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

Step 2— Setting Up for Optimization

Step 3— Setting Up for Acquisition

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

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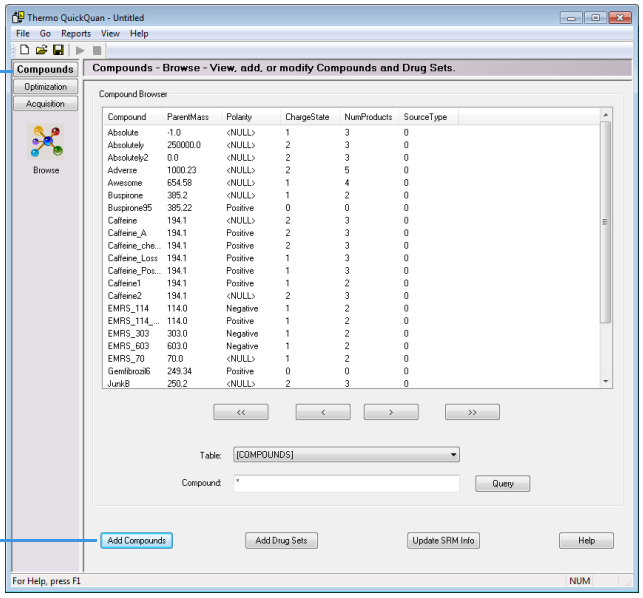
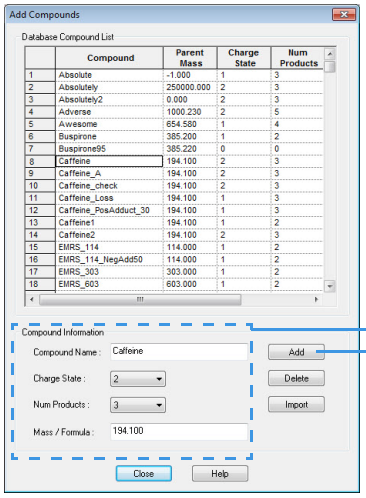
Step 1—Adding Compounds and Drug Sets

❖ 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.



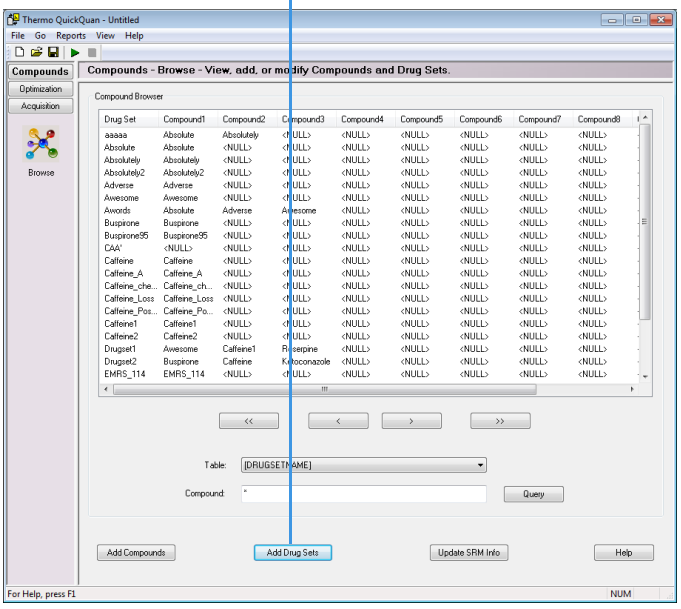


3. Provide the compound information and click **Add**.

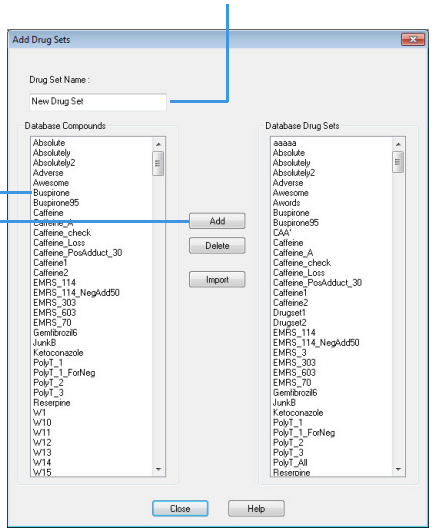
   Or, click **Import** to import the compounds from a text file. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.
4. Click **Close**. The QuickQuan application adds the compounds to the selected database.

❖ 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.

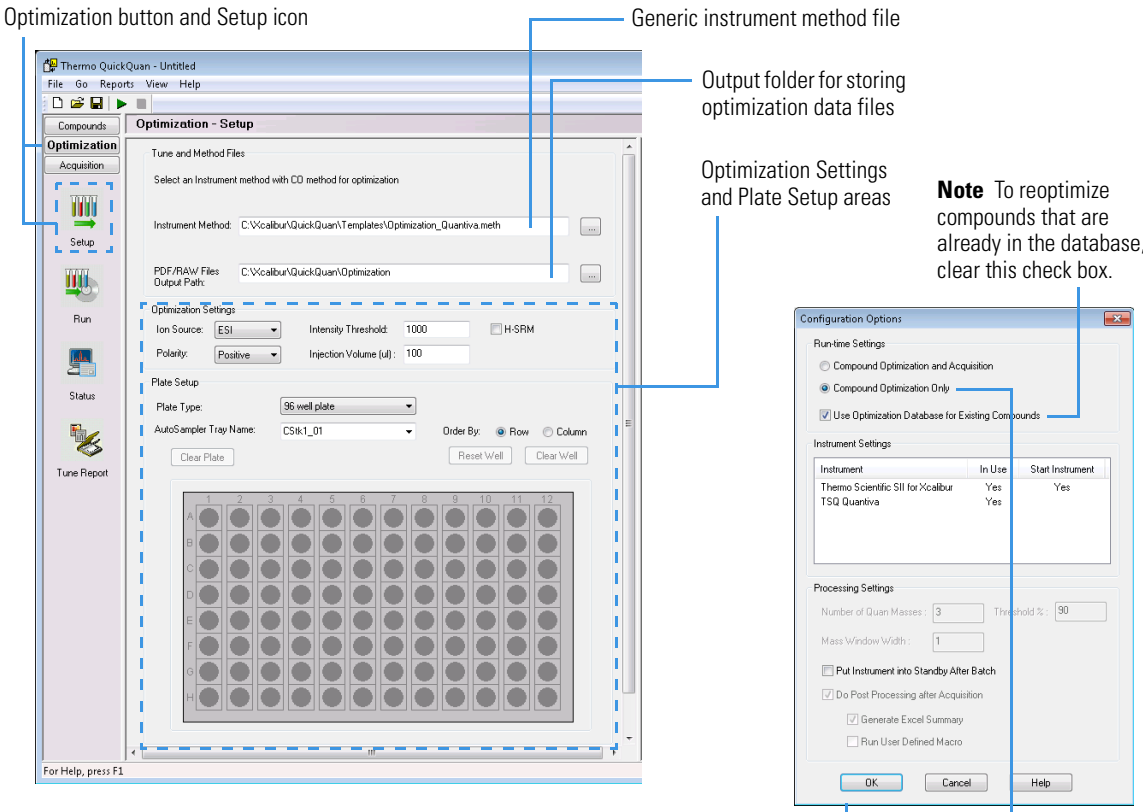
❖ To set up the QuickQuan application for optimization if available

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



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,  , to open the Configuration Options dialog box.
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.

5. 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.
6. Verify the processing settings. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.
7. 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**

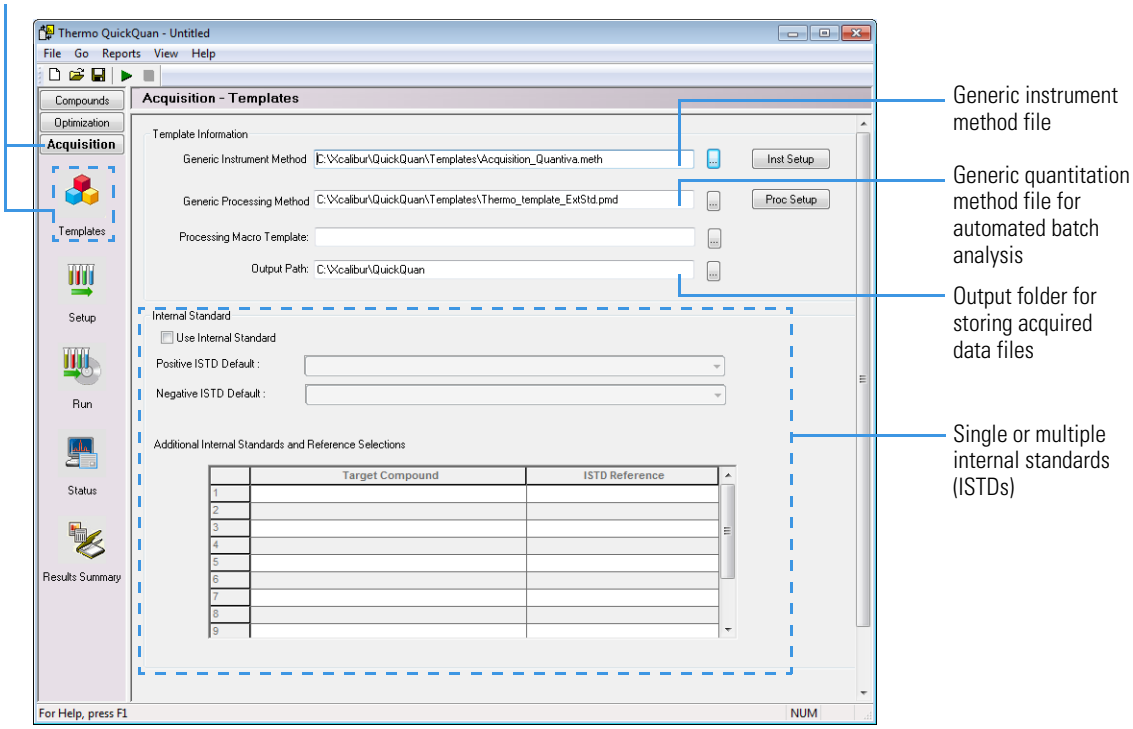
1. Click **Acquisition** and click the **Templates** icon. The Acquisition Templates page appears (see Figure 2).
2. Create the instrument and processing methods. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.

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\

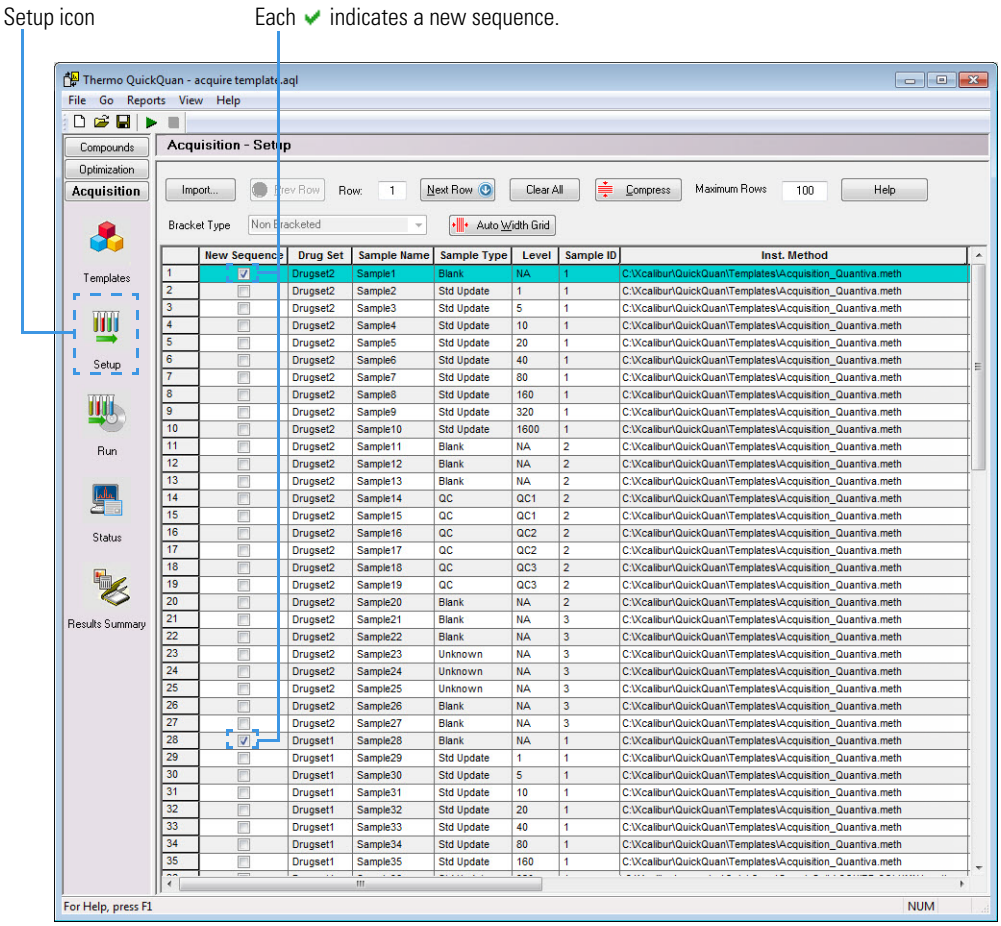
3. Complete the Template Information and Internal Standard areas, if applicable. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.

Figure 2. Acquisition Templates page



4. 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

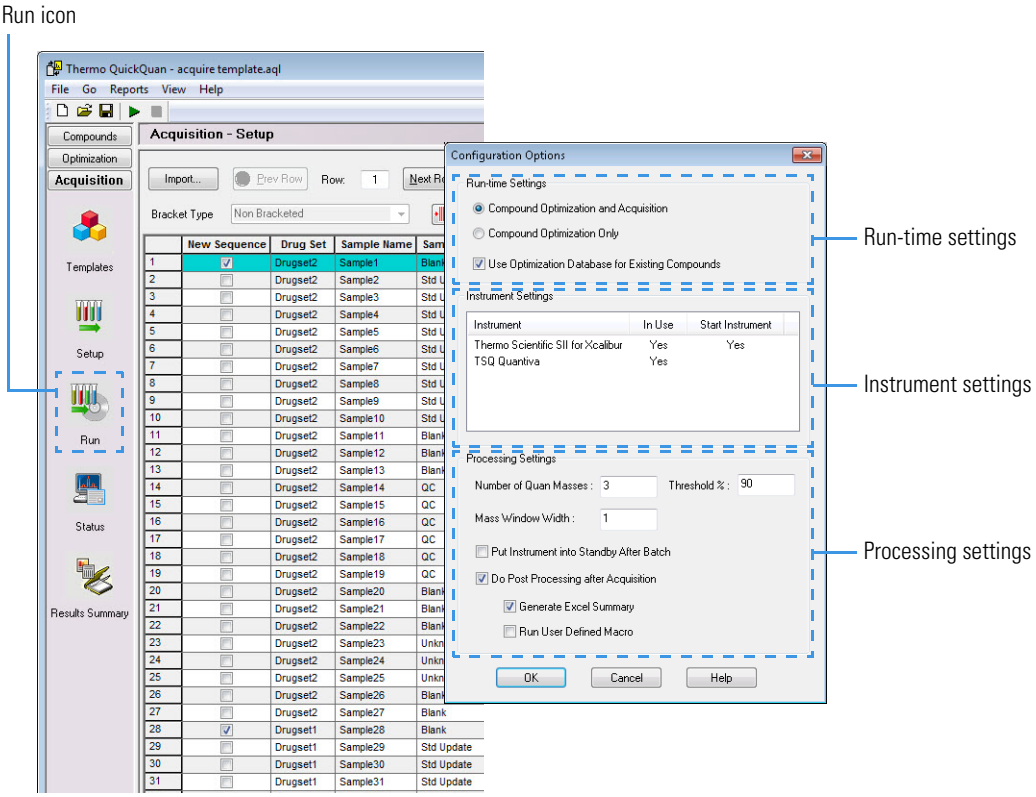


Step 4—Submitting the Samples for Analysis

❖ To submit samples for analysis

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

Figure 4. Configuration Options dialog box



2. In the Run-time Settings area, do the following:
   a. 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.

   b. (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.

3. 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.
4. Verify the processing settings. For details, refer to the *Thermo QuickQuan User Guide* or QuickQuan Help.
5. 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.

Step 5—Reviewing the Results

❖ 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

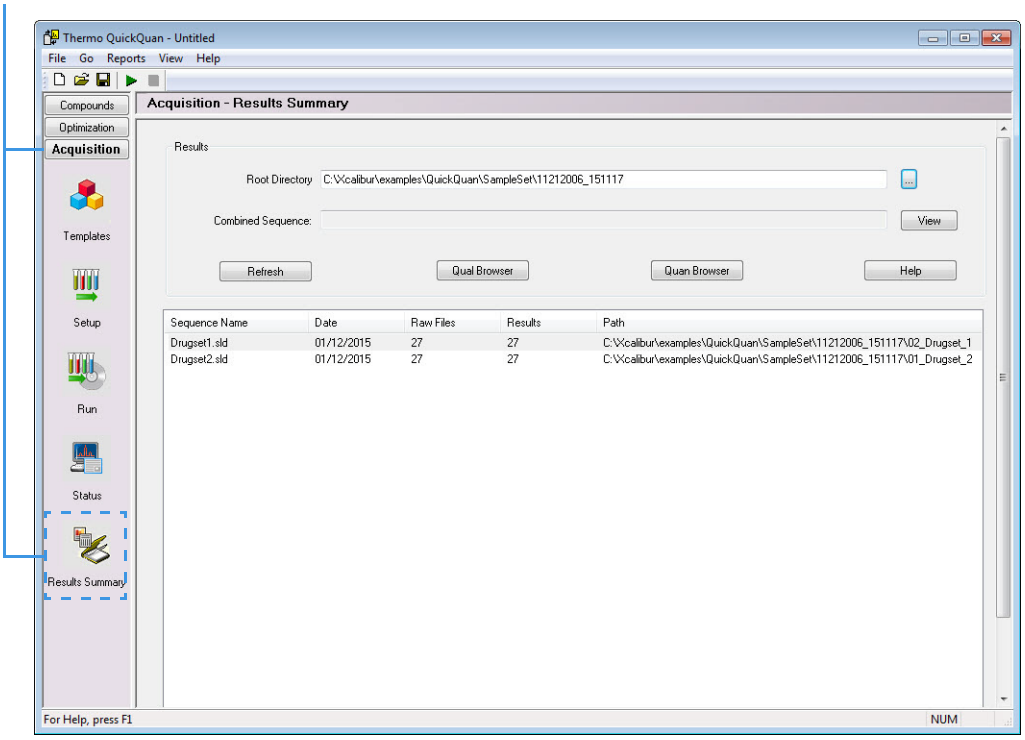
1. Choose **Reports > Acquisition Summary Report**.
2. Select the folder that contains your acquisition data and individual sample report files (.xls), and then click **OK**. The Acquisition Summary Report opens in the Excel application.

–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

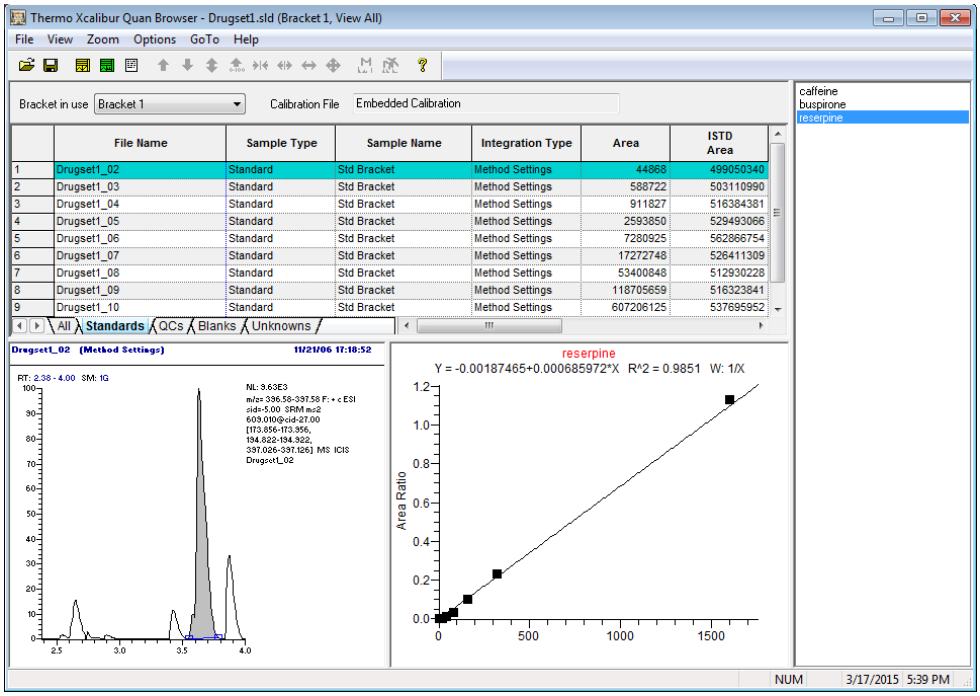


2. For the Root Directory box, click … to search for and select the output folder that the QuickQuan application created, for example:

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

3. Select the sequence whose results you want to view, for example: **Drugset1.sld**.
4. 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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