

Thermo QuickQuan 2.6 Quick Start Guide

This guide provides a brief overview of how to use the Thermo QuickQuan™ 2.6 rapid optimization and acquisition application to perform high-throughput optimization and acquisition for quantitative experiments.

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Workflow Overview

The optimization and acquisition workflow includes the following steps. If you have already optimized the compounds and are performing an acquisition only, start with [Step 3— Setting Up for Acquisition](#).



[Step 1— Adding Compounds and Drug Sets](#)



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Specifying the template information and internal standards (ISTDs), if applicable



Setting up acquisition sequences



[Step 4— Submitting the Samples for Analysis](#)



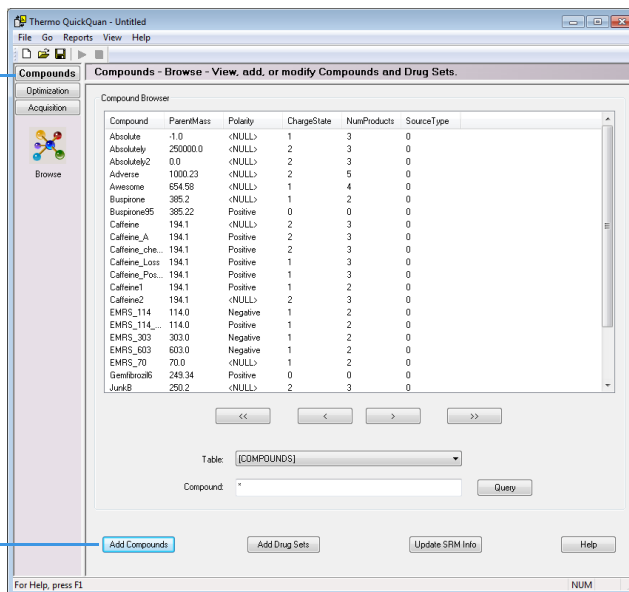
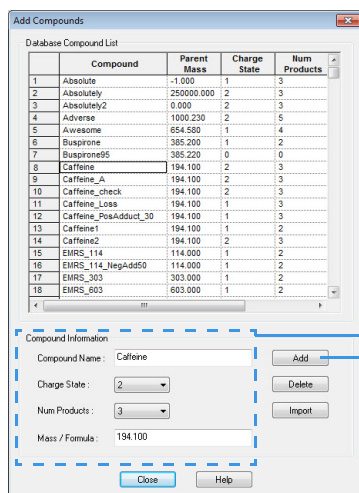
[Step 5— Reviewing the Results](#)

Step 1— Adding Compounds and Drug Sets



❖ To add compounds to the QuickQuan database

1. Click **Compounds**.
The Compounds Browse page appears.
2. Click **Add Compounds** to open the Add Compounds dialog box.



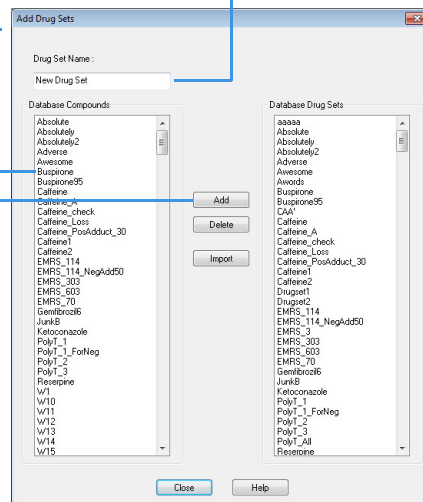
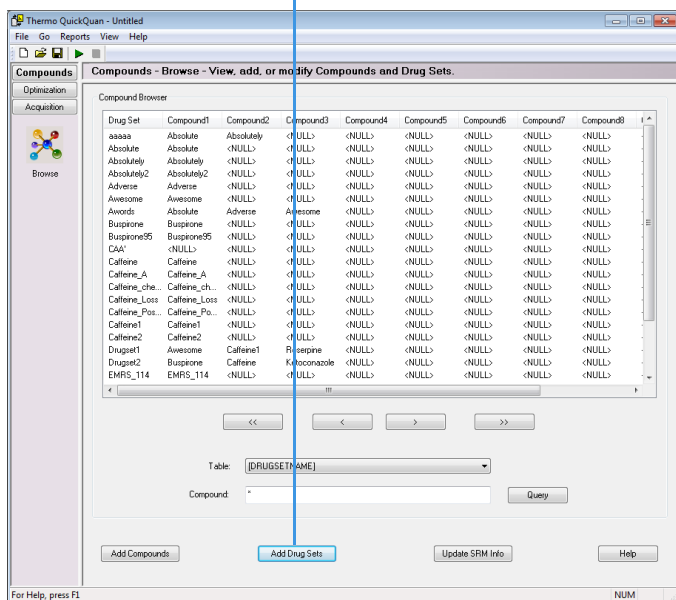
3. Provide the compound information and click **Add**.

Or, click **Import** to import the compounds from a text file. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.

4. Click **Close**. The QuickQuan application adds the compounds to the selected database.

❖ To add drug sets to the QuickQuan database

1. On the Compounds Browse page, click **Add Drug Sets** to open the Add Drug Sets dialog box.
2. Type a drug set name.



3. In the Database Compounds list, select the compounds to add to the drug set and click **Add**.

Or, click **Import** to import the drug sets from a text file.

4. Click **Close**. The QuickQuan application adds the drug sets to the selected database.

Step 2— Setting Up for Optimization



IMPORTANT Before you can set up for optimization, you must configure an autosampler. If you configure an autosampler that is not supported for optimization, the QuickQuan application disables all settings on the Optimization Setup page.

❖ To set up the QuickQuan application for optimization if available

1. Click **Optimization** and click the **Setup** icon. The Optimization Setup page appears (see Figure 1).
2. Specify the generic tune file (only for the TSQ Quantum™ series or TSQ Vantage™ mass spectrometer), generic instrument method file, output folder for storing optimization data files, optimization settings, and tune plate setup as described in the *QuickQuan User Guide* or QuickQuan Help.

Note For the TSQ Endura™ or TSQ Quantiva™ mass spectrometer, the generic instrument method for optimization must be a compound optimization (CO) method. You can locate the default optimization methods in this folder:

drive:\Xcalibur\QuickQuan\Templates

Figure 1. Optimization Setup page

Optimization button and Setup icon

Generic instrument method file


Output folder for storing optimization data files

Optimization Settings and Plate Setup areas

Note To reoptimize compounds that are already in the database, clear this check box.

Instrument	In Use	Start Instrument
Thermo Scientific SII for Xcalibur	Yes	Yes
TSQ Quantiva	Yes	Yes

3. Do one of the following:

- To run an optimization and acquisition, go to “Step 3— Setting Up for Acquisition” on page 4.
- To run an optimization only, click the **Run** icon, ,

4. In the Run-time Settings area:

- a. Select the **Compound Optimization Only** option.
- b. (Optional) Select the **Use Optimization Database for Existing Compounds** check box.

Note If you select the Use Optimization Database for Existing Compounds check box, the QuickQuan application optimizes only the compounds that are considered not tuned in the database. Otherwise, this application optimizes all the compounds in the tune plate.

- If you configure the Aria™ MX or SII driver (same driver for both the pump and autosampler), verify that the Instrument column lists the mass spectrometer and this driver. Otherwise, verify that the Instrument column lists the mass spectrometer, LC pump, and autosampler. Set the Aria MX/SII driver or autosampler as the start instrument. (**Yes** appears in the Start Instrument column.)

If the appropriate instruments do not appear in the Instrument Settings area, exit the QuickQuan application, set up the instruments using the Thermo Foundation™ Instrument Configuration application, and then return to this step.

- Verify the processing settings. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.
- Click **OK**.

The QuickQuan application submits the sequence to start optimization and displays status messages.

Note After you start the optimization run, you can launch other instances of the QuickQuan application if you want to submit additional sequences for optimization or acquisition. Each new instance places the optimization or acquisition sequence into the queue to be processed in the order of submission. Each QuickQuan instance continues processing until the sequence analysis from that instance is complete or you cancel the run.

Step 3— Setting Up for Acquisition



❖ To set up the QuickQuan application for acquisition

- Click **Acquisition** and click the **Templates** icon. The Acquisition Templates page appears (see [Figure 2](#)).
- Create the instrument and processing methods. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.

Note For the TSQ Endura or TSQ Quantiva mass spectrometer, the generic instrument method for acquisition must be a selected reaction monitoring (SRM) method. You can locate the default acquisition methods in this folder:

drive:\Xcalibur\QuickQuan\Templates

- Complete the Template Information and Internal Standard areas, if applicable. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.

Figure 2. Acquisition Templates page

Acquisition button and Templates icon

Generic instrument method file

Generic quantitation method file for automated batch analysis

Output folder for storing acquired data files

Single or multiple internal standards (ISTDs)

	Target Compound	ISTD Reference
1		
2		
3		
4		
5		
6		
7		
8		
9		

- Click the **Setup** icon and specify the acquisition sequences on the Acquisition Setup page (see Figure 3). For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.

Figure 3. Acquisition Setup page

Setup icon Each ✓ indicates a new sequence.



	New Sequence	Drug Set	Sample Name	Sample Type	Level	Sample ID	Inst. Method
1	✓	Drugset2	Sample1	Blank	NA	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
2	✓	Drugset2	Sample2	Std Update	1	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
3		Drugset2	Sample3	Std Update	5	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
4		Drugset2	Sample4	Std Update	10	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
5		Drugset2	Sample5	Std Update	20	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
6		Drugset2	Sample6	Std Update	40	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
7		Drugset2	Sample7	Std Update	80	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
8		Drugset2	Sample8	Std Update	160	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
9		Drugset2	Sample9	Std Update	320	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
10		Drugset2	Sample10	Std Update	1600	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
11		Drugset2	Sample11	Blank	NA	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
12		Drugset2	Sample12	Blank	NA	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
13		Drugset2	Sample13	Blank	NA	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
14		Drugset2	Sample14	QC	QC1	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
15		Drugset2	Sample15	QC	QC1	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
16		Drugset2	Sample16	QC	QC2	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
17		Drugset2	Sample17	QC	QC2	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
18		Drugset2	Sample18	QC	QC3	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
19		Drugset2	Sample19	QC	QC3	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
20		Drugset2	Sample20	Blank	NA	2	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
21		Drugset2	Sample21	Blank	NA	3	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
22		Drugset2	Sample22	Blank	NA	3	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
23		Drugset2	Sample23	Unknown	NA	3	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
24		Drugset2	Sample24	Unknown	NA	3	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
25		Drugset2	Sample25	Unknown	NA	3	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
26		Drugset2	Sample26	Blank	NA	3	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
27		Drugset2	Sample27	Blank	NA	3	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
28	✓	Drugset1	Sample28	Blank	NA	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
29		Drugset1	Sample29	Std Update	1	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
30		Drugset1	Sample30	Std Update	5	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
31		Drugset1	Sample31	Std Update	10	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
32		Drugset1	Sample32	Std Update	20	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
33		Drugset1	Sample33	Std Update	40	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
34		Drugset1	Sample34	Std Update	80	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth
35		Drugset1	Sample35	Std Update	160	1	C:\calbur\QuickQuan\Templates\Acquisition_Quantiva.meth

Step 4— Submitting the Samples for Analysis



❖ To submit samples for analysis

- In the QuickQuan left pane, click the **Run** icon. The Configuration Options dialog box appears (see Figure 4).

Figure 4. Configuration Options dialog box

Run icon

The screenshot shows the 'Acquisition - Setup' window with a table of samples. The 'Run' icon in the left pane is highlighted. The 'Configuration Options' dialog box is open, showing the following settings:

- Run-time Settings:**
 - Compound Optimization and Acquisition
 - Compound Optimization Only
 - Use Optimization Database for Existing Compounds
- Instrument Settings:**

Instrument	In Use	Start Instrument
Thermo Scientific SII for Xcalibur	Yes	Yes
TSQ Quantiva	Yes	Yes
- Processing Settings:**
 - Number of Quan Masses: 3 Threshold %: 90
 - Mass Window Width: 1
 - Put Instrument into Standby After Batch
 - Do Post Processing after Acquisition
 - Generate Excel Summary
 - Run User Defined Macro

- In the Run-time Settings area, do the following:

- Select the **Compound Optimization and Acquisition** option if it is available.

Note If you use an autosampler that is not supported for optimization, the dialog box shows only the Acquisition Only option selected by default.

- (Optional) Select the **Use Optimization Database for Existing Compounds** check box if it is enabled.

Note If you select the Use Optimization Database for Existing Compounds check box, the QuickQuan application optimizes only the compounds that are required for acquisition but considered not tuned in the database. Otherwise, this application optimizes all the compounds in the tune plate required for acquisition before starting the acquisition sequence.

If you use an autosampler that is not supported for optimization, the application automatically selects this check box and you cannot clear it.


- If you configure the Aria MX or SII driver (same driver for both the pump and autosampler), verify that the Instrument column lists the mass spectrometer and this driver. Otherwise, verify that the Instrument column lists the mass spectrometer, LC pump, and autosampler. Set the Aria MX/SII driver or autosampler as the start instrument. (**Yes** appears in the Start Instrument column.)

If the appropriate instruments do not appear in the Instrument Settings area, exit the QuickQuan application, set up the instruments using the Foundation Instrument Configuration application, and then return to this step.

- Verify the processing settings. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.
- Click **OK**. The QuickQuan application starts processing the submitted batch of samples and displays the optimization and/or acquisition status messages.

Note After you start the acquisition run, you can launch other instances of the QuickQuan application if you want to submit additional sequences for optimization or acquisition. Each new instance places the optimization or acquisition sequence into the queue to be processed in the order of submission. Each QuickQuan instance continues processing until the sequence analysis from that instance is complete or you cancel the run.

❖ **To monitor the optimized/acquired data in real time**

On the toolbar of the Xcalibur™ data system Home Page, click  (Real Time Plot View). In the Real Time Plot View window, you can view the real-time updates of status, spectra, and chromatograms from the optimization/acquisition. For details on using the Xcalibur data system, refer to the Xcalibur Help.

❖ **To review the optimization results**

- Choose **Reports > Optimization Summary Report**. The Optimization Summary Report opens in the Microsoft™ Excel™ spreadsheet application.

–or–

1. In the QuickQuan left pane, click **Optimization** and then click the **Tune Report** icon. The Optimization Tune Report page appears.
2. Select a compound from the list on the left. The tune report displays the optimization results for the selected compound.

❖ **To review the quantitation results**

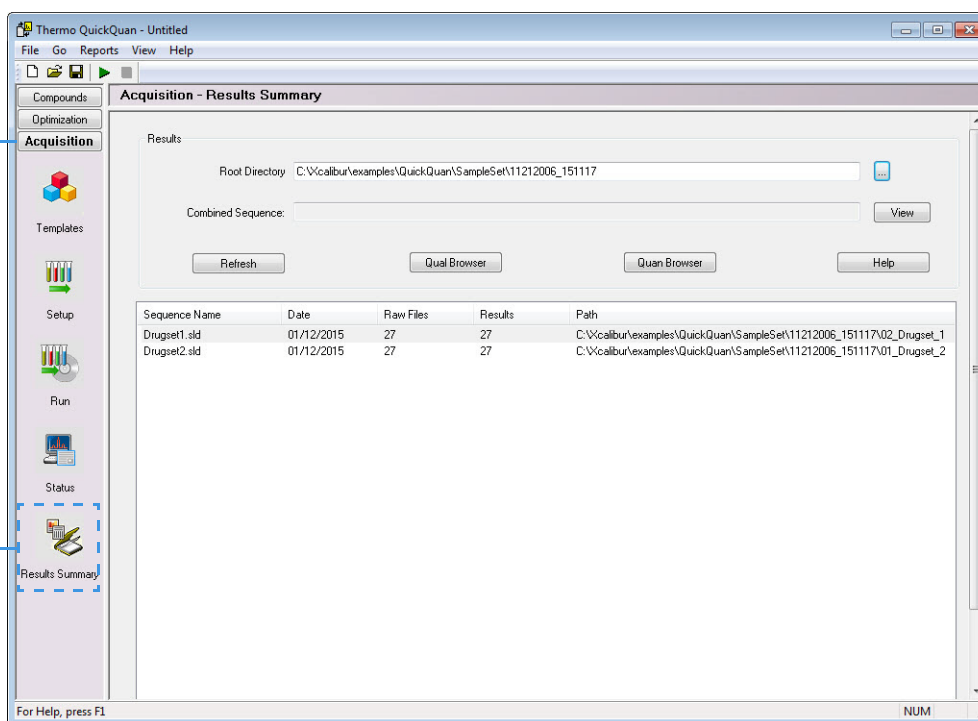
1. Choose **Reports > Acquisition Summary Report**.
2. Select the folder that contains your acquisition data and individual sample report files (.xls), and then click **OK**. The Acquisition Summary Report opens in the Excel application.

–or–

1. In the QuickQuan left pane, click **Acquisition** and then click the **Results Summary** icon. The Acquisition Results Summary page appears (see Figure 5).


Figure 5. Acquisition Results Summary page

Results Summary icon



Step 5— Reviewing the Results

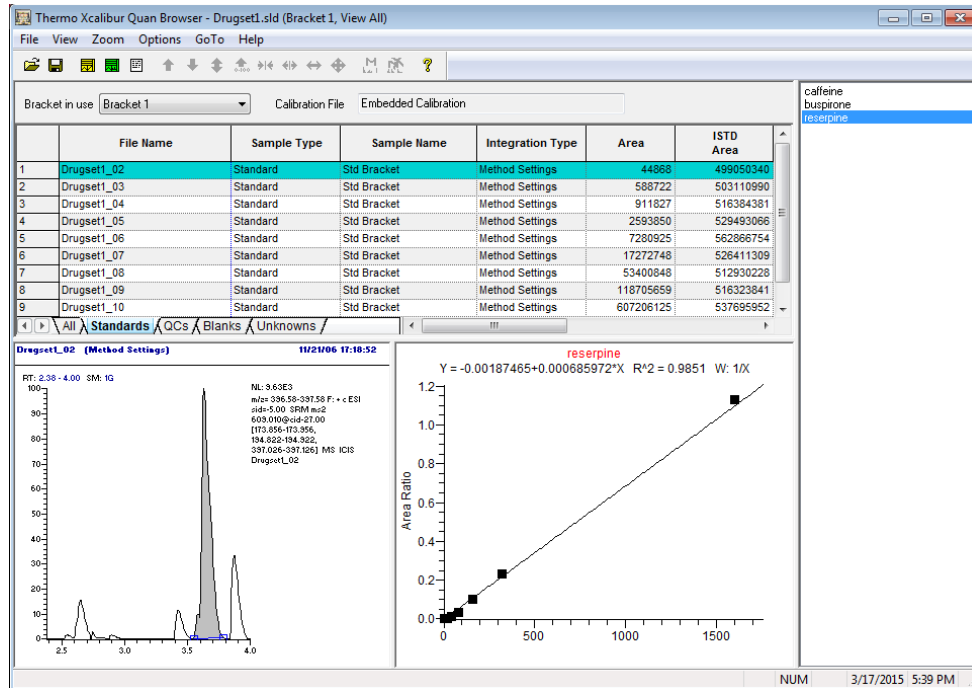


- For the Root Directory box, click  to search for and select the output folder that the QuickQuan application created, for example:

C:\Xcalibur\examples\QuickQuan\SampleSet\11212006_151117

- Select the sequence whose results you want to view, for example: **Drugset1.sld**.
- Click **Quan Browser** to launch the Xcalibur Quan Browser window (see [Figure 6](#)). On the right side of the window, select a component to display the results. For details on the Quan Browser window, refer to the Xcalibur Help.

Figure 6. Quan Browser window



Related Documents

For more information about the QuickQuan application, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.

For more information about the Xcalibur data system, refer to the Xcalibur Help.

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