

TraceFinder Acquisition Quick Reference Guide

This quick reference guide describes the Thermo TraceFinder™ acquisition tasks assigned to the Technician role.

Contents

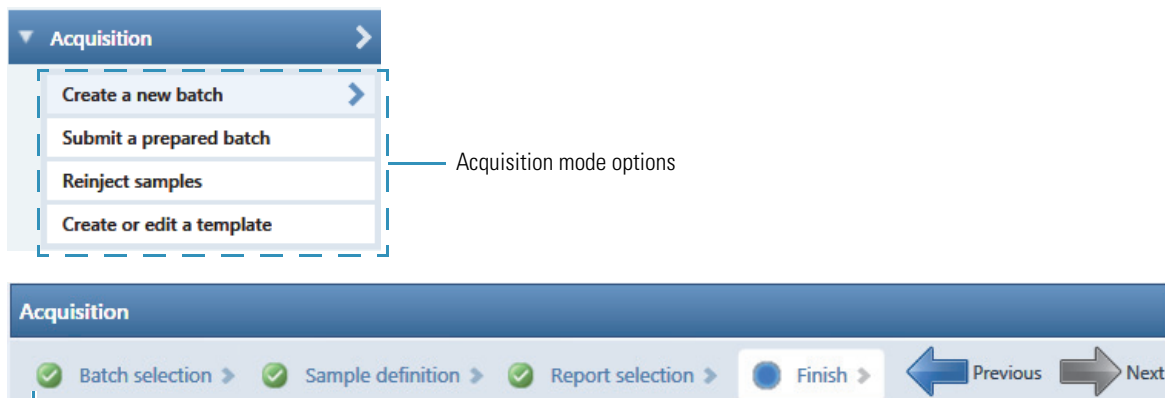
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Acquisition Mode

To open the Acquisition mode, click **Acquisition** from any mode.

Acquisition

Note This mode is available only when you select the Acquisition Batch Wizard style in the Application Configuration mode.



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 subprojects, or use a batch template to start a new batch.

❖ To start a new batch

1. Click **Create a New Batch**.
2. Select either the **Quantitative Batch** option or the **Screening Batch** option.
3. Select a project and subproject where you want to create the new batch.
4. Type a unique name for the new batch in the Batch 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 in the Acquisition mode.

Batch selection | Sample definition | Report selection | Finish

Quantitative batch | Screening batch

Project: Default

Subproject: Default

Batch name: BatchNew3

Available Templates

Template name	Method
Alprazolam_template...	Method_Alprazolam

Template defaults

Project: <none>

Subproject: <none>

Method selection: Alprazolam

Method Compound Data

RT	Compound	Compound type	Active	CAS No	LIMS ID	Use as RT Refer
3.14	Propanenitrile	Target Compound	☒	107120		☐
3.15	Pyrazinamide	Target Compound	☒	98964		☐
3.67	1,3-Dioxolane,...	Target Compound	☒	4359573		☐
4.70	Pyrazinamide ...	Target Compound	☒	98964		☐

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

The Sample Definition page opens. See “Defining the Sample List” on page 5.

❖ To start a new batch from a template

1. Click **Create a New Batch**.
2. Select either the **Quantitative Batch** option or the **Screening Batch** option.
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 project and subproject where you want to create the new batch.
5. (Optional) Select a different method to use for the new batch.

Batch selection | Sample definition | Report selection | Finish

Quantitative batch | Screening batch

Project: Default

Subproject: Default

Batch name: Template_Alprazolam_102212_184358

Available Templates

Template name	Method
Template_Alprazolam	Alprazolam

Template defaults

Project: Default

Subproject: Default

Method selection: Alprazolam

Method Compound Data

RT	Compound	Compound type	Active	CAS No	LIMS ID	Use as RT Refer
3.14	Propanenitrile	Target Compound	☒	107120		☐
3.15	Pyrazinamide	Target Compound	☒	98964		☐
3.67	1,3-Dioxolane,...	Target Compound	☒	4359573		☐
4.70	Pyrazinamide ...	Target Compound	☒	98964		☐

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

The Sample Definition page opens. See “Defining the Sample List” on page 5.

❖ To select a prepared batch

1. Click **Submit a Prepared Batch**.

The application displays all your unacquired, saved batches. The TraceFinder application stores all unacquired batches in the following folder:

...\Thermo\TraceFinder\3.0\General\Projects\projectname\subprojectname

2. Select the batch that you want to acquire.

Batch selection >				Previous	Next
Batch name	Project	Subproject	Last modified		
Batch_Alprazolam_1	Default	Default	8/27/2012 2:16:48 PM		
Batch_Alprazolam_2	Default	Default	8/27/2012 10:56:06 AM		

3. 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 samples list for this batch.

4. Do one of the following:

- To prepare the batch for acquisition, click **Submit**,  **Submit** .
For detailed instructions, see “Submitting the Batch” on page 11.

–Or–

- To edit the samples list, click **Previous**.
For detailed instructions about editing a samples list, see “Defining the Sample List” on page 5.

–Or–

- To save the batch to be acquired later, click **Save**,  **Save** .

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

The TraceFinder application saves batches to the following folder:

...\Thermo\TraceFinder\3.0\General\Projects\projectname\subprojectname

❖ To select a previously acquired batch

1. Click **Reinject Samples**.

From this page, you can resubmit a previously acquired batch, edit the batch, or save it to be acquired later.

2. In the Project pane, select a project name.

3. In the Subproject pane, select a subproject name.

The Batch pane displays all previously acquired batches included in the selected subproject, both quantitative and screening.

4. In the Batch pane, select the batch that you want to reacquire.

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

The Sample Definition page opens. See “Defining the Sample List” on page 5.

❖ **To create a batch template**

1. Click **Create or Edit a Template**.

From this page, you can begin a new batch template.

2. Select either the **Quantitative Batch** option or the **Screening Batch** option.
3. Select the project and subproject 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	Compound type	Active	CAS No
▶	3.14	Propanenitrile	Target Compound	☒	107120
	3.15	EDIFENPHOS-CE5-R20-T...	Target Compound	☒	17109498
	3.67	1,3-Dioxolane, 2-heptyl-	Target Compound	☒	4359573
	4.70	Pyrazinamide	Internal Standard	☒	98964

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

The Sample Definition page opens. See [“Defining the Sample List”](#) on [page 5](#).

Defining the Sample List

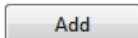
Use the Sample Definition page (see “[Sample Definition Page](#)” on [page 8](#)) of the Acquisition mode to create a list of samples for the batch. You can add samples, insert samples, import a sample list, or remove samples from the list.

As you enter sample values, you can use the Copy Down and Fill Down commands to quickly enter column values. For detailed instructions about using the Copy Down and Fill Down commands to enter column values, refer to the “Using Copy Down and Fill Down” chapter 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](#)” on [page 9](#).
- If you are editing a previously acquired batch or a prepared batch, the Finish page opens. See “[Submitting the Batch](#)” on [page 11](#).

❖ 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 in the sample list and choose **Add Sample** from the shortcut 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	Unknown
Cal Std	QC 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 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 LabDirector permissions to edit the method and specify the levels.

For detailed instructions about defining sample levels, refer to “Using the Method Development Mode” in the *TraceFinder User Guide*.

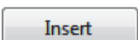
5. For each sample, type a vial position in the Vial Position column.

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

❖ To 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.

Inserted samples

	Status	Filename	Sample type	Qual Processing	Level	Sample ID
1		cal_std_5	Cal Std	☐	5	cal std = 5
2		Unknown2	Unknown	☐		
3		Unknown1	Unknown	☐		
4		cal_std_10	Cal Std	☐	10	cal std = 10

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 “Using the Method Development Mode” in the *TraceFinder User Guide*.

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

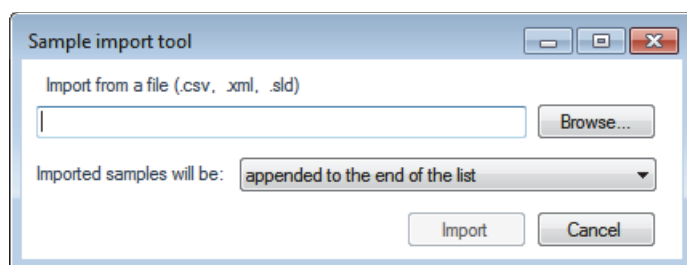
Tip Use the Fill Down command to make entering vial positions easier.

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.



2. Click **Browse** 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 file format must match the TraceFinder file format.

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

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

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

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 LabDirector permissions to edit the method and specify the levels.

For detailed instructions about defining sample levels, refer to “Using the Method Development Mode” in the *TraceFinder 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.

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

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

- (Optional) When using multiplexing, select a channel for each imported sample.

Imported samples default to Auto.

❖ **To remove samples from the list**

- Select the samples you want to remove.

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

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

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

- In the sample list, select the sample that you want to reinject.
- Right-click and choose **Reinject Selected Samples** 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.

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).

	cal_std_50_INJ001	Cal Std	10
	cal_std_50	Cal Std	10
	cal_std_100_INJ001	Cal Std	10
	cal_std_100	Cal Std	10

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

Sample Status Color Codes

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

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

Sample Definition Page

☒ Batch selection >
 ☒ Sample definition >
 ☒ Report selection >
 ☒ Finish >
 Previous Next

Samples		Reference Samples														
	Status	Filename	Sample type	Qual Processing	Level	Sample ID	Sample name	Vial position	Injection volume	Conversion Factor	Channel	Barcode Expected	Sample Volume	Dilution Factor	Sample Weight	Calculation Type
1		Unknown1	Solvent	☐				CStd1-01:1	10.0	1.000	Channel 1		1	1	1	Liquid
2		Unknown2	Unknown	☐				CStd1-01:3	10.0	1.000	Auto		1	1	1	Liquid
3		Unknown3	Matrix Blank	☐				CStd1-01:4	10.0	1.000	Auto		1	1	1	Liquid

Sample Controls: Add Insert Import

Multiplexing Channels: ☒ All Channels ☒ Channel 1 ☒ Channel 2 ☒ Channel 3 ☒ Channel 4

Parameter	Definition
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.
Multiplexing Channels	
	Available only when you have activated multiplexing. Refer to “Using the Application Configuration Mode” in the <i>TraceFinder User Guide</i> .
All Channels	Uses all configured channels to acquire this batch.
Channel 1- <i>n</i>	Uses only the selected channels to acquire this batch.
Previous	Returns you to the previous Acquisition mode page.
Next	Takes you to the next Acquisition mode page.
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.
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 <i>TraceFinder User Guide</i> .
Enable/Disable 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 another application, such as a Microsoft™ Excel™ spreadsheet. 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 another application, such as an Excel spreadsheet. You cannot paste this data back into the method development compound list.
Paste	Pastes one column of copied data from another application, such as an Excel spreadsheet, into the selected column.
Undo Last Paste	Undo 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.

Selecting and Reviewing Reports

Use the Report Selection page (see “[Report Selection Page](#)” on [page 10](#)) of the Acquisition mode to specify the types of reports that you want to create. For a complete list of report types and examples of output files, refer to “Reports” in the *TraceFinder User Guide*.

The Report Selection page lists all the available reports. The Report Selection page displays the report name, report description, report type, and the options to create printed, PDF, XML, or XLSM outputs.

For each standard report that you generate, you can create a hardcopy printout, a PDF (.pdf) file, or an XML (.xml) file. In addition to the report type, you can specify a report title for each of your reports.

For each custom report that you generate, you can create a hardcopy printout or an XLSM file.

For each target screening report you generate, you can create a hardcopy printout or a PDF file.

After specifying your report options, click **Next** to go to the Finish page and submit your batch. See “[Submitting the Batch](#)” on [page 11](#).

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

...\\TraceFinder\\3.0\\General\\Projects*projectname**subprojectname**batchname*\\Reports

❖ To edit a report description

Select the text in the Report Description column and edit the default name.

The default report description is the same as the report name.

❖ To preview a standard report

1. Click  (magnifier icon) to view an example of the report type as a PDF file.

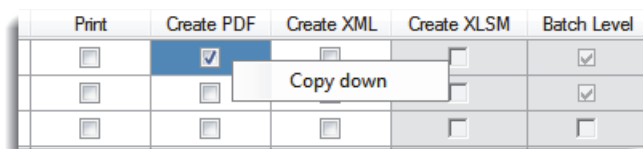
The right pane of the page displays an example PDF report with typical PDF viewer controls.

Note Only Standard report types have preview documents.

2. To minimize the PDF viewer, click .

❖ To specify a standard report in hardcopy print, as a PDF file, or in XML format

1. For each report that you want to create, select the check box in the Print, Create PDF, or Create XML columns.
2. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.



Print	Create PDF	Create XML	Create XLSM	Batch Level
☐	☒	☐	☐	☒
☐	☐	☐	☐	☒
☐	☐	☐	☐	☐

All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell. This action applies only to report types that make this output format available.

❖ To specify a custom report in hardcopy or XLSM format

1. For each custom report that you want to create, select the check box in the Print or Create XLSM columns.
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. This action applies only to report types that make this output format available.

❖ To specify a ToxID or target screening report in hardcopy format or as a PDF file

1. For each ToxID or target screening report that you want to create, select the check box in the Print or Create PDF columns.
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. This action applies only to report types that make this output format available.

❖ To export the reports to a specific folder

1. Select the **Export Results** check box at the bottom of the page.



You can export your reports to any directory.

2. Locate and select the folder where you want to save the reports.
3. To create a new reports folder within the selected folder, click **Make New Folder** and type the new folder name.
4. Click **OK**.

The application saves all reports in the specified folder in addition to the batch Reports folder.

Report Selection Page

Example	Report Name	Report Title	Report Type	Print	Create PDF	Create XML	Create XLSM	Batch Level
	Batch Report	Batch Report	Standard	☐	☒	☐	☐	☒
	Alternate BatchReport	Alternate BatchReport	Custom	☐	☐	☐	☐	☒
	Target Screening Su...	Target Screening Su...	Target Screenii	☐	☐	☐	☐	☐
	Target Screening Su...	Target Screening Su...	ToxID	☐	☐	☐	☐	☐

Parameter	Description
Example	(For standard reports only) Displays an example PDF for the report type. This example provides a model of the report type only; it does not reflect your data.
Report Name	The name of a report.
Report Title	User-editable description to be used on a report.
Report Type	The type of report: Standard, Custom, ToxID, or Target Screening.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files.
Create XML	Reports to be exported in XML format.
Create XLSM	Reports to be exported in XLSM format.
Batch Level	Instead of creating separate reports for each sample, the application uses a composite of the data from all the samples to create a single report for the entire batch. Batch-level reports have a B prefix to differentiate them. You cannot select this option from the Report Selection page. You must select the Batch Level option for the report in the report configuration.
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.

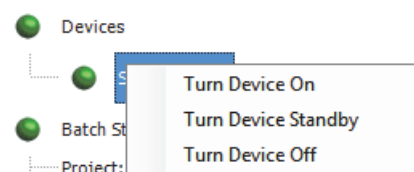
Submitting the Batch

Use the Finish page (see “[Finish Page](#)” on [page 14](#)) 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, right-click the name of the device, and then choose a device state from the shortcut menu.



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.

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

System startup method:

System shutdown method:

❖ To automatically update the timed selected reaction monitoring information

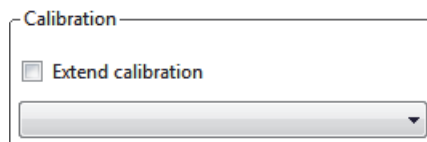
Select the **Auto TSRM Update** check box.

☐ **Auto TSRM Update**

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, select a calibration (.calx) file from the list.



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

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

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

From the Finish page, click **Save**,  **Save** .

The TraceFinder application saves your batch as a prepared file, closes the Acquisition mode, and returns you to the application dashboard.

❖ **To start an acquisition**

1. Click **Submit**,  **Submit** .

The Submit Options dialog box opens. See [Submit Options Dialog Box](#).

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

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

3. Select the **Use** check box for the device that you want to use for this acquisition.
4. (Optional) Select the **Start Device** check box to indicate which device initiates the communication with the other instruments.
This is usually the autosampler.
5. (Optional) Select the **Start When Ready** check box to have all instruments start together when they are all ready.
When you clear this option, individual instruments can start at different times and then have to wait for the last instrument to be ready.
6. (Optional) Select the **Priority Sequence** check box and then select one of the priority options to place the batch in the queue.
 - Select **Next Available Batch** to place the batch immediately after the currently acquiring batch.
 - Select **Next Available Sample** to place the batch immediately after the currently acquiring sample.

Note When you are using multiplexing features, the application acquires the priority batch on the next available channel or the assigned channel.

7. Do one of the following:
 - To start the selected processes, click **OK**.
The selected processes begin, and the TraceFinder application returns you to the dashboard and shows the real-time display at the bottom of the dashboard. The real-time display is visible from the dashboard and all modes. You can begin another batch in Acquisition mode while you watch the real-time display of the currently acquiring batch.
 - Click **Cancel** to exit Acquisition mode without performing any tasks.

Submit Options Dialog Box

Submit Options

User name:

Samples:

☒ Acquire data

☒ Process data

☐ Create reports

Priority

☐ Priority Sequence

☒ Next Available Batch

☐ Next Available Sample

Acquisition

Device Name	Use	Start Device
Accela AS	☒	☒

☒ Start when ready

Post-run system state:

Programs

Pre-acquisition:

☐ Wait for program completion

Post-acquisition:

☐ Wait for program completion

Parameter	Description
User Name	Displays the name of the current user.
Samples	Reports the batch number and number of samples.
Acquire Data	(Default) Submits the current batch to acquisition.
Process Data	(Default) Processes the data for the current batch.
Create Reports	Creates reports for the current batch.
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.
Priority Sequence	With multiplexing activated, places the batch immediately after the currently acquiring batch. Without multiplexing 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 Application Configuration mode, these options are unavailable because the current batch and the current sample are, in effect, the same thing.	
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 locate the output files

Locate the files to view from the following directories:

- The TraceFinder application writes saved batches to the subproject folder:
`...\\TraceFinder\\3.0\\General\\Projects\\projectname\\subprojectname`
- For each acquired sample, the application writes an RSX file to the batch Data folder:
`...\\projectname\\subprojectname\\batchname\\Data`
- The application saves method information to the batch Methods folder:
`...\\projectname\\subprojectname\\batchname\\Methods\\methodname`
- The application writes the reports to the batch Reports folder:
`...\\projectname\\subprojectname\\batchname\\Reports`

Finish Page

Parameter	Description
System Status	The System Status pane displays the following: • The devices used for the acquisition • The project, subproject, and name of the batch • The number of samples in the batch • The number of reports to be printed or saved as PDF, XML, or XLSM files • The local method and instrument method used for the batch • The number of compounds in the method
System Startup Method	The instrument method that runs before the batch. No autosampler injection takes place. This feature is not available for all instruments.
System Shutdown Method	The instrument method that runs after the batch. No autosampler injection takes place. This feature is 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 mode page.
Cancel	Confirms that you want to exit Acquisition mode. Your edits are not saved.
Save	Saves the current batch as a prepared file.
Submit	Opens the Submit Options dialog box where you can optionally choose to generate reports.

Quick Acquisition

Use the quick acquisition feature to quickly submit a single sample from any page of the Acquisition mode.

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

❖ To run a quick acquisition

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

The Quick Acquisition dialog box opens.

2. Select an instrument method.
3. Type a name for the raw data file that you acquire.
4. For the path, browse to a folder where you want to write the acquired raw data file.
5. Select either the manual injection or the autosampler option:
 - To perform manual injection, do the following:
 - i. Select the **Manual Injection** option.
 - ii. Click **OK**.

The application submits the sample to the Acquisition queue.

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

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

- iv. Click **OK**.

The Quick Acquisition dialog box opens.

Device Name	Use	Start Device
Accela AS	☒	☐

- v. (Optional) Select the **Start Device** check box to indicate the device that will initiate communication with the other instruments.
This is usually the autosampler.
- vi. (Optional) Select the **Start When Ready** check box, which starts all instruments together when they are all ready.
When this is cleared, individual instruments can start at different times and then must wait for the last instrument to be ready.
- vii. (Optional) Select the **Priority** check box to place the sample immediately after any currently acquiring sample.
- viii. (Optional) Select a value for the Post-run System State: **Unknown**, **On** (default), **Off**, or **Standby**.
The application sets the system to this state after it acquires the last sample.
- ix. Click **OK**.

The application submits the sample to the Acquisition queue.

Trademarks

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