# Thermo Xcalibur 4.1 Quick Start Guide

This guide describes the new Roadmap view for the Thermo Xcalibur™ 4.1 data system. It also describes how to set up the instrument configuration, view the instrument status, create instrument methods, and create and run acquisition sequences.

For complete information about acquiring raw data files (.raw), refer to the *Xcalibur Data Acquisition and Processing User Guide*.

### Contents

❖ **To open the Xcalibur data system**

- From the taskbar, choose **Start > All Programs > Thermo Xcalibur > Xcalibur**.

–or–

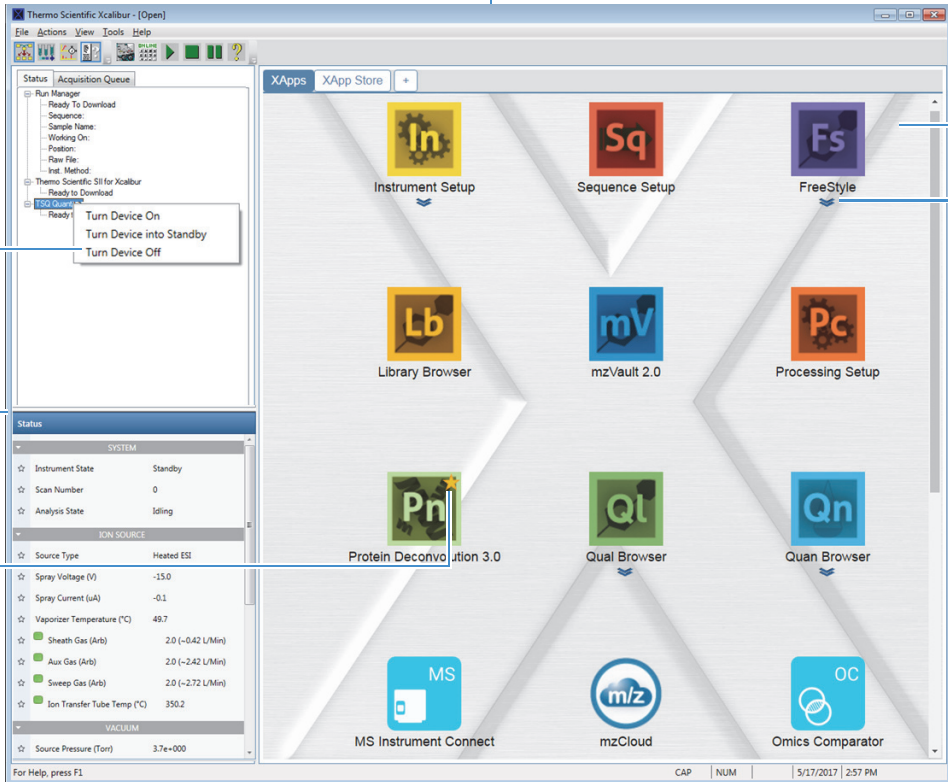- On the desktop, double-click the **Xcalibur** icon, .

The home page window opens with the Info view on the left and the Roadmap view (open to the XApps page) on the right.

The XApps page provides access to the Xcalibur data system and other Thermo Scientific applications that are installed on the data system computer. The XApp Store page—which opens when you click the XApp Store tab—provides access to Thermo Scientific applications that are available for trial and purchase (see Installing Trial Versions of Applications for more information).

The Status page of the Info view displays the instrument status and the Acquisition Queue page displays the status of the injection sequences that you submit.

❖ **To navigate the Xcalibur data system**

To navigate the home page views (Roadmap, Sequence Setup, Real Time Plot, and Info), use the View menu or the View toolbar, .



Info view

Shortcut menu

Complete status information for the selected instrument in the directory tree

The star indicates that a later version of this application is available in the XApp Store.

Roadmap view

Clicking the double chevron below the application icon opens a menu.

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❖ **To open the Help topic for the current item**

- In the toolbar, click the **Help** icon, ❓.
- From the menu bar, choose **Help > Help on Current Item**.

—or—

- On the computer keyboard, press the F1 key, ⌨.

❖ **To open the Help to the Welcome topic**

From the menu bar, choose **Help > Xcalibur Help**.

❖ **To close the Xcalibur data system**

- Click the **Close** icon, ❌, in the upper right corner of the Xcalibur window.

—or—

- Right-click the **Xcalibur** icon in the taskbar and choose **Close Window** from the shortcut menu.

## Working with the Xcalibur Roadmap View

The XApps page contains the following icons:

- The first row contains icons for the Instrument Setup window, the Sequence Setup view, and the FreeStyle™ application.
- The remaining Xcalibur applications and other installed Thermo Scientific applications populate the page in alphabetical order from left to right and top to bottom.
- The last row contains icons for the mzCloud™, Planet Orbitrap, and Thermo Fisher Cloud application websites.

The data system automatically detects the installed applications. If the XApp Store contains a later version of an installed application, a star (⭐) appears in the upper right corner of the application icon. You cannot hide or rearrange the icons on the XApps page.

### Adding Custom Pages to the Roadmap View

You can customize the Roadmap view by adding pages that provide access to your preferred set of Thermo Scientific applications.
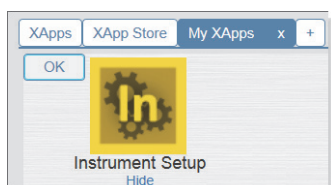
❖ **To add custom pages to the Roadmap view**

In the Roadmap view, click the **My XApps** icon, ⊞. A new My XApps page opens with the same icons as the XApps page.
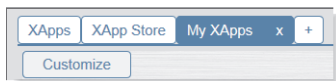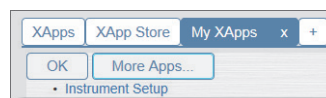


❖ **To hide applications on a custom page**

1. Click **Customize**. "Hide" appears below each application icon and the OK button replaces the Customize button.



2. To hide an application, click **Hide**. The application icon disappears from the page. Once you hide at least one application, the More Apps button appears to the right of the OK button.

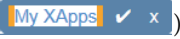3. Click **OK** to save the changes.

❖ **To show installed applications on a custom page**

1. Click **More Apps**. A list of the hidden applications appears below the button. If the More Apps button is not visible, the custom page already contains icons for all the installed applications.



2. From the More Apps list, select the hidden application that you want to show on your custom page.

❖ **To rename a MyXApps tab**

1. Double-click the **MyXApps** tab ().

2. Select the tab text.

3. Type a new name.

4. Click ✔.

## Installing Trial Versions of Applications

Use the XApps Store to install trial versions of Thermo Scientific applications.

❖ **To install a trial version of an available application**

1. Click the **XApps Store** tab. The XApp Store opens.
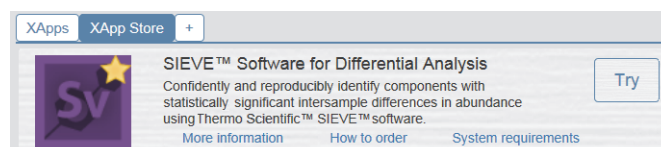


2. Click **Try** to the right of the application that you want to install. The Life Sciences and Mass Spectrometry (LSMS) website for software downloads opens to the Login page.

3. If you do not have a login ID, click **Register** to set one up. After you receive a confirmation email, log in. The Product Download page appears.

4. Download the compressed folder that contains the application.

## Setting Up the Instrument Configuration

If the icons for your instruments are not displayed in the Instrument Setup window or you want to change the hardware configuration of one or more of the instruments, close the Xcalibur data system and open the Foundation™ Instrument Configuration application.

❖ **To set up the Foundation instrument configuration**

1. From the computer desktop, choose **Start > All Programs (or Programs) > Thermo Foundation x.x > Instrument Configuration**. The Thermo Foundation Instrument Configuration application opens.

2. Add the instruments that make up your GC, LC, GC/MS, or LC/MS system to the Configured Devices list.

3. To set up or modify the configuration of a specific instrument, double-click its icon in the Configured Devices list and modify the settings in the instrument's configuration dialog box.

4. Click **Done** to close the Instrument Configuration application.

## Viewing the Instrument Status

Use the Info view to view the status of your instruments.

❖ **To open the Info view if it is hidden**

In the View toolbar, click the **Information View** icon, ▣.

❖ **To view the status of the system instruments**

1. Click the **Status** tab to open the Status page. The Status page contains a directory tree on top and the *Instrument* Status view on bottom (see the figure on page 1).

   The *Instrument* Status view is empty until you select an instrument in the directory tree.

2. To check the instrument's state, click the expand icon to the left of the instrument's name.

   The possible states for the mass spectrometer include Ready to Download, Preparing for Run, Ready for Run, Waiting for Contact Closure, Running, and Off.

3. To display the Status view for a particular instrument, select the instrument in the directory tree. The instrument's status view appears.

## Creating Instrument Methods

Use the Instrument Setup application to create instrument methods and to access the direct controls (when available) for each instrument. An instrument method contains the chromatographic settings for the GC or LC, the injection program for the autosampler, and the data acquisition settings for the detector or detectors.

❖ **To create an instrument method**

1. Click the **Instrument Setup** icon. The Instrument Setup window opens with the default parameter settings for each instrument. Or, click the double chevron, ⤓, below the application icon and choose **Last Used Method**. The Instrument Setup window opens with the parameter settings from the last method that you ran.

   The View bar on the left displays icons for the configured instruments.

2. Do the following for each instrument:

   a. In the View bar, click the instrument's icon.

   b. Set up the instrument's method parameters. For information about the method parameters, press the F1 key to open the Help topic for the current window, dialog box, or page.

3. From the Instrument Setup menu bar, choose **File > Save** to open the Save As dialog box and save the instrument method.

## Creating and Running Acquisition Sequences

Use the Sequence Setup view to create and run acquisition sequences.
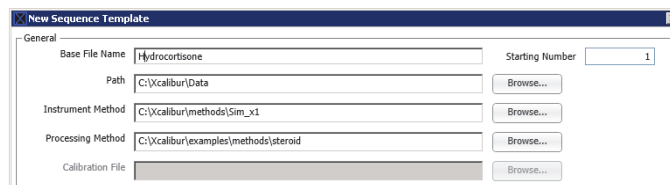
### Creating an Acquisition Sequence

To acquire raw data files, each row in the sequence table must include an instrument method, a file name, a directory path, a vial position, and an injection volume (if the method does not specify an injection volume). The vial position nomenclature varies by autosampler model.

❖ **To create a multi-sample sequence**

1. In the Roadmap view, click the **Sequence Setup** icon. The Sequence Setup view opens with a single-row table.

   | | Sample Type | File Name | Path | Inst Meth | Position | Inj Vol |
   |---|---|---|---|---|---|---|
   | * | | | | | | 0.00 |

2. From the menu bar, choose **File > New**. The New Sequence Template dialog box opens.
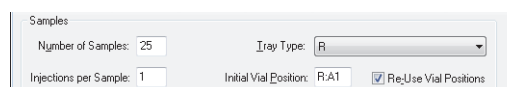


3. In the General area, enter the base name for the raw data files (.raw), browse to the directory folder where you want to store the files, and browse to an instrument method (.meth). With the default starting number set to 1, the data system appends values from 01 to 4000 to the file name.

4. Specify the number of samples of Unknown sample type as follows:

   a. In the Number of Samples box, type the number of samples (from **1** to **4000**).

   b. In the Injections per Sample box, type number of injections per sample. To make the replicate injections from the same vial, select the **Re-Use Vial Positions** check box.

   The data system creates one row for each injection up to the maximum number of 4000.



5. Set up the vial positions as follows:

   a. If the Tray Type list is available, select the tray type that you installed in the autosampler tray compartment.

   b. In the Initial Vial Position box is available, type the position for the first injection.

   For information about the vial nomenclature for your autosampler model, refer to the *Autosampler* Help.

6. Click **OK**. An editable sequence table appears in the Sequence Setup view. You can change the sample type, the file name, the instrument method, and so on. You cannot change the bracketing type. For information about setting up sequence bracketing in the New Sequence Template dialog box, refer to the Help.

❖ **To specify the injection volume for each injection**

To overwrite the injection volume in the instrument method (or if the instrument method does not include the injection volume), type a numeric value in the Inj Vol column.

> **Tip** To copy a value to multiple rows, select the range including the row that you want to copy. Then choose **Edit > Fill Down**. The Fill Down dialog box opens.

❖ **To save the sequence**

1. From the menu bar, choose **File > Save As**. The File Summary Information dialog box opens.

2. In the Comment box, type an appropriate description. Then click **OK**. The Save As dialog box opens.

3. Browse to the folder where you want to save the sequence, and in the File Name box, type a file name. Then click **Save**.

## Starting a Sequence Run

> **IMPORTANT** Make sure that the autosampler tray contains vials (or microwell plates) in the specified positions.

❖ **To start a single run or sequence run**

1. Select the rows that you want to run. When you select more than one sequence row, the Run Sample icon becomes unavailable.

2. In the Sequence Editor toolbar, do one of the following:

   • To run multiple rows, click the **Run Sequence** icon, 📋.

   • To run a single row, click the **Run Sample** icon, ⬦.

   The Run Sequence dialog box opens.

   –or–

   If the data system detects a new instrument configuration, a message box appears. Closing the message box opens the Change Instruments In Use dialog box where you can change the start instrument by clicking the Start Instrument column. Closing the Change Instruments In Use dialog box opens the Run Sequence dialog box.
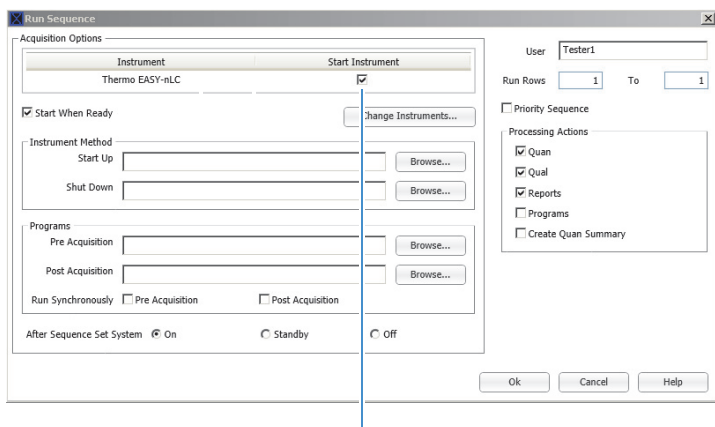


Selecting the Start Instrument check box next to the instrument name indicates that it triggers data acquisition.

3. Do the following:

   a. In the Acquisition Options area, check whether the appropriate instrument is listed as the Start Instrument.

   b. If necessary, open the Change Instruments in Use dialog box by clicking **Change Instruments** and select the appropriate start instrument.

   c. In most cases, keep the remaining default settings.

   > **Note** By default, the Start When Ready check box and Priority Sequence check boxes are selected and the post-sequence status of the system is set to On. If you clear the Start When Ready check box, you must click the **Start Analysis** icon, ▶, to start each run.

   d. To submit the run to the acquisition queue, click **OK**.

## Pausing and Stopping Sequences

Use the Stop Analysis icon ■, to stop a sequence. Use the Pause/Resume Sequence Queue icon, ▐▐, to pause and restart a sequence.

   • Actions > Pause ( ▐▐ )—The sequence is running.

   • Actions > ✓ Pause ( ▐▐ )—The sequence is paused.

❖ **To stop the current run and go to the next sample**

1. In the Sequence Editor toolbar, click the **Stop Analysis** icon. The data system immediately stops the current run and acquires the raw data file.

2. To resume the sequence, click the **Pause/Resume Sequence Queue** icon. The data system resumes the sequence at the next sample in the queue.

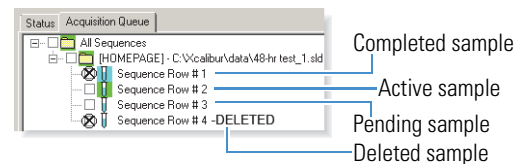❖ **To pause an active sequence**

In the Sequence Editor toolbar, click the **Pause/ Resume Sequence Queue** icon. The data system continues to acquire data for the current sample until the run time specified in the instrument method expires. At the end of the run, the data system acquires the raw data file.

❖ **To restart a paused sequence**

Click the **Pause/Resume Sequence Queue** icon. The data system resumes the sequence with the next sample in the queue.

## Deleting Samples from the Acquisition Queue

During a sequence run, the All Sequences folder, the folder for the active sequence, and the vial icon for the active sample have green backgrounds. The vial icon for a completed sample has a blue background and a large cross (⊗) in its check box. The vial icon for a pending sample has a white background.



❖ **To delete pending samples from an active sequence**

1. Open the Acquisition Queue by clicking the **Acquisition Queue** tab in the Info view.

2. Select the check boxes to the left of the pending samples that you want to delete.

3. Press the DELETE key. The data system appends "DELETED" to the deleted samples.

## Viewing the Data as It Is Acquired

Use the Real Time Plot view to view the data as it is acquired. Use the Plot toolbar to lock and unlock the display and to zoom in or out on the chromatogram and spectrum views.

❖ **To view data as it is acquired**

1. In the View toolbar, click the **Real Time Plot View** icon, 📈. The Real Time Plot view opens.

2. To monitor the real-time progress of a run, lock the display by clicking the **Lock Display** icon.

- View > Lock Display ( 🔓 )—The display is unlocked, and you can review the data that has already been acquired for the current run on the screen, but you cannot view the real-time acquisition of data.<<update>>

- View > ✓ Lock Display ( 🔒 )—The display is locked, and you can view the real-time acquisition of data for the current run, but you cannot review the data.

## Associating Raw Data Files with the Qual Browser Application

Associate Raw data files with the Thermo Qual Browser application from Microsoft™ Windows™ Explorer if you want them to open in Qual Browser by default.

❖ **To associate Raw data files with Qual Browser**

1. From Windows Explorer, right-click any Raw (.raw) file.

2. Choose **Open With**.

   The Open With dialog box appears and displays a list of applications.

3. Under Recommended Programs, select **Qual Browser**. If the application is not listed, double-click **Other Programs** and then select **Qual Browser** from the list.

   > **Tip** The Qual Browser application (QualBrowser.exe) is located in the Xcalibur installation directory. The default installation path is:
   >
   > C:\Xcalibur\system\programs

4. Select the **Always Use the Selected Program to Open This Kind of File** check box, and then click **OK**.

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