watch the real-time display of the currently acquiring batch.

IMPORTANT When your batch uses unknown screening features, after the first processing, you might see an error message stating that the total number of results is too large for a single batch (more than 500 000). Return to the Processing pages for the unknown screening features and make one or more of these parameter adjustments:

- Limit the RT range.
- Shorten the signal range.
- Specify a lower value for the Number of Top Matches.
- Specify a Simple Search instead of an Exhaustive Search.
- Specify Top Peaks instead of All Peaks.
- Limit the number of search types.

Submit Options Dialog Box

Table 2. Submit Options dialog box parameters (Sheet 1 of 2)

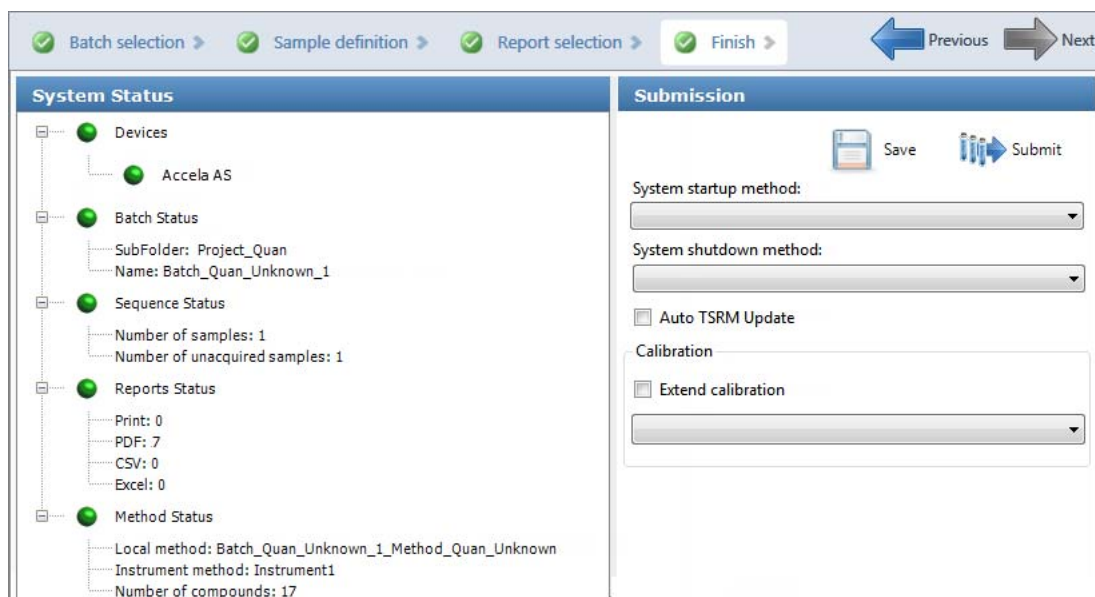| Parameter	Description
User Name	Displays the name of the current user.
Samples	Reports the batch number and number of samples.
Method Types	Lists the types of methods (quantitation, target screening, or unknown screening) used in the submitted batches.
Workflow Steps to Perform	
Acquire Data	Submits the current batch to acquisition.
	• When all submitted samples have been previously acquired, this option is (by default) not selected.
	• When there are any samples in the batch that have not been acquired, this option is (by default) selected.

Table 2. Submit Options dialog box parameters

Parameter	Description
Process Data	Processes the data for the current batch using any of the following options:
	Peak Detect: Performs peak detection for all method types. You can process the data with or without performing peak detection. For example, you might want to turn off peak detection when reprocessing samples.
	Quantitate: Performs quantitation for quantitation methods.
	Identify: Performs identification for unknown screening methods.
	Identify and Confirm: Performs both identification and confirmation for target screening methods.
	With RT Alignment: Performs retention time alignment for unknown screening methods. This produces the heat map and group averages data in the Unknown Screening View. When you select this option, the application automatically selects the Peak Detect option.
Create Reports	Creates reports for the current batch.
Submit as a Priority Sequence?	
Priority Sequence	With the Multi-Channel LC feature activated, places the batch immediately after the currently acquiring batch.
	Without the Multi-Channel LC feature activated, specifies one of the following priority options to place the batch in the queue:
	Next Available Batch: Places the batch immediately after the currently acquiring batch.
	Next Available Sample: Places the batch immediately after the currently acquiring sample.
	Note When you select Full Sequence Submission in the Configuration console, these options are unavailable because the current batch and the current sample are, in effect, the same thing.
Acquisition pane	
Device Name	Lists all configured instruments. If the instrument that you want to use is not configured, close the TraceFinder application, configure the instrument, and then reopen the application. You cannot configure an instrument while the TraceFinder application is running.
Use	Specifies the instruments used for this acquisition.
Start Device	Specifies the instrument that is used to initiate the communication with the other instruments. This is usually the autosampler.
Start When Ready	Starts the specified device when all the instruments are ready to acquire data.
Post-run System State	Specifies the system state after it acquires the last batch: On (default), Standby, or Off.
Buttons	
Hide/Show Details	Collapses or expands the acquisition details of the Submit Options dialog box.
OK	Begins the selected processes.
Cancel	Closes the Submit Options dialog box without submitting any tasks.

❖ **To view the output files**

Locate the files to view from the following directories:

- The application writes saved batches to the project folder:

  …\TraceFinderData\Projects\…

- For each acquired sample, the application writes an RSX file to the batch Data folder:

  …\TraceFinderData\Projects\…\Data

- The application saves method information to the batch Methods folder:

  …\TraceFinderData\Projects\…\Methods

- The application writes the reports to the batch Reports folder:

  …\TraceFinderData\Projects\…*batchname*\ReportOutput

Finish Page

| Parameter	Description
System Status	The System Status pane displays the following: • Devices used for the acquisition • Project, subproject, and name of the batch • Number of acquired and unacquired samples in the batch • Number of reports to be printed and saved as PDF, CSV, or Excel files • Local method and instrument method used for the batch • Number of compounds in the method
System Startup Method System Shutdown Method	The instrument methods that run before and after the batch. No autosampler injection takes place. These features are not available for all instruments.
Auto TSRM Update	Updates the TSQ method with mass transitions, collision energy, and other appropriate data for TSRM functionality.
Calibration	• Use calibration: Uses the selected calibration file to process the current data. • Extend calibration: Adds calibration data from the current batch to the selected calibration file.
Previous	Returns you to the previous Acquisition page.
Save	Saves the current batch as a prepared file.
Submit	Opens the Submit Options dialog box.

Using Quick Acquisition

Use the quick acquisition feature to quickly submit samples from any mode in the application.

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

❖ **To run a quick acquisition**

1. Choose **Tools > Quick Acquire Sample** from the main menu or click the **Quick Acquire Sample** icon, .

   The TraceFinder Quick Acquisition window opens.
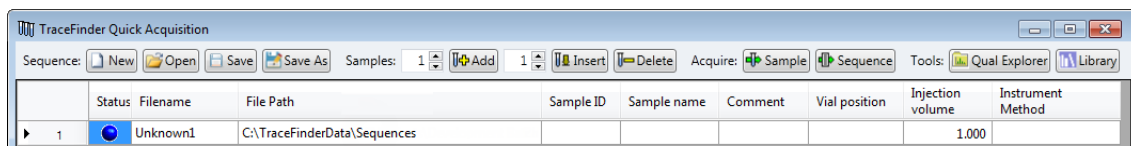
2. To create the sequence of samples that you want to acquire, do any of the following:

- Use the Sequence buttons in the toolbar to open and save Xcalibur sequence (.sld) files.

Sequence: New | Open | Save | Save As
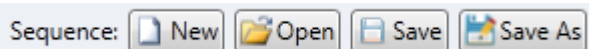
Button	Description
New	Replaces the current sequence with a new sequence that contains one Unknown sample.
Open	Opens a saved SLD file.
Save	Saves the current sequence as an SLD file in the …\TraceFinderData\Sequences folder.
Save As	Saves the current sequence to a new file name or location.

- Use the Samples buttons in the toolbar to create a sequence of samples.

Samples: 1 Add | 1 Insert | Delete
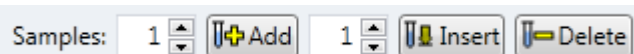
Button	Description
1 Add	Adds the specified number of new, empty samples to the end of the sample list.
1 Insert	Inserts a new, empty sample or samples above the selected sample.
Delete	Removes the selected samples from the sample list.

- Use the Tools buttons in the toolbar to open a qualitative browser or the NIST™ library browser.

Tools: Qual Explorer | Library
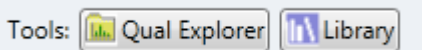
Button	Description
Qual Explorer	Opens the qualitative explorer that you configured as your default qualitative explorer in the Configuration console.
Library	Opens the NIST library browser.

3. When you have completed your sequence of samples, click either of the Acquire buttons.

Acquire: Sample | Sequence
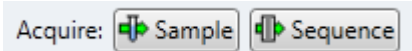
Button	Description
Sample	Submits only the selected samples for acquisition, processing, or report generation.
Sequence	Submits the sequence for acquisition, processing, or report generation.

The application submits the samples for acquisition, processing, and report generation.

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