

SII for Xcalibur

Quick Start Guide

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Document history

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About the documentation

This chapter provides an overview of the guide including the different conventions used throughout the document to indicate text with special importance.

About this document

You can use Thermo Scientific™ Standard Instrument Integration (SII) for Xcalibur™ software to acquire data and control a wide range of instruments via the Thermo Scientific™ Xcalibur™ data system. SII for Xcalibur is based on the Thermo Scientific™ Dionex™ Chromeleon™ 7 Chromatography Data System and uses certain key Chromeleon features. This guide provides an overview of operation when SII for Xcalibur is installed.

NOTE: For access to Chromeleon features other than those required by SII for Xcalibur, you must purchase the appropriate licenses. Contact your local Thermo Scientific sales representative for details.

Documentation conventions

The following formatting is used throughout the documentation to indicate text with special importance.



CAUTION: Indicates instructions that must be followed carefully to avoid potential problems.

NOTE: Indicates information of special interest.

TIP: Indicates information that helps you work more efficiently.

Other documents

In addition to this quick start guide, Thermo Fisher Scientific provides the following documentation: application-specific Help available from within Chromeleon and Xcalibur.

For detailed information about the Chromeleon data system, refer to the *Chromeleon Help*:

- In the Thermo Xcalibur Instrument Setup window, select **Help > Thermo Scientific SII for Xcalibur Contents and Index**.
–or–
- Press **F1** from the Direct Control window.

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

Contact us

For Technical Support for Dionex products

In the U.S. and Canada, call 1-800-532-4752.

Outside the U.S. and Canada, call the nearest Thermo Fisher Scientific office.

For additional contact information

Go to www.thermofisher.com/us/en/home/technical-resources.html.

Overview

Instrument control

For a list of instruments supported by SII for Xcalibur, refer to the *SII for Xcalibur List of Supported Instruments*, provided on the SII for Xcalibur installation medium.

When SII for Xcalibur is installed, the following options are available from Xcalibur for control (and monitoring) of instruments supported by SII for Xcalibur:

- Automated control from Xcalibur instrument methods (required to run a single injection or a sequence of injections)
Automated control requires an instrument method. The SII for Xcalibur Instrument Method Wizard supports the creation of HPLC and IC instrument methods from within Xcalibur. These methods are stored in the Xcalibur instrument method (a *.meth file).
- Direct control from Chromeleon ePanels (recommended for most users)
ePanels are windows that contain controls for the most frequently used instrument properties or commands. A typical HPLC or IC system is controlled from multiple related ePanels, known collectively as an ePanel Set. Note that ePanels may not fully support older instruments or nonstandard configurations.
- Direct control from the Chromeleon Command window (recommended for advanced or expert users only)
The Command window provides access to all properties and commands for a particular instrument. Use the window to access controls that are not available on ePanels.

Data acquisition and storage

Detector signals (including conductivity and UV absorbance) and other channel data (for example, pump pressure and column oven temperature) are digitally transferred from SII for Xcalibur to Xcalibur for permanent

storage. A temporary copy of the data is stored in a Chromeleon data vault (a database of chromatographic data). SII for Xcalibur generates three types of temporary data:

- Chromeleon sequences
- Chromeleon audit trails
- SII for Xcalibur daily log files

Data processing and reporting

Data processing and results reporting are executed in Xcalibur as usual. For details, refer to the *Xcalibur Help*.

Start the software

The startup instructions assume that you have completed installation of the analytical system software and hardware, including configuration of the instrument in the Chromeleon Instrument Configuration Manager. For instructions, refer to the *SII for Xcalibur Installation Guide*, the Chromeleon, Xcalibur, and Thermo Scientific™ Foundation™ manuals, and the hardware manuals.

Start Xcalibur and SII for Xcalibur

Procedure

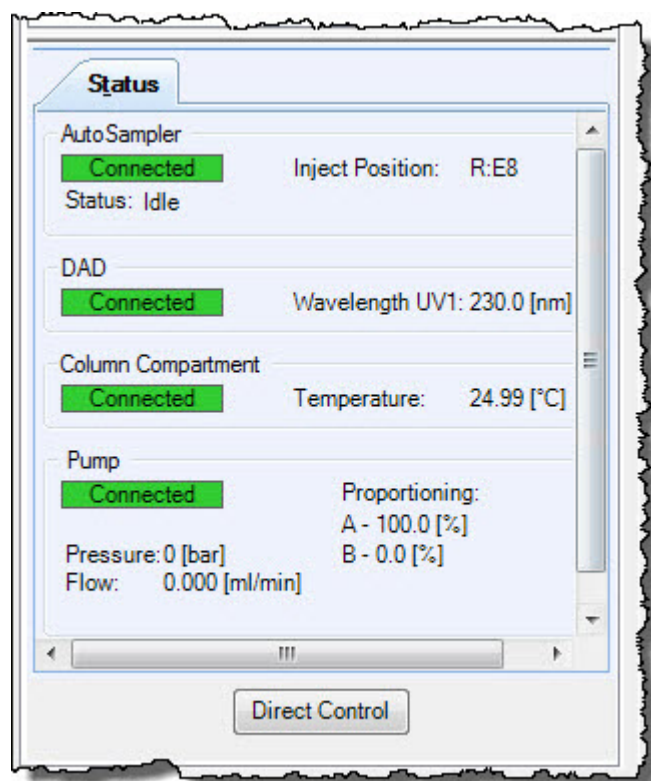
1. If it is not already running, start the Chromeleon Instrument Controller Service (refer to the *SII for Xcalibur Installation Guide* for details).
2. Select **Start > All Programs > Thermo Xcalibur > Xcalibur**.

The Roadmap view of the Home page window appears.

3. On the Status page of the Information view, select **Thermo Scientific SII for Xcalibur**.

A simplified version of a Chromeleon ePanel appears in the SII for Xcalibur Status pane. Use this ePanel to monitor basic operating parameters (pump flow rate, autosampler status, and so on). To open a standard Chromeleon ePanel Set and allow for direct control and in-depth monitoring of the HPLC or IC system, select **Direct Control** below the ePanel.

Figure 1 SII for Xcalibur status pane



Equilibrate the system

Before starting an analysis, equilibrate the chromatography system (flush the system, turn on all temperature-controlled devices, monitor the pump pressure and detector signal, and so on). For details about the steps required to equilibrate a particular system, refer to the operator's manual for the system.

Select one of the following methods to perform equilibration:

- Select operating commands and parameters directly from the Chromeleon ePanel Set.
- Create and run an equilibration instrument method to automate the process.

Direct control of the system

Direct control of instruments is possible from the Chromeleon ePanel Set or the Chromeleon Command window. Both locations are accessed from the SII for Xcalibur Direct Control window.

Open the Direct Control window

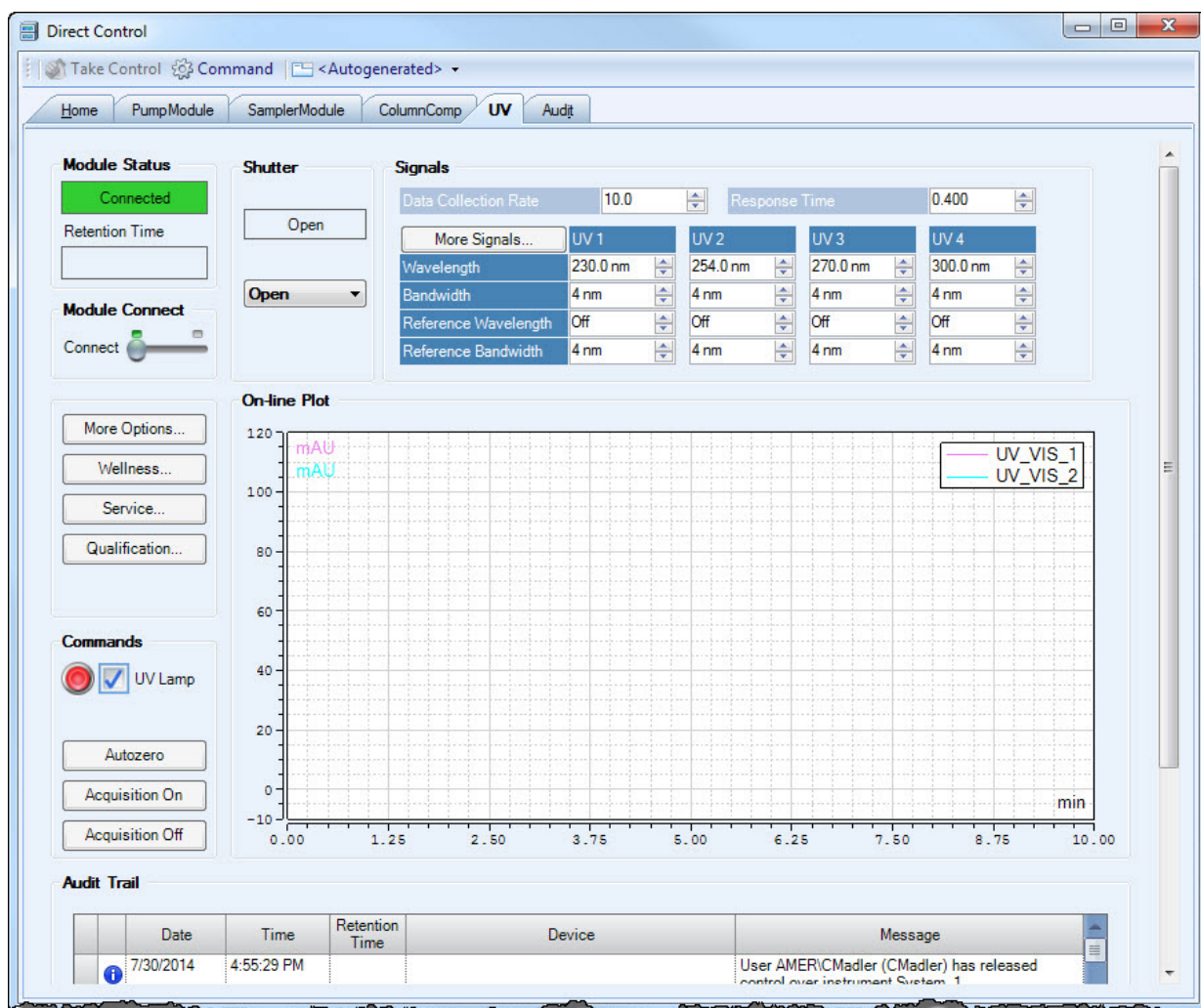
Procedure

- Select **Direct Control** in the SII for Xcalibur Status pane (see [Figure 1: SII for Xcalibur status pane](#)).

By default, the Chromeleon ePanel Set appears in a maximized window.

TIP: ePanels are best viewed in a maximized window; this size ensures that all ePanel controls and readouts are visible.

Figure 2 SII for Xcalibur Direct Control window



The toolbar of the Direct Control window provides access to the following commands:

- **Take Control and Release Control**

The instrument is usually controlled by Xcalibur. The Take Control command places the instrument under user control and is required to perform manual actions from an ePanel or to take over control of the system from either Xcalibur or another user. The Release Control command places the system in a neutral state until Xcalibur or a user takes control again.

Xcalibur automatically takes control of the instrument whenever necessary. When this happens, controls in the Direct Control window are disabled.



WARNING: You can use ePanels for detailed instrument monitoring during data acquisition. However, be careful not to take control manually and interfere with the acquisition in progress.

- **Command**

Opens the Command window. For details, see [Control an instrument from the Command window](#).

- **<ePanel Set>**

- **<Autogenerated>** When you first start Chromeleon and connect to the instrument, Chromeleon automatically generates an ePanel Set that is based on the current instrument configuration. For example, if the configuration includes three modules (autosampler, pump, and detector), the <Autogenerated> ePanel Set includes a default ePanel for each module.

If you want to assign a different ePanel Set to the instrument: On the toolbar, select the down arrow on the **<Autogenerated>** button, select **Manage ePanel Set**, and select a different ePanel from the ePanel Set Manager dialog box.

- **Custom** If you want to use a modified version of the <Autogenerated> ePanel Set, add or remove ePanels as required, and then save the ePanel Set to a different name: On the toolbar, select the down arrow on the **<Autogenerated>** button, select **Save ePanel Set As**, and enter the new name.
- **<Last Used>** When you modify an ePanel Set, Chromeleon saves the changes in an ePanel Set called <Last Used>. Modifying an ePanel Set also modifies the <Last Used> ePanel Set for the instrument. To reuse a custom ePanel Set and ensure that it is not overwritten by newer changes, save it to a different name.

Control an instrument from the ePanel Set

Procedure

1. If necessary, open the Direct Control window (see [Figure 2: SII for Xcalibur Direct Control window](#)).
2. To access module-specific properties, select the corresponding tab on the ePanel Set. For example, if you want to change the pump flow rate, select the Pump tab.

- To control an instrument function, locate the control (for example, a button, slider, or gauge) for the command or property that you want to change. Select the button or enter the preferred property value.

After you execute a command or change a property value, Chromeleon checks the status of the instrument to verify that the change can be executed:

- If there are no problems, the change is executed immediately.
- If a problem is detected, a message appears. Serious problems must be resolved before Chromeleon will execute the change.

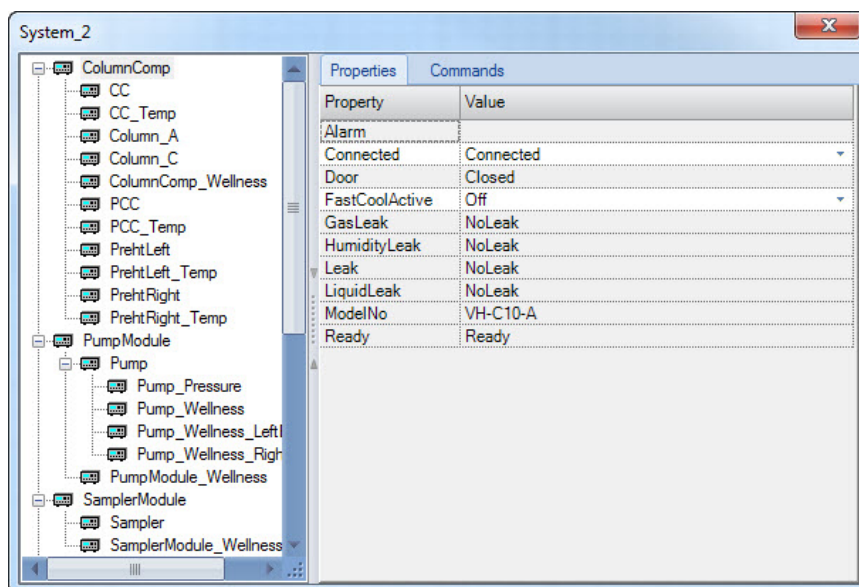
NOTE: Changes to commands and properties are recorded in the Instrument Audit Trail. To view the Instrument Audit Trail, select the **Audit** tab on the ePanel Set.

Control an instrument from the Command window

Procedure

- If necessary, open the Direct Control window (see [Figure 2: SII for Xcalibur Direct Control window](#)).
- Select **Command** from the toolbar to display the Command window.

Figure 3 SII for Xcalibur Command window



The left pane of the Command window displays a device tree. The tree lists each module configured in the instrument, as well as any sub-devices associated with the module. For example, if the instrument includes a detector, the detector module is shown as a top-level device and each of its signals is listed as a sub-device below.

3. Select a module or sub-device to view its properties and commands in the right pane of the Command window:
 - The Properties tab page displays the properties available for the selected module or device, as well as their current values. Properties that can be changed are displayed on a white background. Read-only properties are displayed on a shaded background.
 - The Commands tab page displays the commands available for the selected module or device.

TIP: You can filter the list of properties and commands to increase or decrease the number of entries. Right-click anywhere in the Command window, and then select the preferred option:

- **Normal:** Displays properties and commands relevant for basic operation.
- **Advanced:** Displays properties and commands relevant for basic and advanced operation.
- **Expert:** Displays all properties and commands, including additional ones relevant for expert operation (for example, diagnostic properties).

4. To change a property value:
 - a. Select the **Properties** tab.
 - b. In the property box, enter a new value. If only predefined values are allowed, select a value from the dropdown list.
5. To execute a command:
 - a. Select the **Commands** tab.
 - b. If the command does not require any parameters, select the button next to the command name.
 - c. If the command includes parameters, enter values for the parameters in the Parameters box, and select **OK**. Then, select the button next to the command name.

After you execute a command or change a property value, Chromeleon checks the status of the instrument to verify that the change can be executed:

- If there are no problems, the change is executed immediately.
- If a problem is detected, a message appears. Serious problems must be resolved before Chromeleon will execute the change.

NOTE: Changes to commands and properties are recorded in the Instrument Audit Trail. To view the Instrument Audit Trail, select the **Audit** tab on the ePanel Set.

Automated control of the system

You can create and edit the part of the instrument method with HPLC or IC instrument parameters. Additionally, you can create and edit mass spectrometer parameters in the Xcalibur Instrument Setup as usual. For details, refer to the *Xcalibur Help*.

TIP: If the instrument configuration does not contain a mass spectrometer, the HPLC or IC front-end system can be operated alone via Xcalibur and SII for Xcalibur.

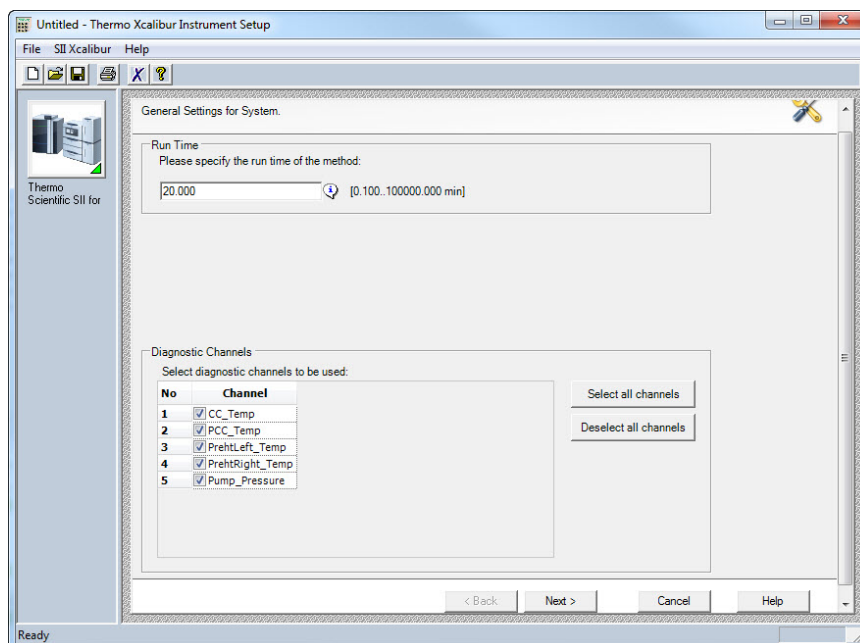
Create an instrument method

Procedure

1. From the Xcalibur Home page window, select **GoTo > Open Instrument Setup**.

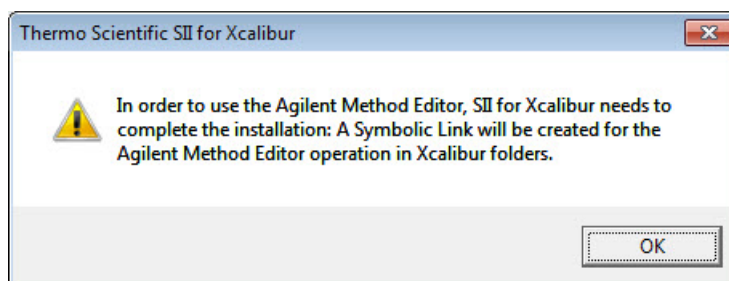
The Instrument Setup window appears. By default, the first page of the SII for Xcalibur Instrument Method Wizard is displayed.

Figure 4 SII for Xcalibur Instrument Method Wizard: General Settings page



If the instrument is being controlled by the Agilent Drivers for Chromeleon, when you launch the Instrument Method Wizard for the first time, a prompt appears.

Figure 5 Thermo Scientific SII for Xcalibur prompt



2. At the prompt, select **OK**.
3. In the Windows User Account Control dialog box, select **Yes** to enable the proper operation of the Agilent Method Editor.
4. Follow the instructions on the Instrument Method Wizard pages to select the method parameters. Be sure to select the acquisition channels that you want to acquire and store in Xcalibur.

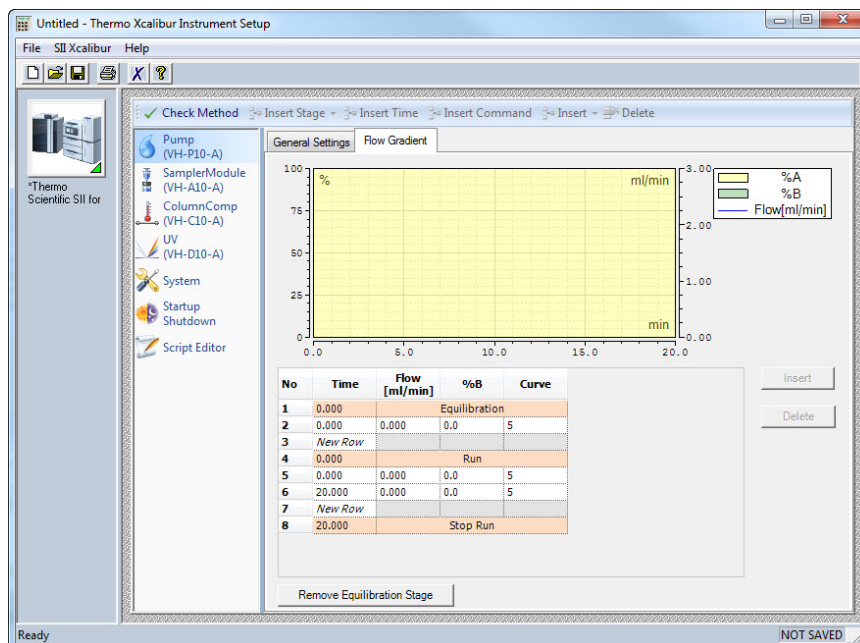


CAUTION : To acquire a data channel in Xcalibur, the channel must have been enabled in the Chromeleon Instrument Configuration Manager (refer to the *SII for Xcalibur Installation Guide* for details) and the data acquisition of the channel must be turned on in the HPLC or IC part of the instrument method.

- When you finish selecting parameters, select **Finish**.

The Module view of the wizard appears.

Figure 6 SII for Xcalibur Instrument Method Wizard: Module view



In the left pane, each module in the instrument is represented by an icon. The right pane displays a series of tab pages (similar to the Instrument Method Wizard pages) with commands for the currently selected module. The module view is an easy way to edit the most important method commands. For details, see [Edit an instrument method](#).

The left pane contains two additional icons: Startup/Shutdown and Script Editor.

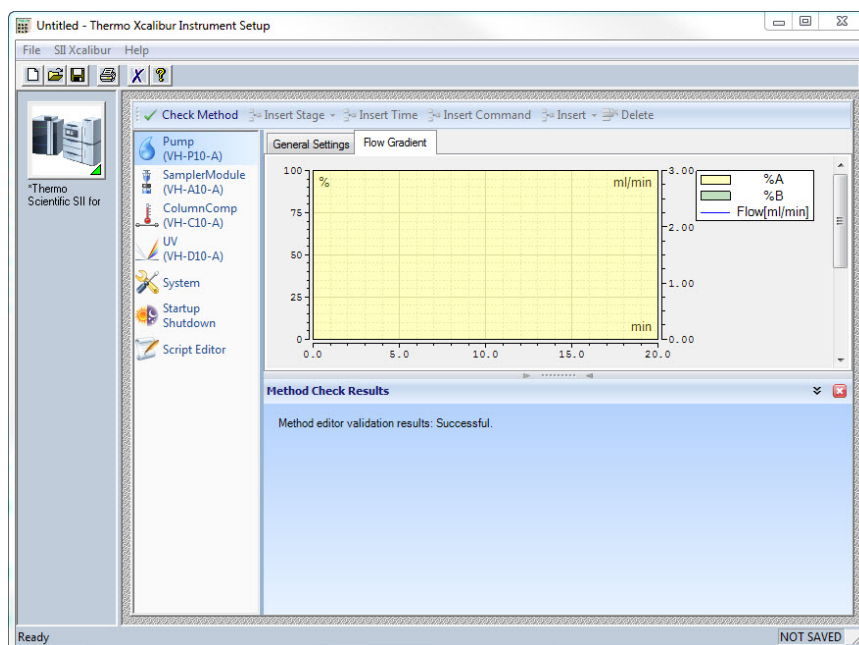
- Select an icon from the left pane:
 - Select **Startup/Shutdown** to view and customize parameters for standby and shutdown modes for supported instruments. For details, see [Edit a Standby \(Smart Standby\) or Off \(Smart Shutdown\) state](#).
 - Select **Script Editor** to display a chronological list of all steps defined in the Instrument Method Wizard. You can review and customize method parameters, line-by-line. For details, see [Edit an instrument method](#).
- Select **Check Method** on the toolbar to have SII for Xcalibur check the HPLC or IC part of the method for errors in syntax or semantics (logic).

When the process is complete, the Method Check Results window appears in the lower half of the Instrument Method Wizard page. The window identifies any problems that were detected. Serious problems must be resolved before Chromeleon will execute the method.



CAUTION: Some error conditions cannot be detected until data acquisition is about to start.

Figure 7 SII for Xcalibur Method Check Results window



8. Correct the problems as necessary.
9. To temporarily hide the Method Check Results window, select  on the title bar of the window.

–or–

To close the Method Check Results window, select  on the title bar.

10. Select **File > Save** and enter a method name, as well as any comments that you want to save with the method.

NOTE: Methods created can be used as acquisition methods, Xcalibur Start Up methods, or Xcalibur Shut Down methods.

Edit an instrument method

Methods are usually edited in the Module view, which displays the most important module-related commands. However, you must use the Script Editor to make the following changes:

- Add commands that are not available in the Module view
- Add new time steps or stages
- Create conditional statements

- Create trigger blocks

NOTE: The Script Editor is recommended for use by *advanced* users only. The creation of conditional statements or trigger blocks is recommended for *expert* users only; for instructions on how to create them, refer to the *Chromeleon Help*.

Open an instrument method

Procedure

1. From the Xcalibur Home page window, select **GoTo > Open Instrument Setup**.

The SII for Xcalibur Instrument Method Wizard appears.

2. Select **File > Open** and select the method to edit.
3. Select **Thermo Scientific** in the left pane of the Instrument Method Editor window.

The embedded SII for Xcalibur Instrument Method Editor appears in the main part of the window. By default, the selected file appears in the Module view. (This view resembles the SII for Xcalibur Instrument Method Wizard pages.)

Edit an instrument method in the Module view

Procedure

1. Select the appropriate module icon in the left pane of the SII for Xcalibur Method Wizard (see [Figure 7: SII for Xcalibur Method Check Results window](#)).
2. On each page, modify the parameters as needed.
3. When you are finished editing, check the file for errors (see [Control an instrument from the ePanel Set](#)).
4. Select **File > Save**.

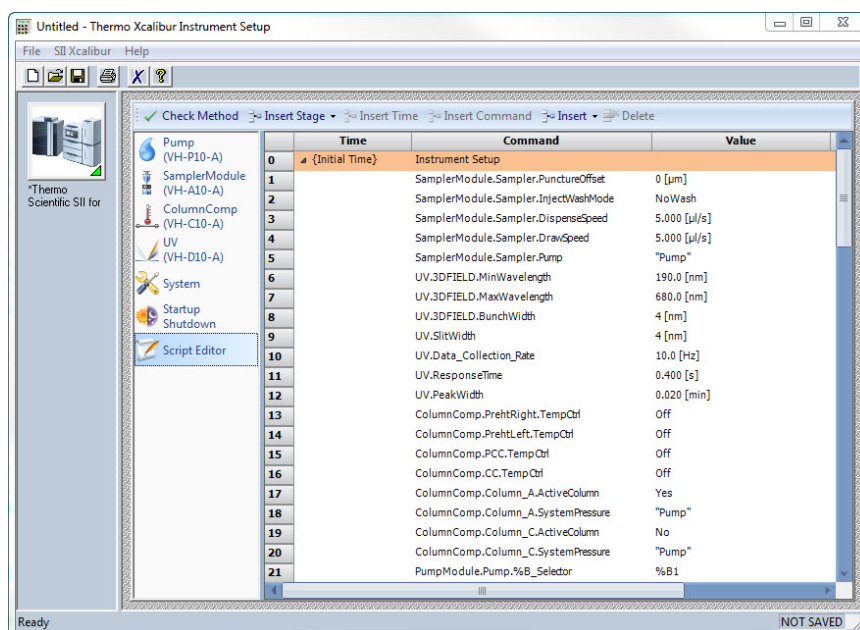
Edit an instrument method in the Script Editor view

Procedure

1. Select **Script Editor** in the left pane of the SII for Xcalibur Method Wizard to display the method script.

Control commands in the script are subdivided into predefined sections (called *stages*) in which related commands are grouped by function (for example, instrument setup or equilibration). Stage names are displayed on an orange background.

Figure 8 SII for Xcalibur Method Wizard: Script Editor view



2. Edit the method as required.

NOTE: For detailed information, refer to the *Chromeleon Help*.

TIP: Most editing commands on the toolbar are also available on a context menu. To access the context menu, right-click any line in the script.

3. When you are finished editing, check the file for errors (see [Control an instrument from the ePanel Set](#)).
4. Select **File > Save**.

Edit the value or property of a command

Procedure

1. Select the **Value** column.

2. Enter a value in the box or select a value from the dropdown list.

Insert a new command

Procedure

1. Select the line where you want to insert the new command.
2. Select **Insert Command** from the toolbar.
3. Select the down arrow in the Command column of the new line to display a list of available commands.
4. Select the required command to insert it into the table.
5. Select the **Value** column.
6. Enter a value in the box or select a value from the dropdown list.

Delete a command

Procedure

1. Select the line with the command that you want to remove.
2. Select **Delete** from the toolbar.

Add a comment

Procedure

1. Select the **Insert** down arrow from the toolbar and select **Comment**.
2. Enter your comment in the Comment column.

Delete a comment

Procedure

- Select the **Delete** down arrow from the toolbar and select **Comment**.

Insert a new time step

NOTE: A new time step can be inserted in only two locations: before an existing time step or before a stage.

Procedure

1. Select the line where you want to insert the new time step.
2. Select **Insert Time** from the toolbar.
3. Enter a time in the Time column.

Delete a time step

Procedure

1. Select the time step.
2. Select **Delete Time** from the toolbar.

Insert a new stage

Procedure

1. Select the line where you want to insert the new stage.
2. Select the **Insert Stage** down arrow from the toolbar and select an option.
3. Insert the commands required for the new stage.

Delete a stage

Procedure

1. Select the line with the stage that you want to remove.
2. Select **Delete** from the toolbar.

Edit On, Off, and Standby states

If the system will not be in operation for a while, you may want to use a Smart Standby or Smart Shutdown method in SII for Xcalibur to automate the process of preparing the chromatography system for downtime. Smart Standby and Smart Shutdown methods (if supported by the instrument) are created and executed automatically, based on the last method used.

If you change a value in the instrument method, verify that the associated Smart Standby or Smart Shutdown method is updated accordingly. SII for Xcalibur executes the Smart Standby or Smart Shutdown method after the last injection or the shutdown method (whichever occurs later).

The Xcalibur Shut Down method (not the Smart Shutdown method) runs between the last injection and the start of the On, Off, or Standby state (see [Specify the post-sequence state](#)). Thermo Fisher Scientific recommends the following options:

- Run a shutdown method when the On state is selected.
- Do not run a shutdown method when the Off or Standby state is selected.



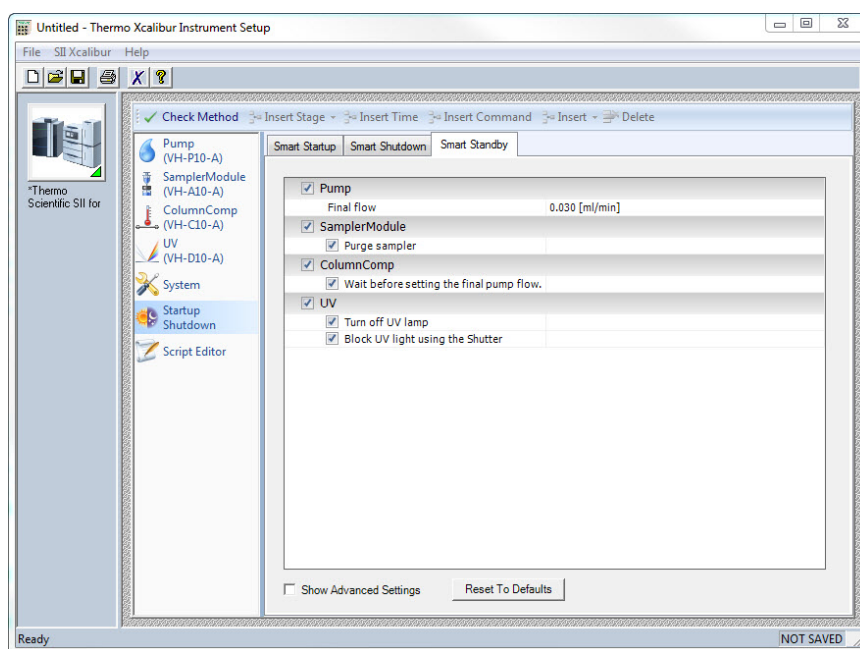
WARNING: Before editing a Smart Standby or Smart Shutdown method, familiarize yourself with any relevant requirements for the front-end system and the mass spectrometer.

Edit a Standby (Smart Standby) or Off (Smart Shutdown) state

Procedure

1. Open the instrument method that will run last.
2. In the left pane of the SII for Xcalibur Instrument Method Wizard, select **Startup Shutdown**.
3. Select the **Smart Standby** or **Smart Shutdown** tab to display the corresponding tab page.

Figure 9 SII for Xcalibur Instrument Method Wizard: Smart Standby page



4. Modify the method as required (change a parameter value, exclude a module or parameter from the method, and so on).

TIP: To quickly restore all modified parameter values to their initial settings, select the **Reset to Defaults** button at the bottom of the tab page. To restore the value of a single parameter, right-click the parameter and select the **Reset to Default** option.

5. Select **File > Save**.

Run a sequence

When SII for Xcalibur is installed, you can create and edit sequences in Xcalibur as usual.

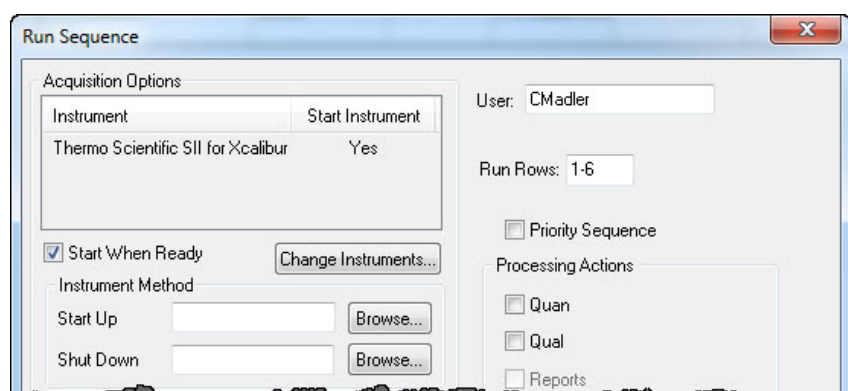
Change the start instrument

In the Xcalibur Run Sequence dialog box, the Start Instrument is usually Thermo Scientific SII for Xcalibur. If necessary (for example, if an external autosampler is configured as the start instrument), change the setting before starting the sequence.

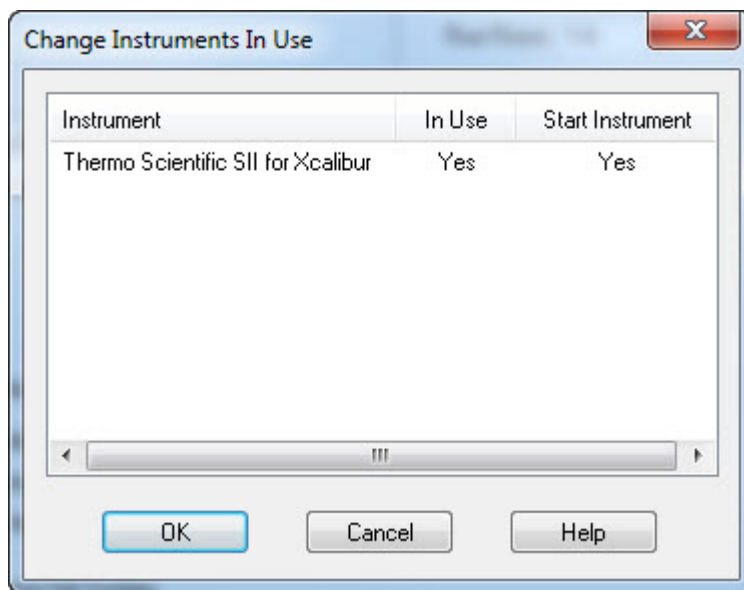
Procedure

1. From the Sequence Setup view of the Home page window, select **Actions > Run This Sample** or **Actions > Run Sequence** to open the Run Sequence dialog box.

Figure 10 SII for Xcalibur Run Sequence dialog box: Start Instrument parameter



2. Select **Change Instruments** to open the Change Instruments In Use dialog box.

Figure 11 SII for Xcalibur Change Instruments In Use dialog box

3. In the row for the instrument that you want to use as the start instrument, select the **Start Instrument** column to change the blank entry to **Yes**.
4. Select **OK** to save the changes and close the dialog box.

Monitor samples

While a sequence is running, there are three ways to monitor samples:

- If your focus is front-end system signals and parameters, SII for Xcalibur direct control is recommended. Select **Direct Control** in the SII for Xcalibur status pane (see [Figure 1: SII for Xcalibur status pane](#)) to display the Chromeleon ePanel Set.
- Otherwise, use the Xcalibur Qual Browser (recommended for viewing the mass spectrometer signal) or the Xcalibur Real Time Plot view.

Specify the post-sequence state

When a sequence finishes running, Xcalibur places instruments into one of three states:

- **On:** Select the On option to leave the system in the On state when the current sequence is completed. After the last injection or the shutdown method (whichever occurs later), SII for Xcalibur will not execute any commands. Select the On option to run another sequence without waiting.

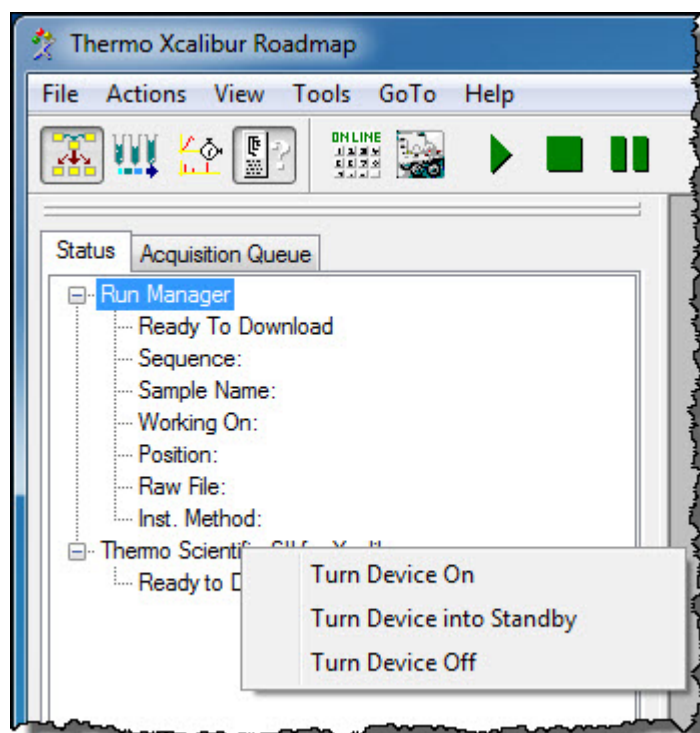
- **Standby:** Select the Standby option to place the system in the Standby state when the current sequence is completed. After the last injection or the shutdown method (whichever occurs later), SII for Xcalibur will execute the SmartStandby portion of the last instrument method that was used. Select the Standby option to run another sequence with only a short delay.
- **Off:** Select the Off option to place the system in the Off state when the current sequence is completed. In the Off state, power to devices in the system (such as a suppressor) is turned off. After the last injection or the shutdown method (whichever occurs later), SII for Xcalibur will execute the SmartShutdown portion of the last instrument method that was used.

Manually implement the post-sequence state (On, Standby, or Off state)

Procedure

1. On the Status page of the Xcalibur Information view, right-click **Thermo Scientific SII for Xcalibur**.
2. On the context menu, select either **Turn Device into Standby** or **Turn Device Off**.

Figure 12 SII for Xcalibur Device commands context menu



NOTE: The Turn Device On command is currently reserved for error recovery.

View chromatographic data

You can view the chromatographic data acquired via SII for Xcalibur in the Xcalibur Qual Browser. For details, refer to the *Xcalibur Help*.

Troubleshooting

SII for Xcalibur provides complete error notification and easy recovery (see [Table 1: Error messages](#)):

- After creating or editing an instrument method, you can immediately check the method for possible errors in the syntax or semantics, by selecting **Check Method** from the toolbar in the SII for Xcalibur Method Wizard.
- Some instrument method errors cannot be detected until data acquisition is about to start. When this type of error occurs, an error prompt is displayed.
- If a preflight error related to an LC device driver occurs, an error prompt is displayed and the message is logged in the Chromeleon audit trail. To view the audit trail, select the **Audit** tab on the ePanel Set.
- Minor problems that occur during operation are logged in both the Chromeleon audit trail and the Xcalibur raw data files (which can be viewed via the Xcalibur Qual Browser).

NOTE: If the Foundation auditing database is configured, Chromeleon error and warning messages are logged and viewable in both the Foundation Audit Viewer and the Chromeleon audit trail. The Foundation Audit Viewer limits messages to 600 characters. If a message exceeds 600 characters, check the Chromeleon audit trail to view the entire message.

- When an Abort error occurs, an error prompt is displayed and the sequence is aborted.

Table 1 Error messages

Error message	Remedy
Preflight check failed: <Description of error.>	Procedure 1. Select OK on the error prompt to dismiss the message. 2. Select Actions > Stop Analysis in Xcalibur.

Error message	Remedy
	3. Select Actions > Start Analysis in Xcalibur. NOTE Xcalibur will resume the sequence at the sample immediately after the failed sample in the queue. If all samples after the failed sample have the same type of error, consider deleting the submitted sequence; this is more efficient than correcting samples individually.
Method validation failed Row <row number>.	Procedure 1. Edit the method in the SII for Xcalibur Method Wizard. 2. Select Check Method to validate the method. NOTE The sequence may contain more than one problem; only the first failed method is reported.
Device abort.	Procedure 1. Select OK to close error prompt. 2. Select the Chromeleon Audit Trail or the Foundation Audit Viewer for an explanation of the problem. 3. Correct the problem. 4. On the Xcalibur Status page, right-click Thermo Scientific SII for Xcalibur and then select Turn Device On. This restores the software to the Ready to Download state. 5. Select Actions > Start Analysis in Xcalibur.
SII for Xcalibur has encountered an error due to one of the following issues: a) Chromeleon 7 framework services may not be available. b) SII license may not be enabled. c) Access privileges may be set incorrectly.	Enable the Chromeleon framework services: Procedure 1. Select Start and enter <i>services.msc</i> in the search box. In the search results, select services.msc. 2. In the list on the right side of the Services window, right-click the name of each Chromeleon service and then select Start. Enable the SII for Xcalibur license: Procedure 1. Select Start > All Programs > Thermo Chromeleon 7 > Administration Console.

Error message	Remedy
	2. Select User Database and then select the Roles folder. Expand the name of the appropriate Role. 3. On the License tab, select the Standard Instrument Integration License checkbox. Specify the required access privileges: Procedure 1. Select Start > All Programs > Thermo Chromeleon 7 > Administration Console. 2. Select User Database and then select the Roles folder. Expand the name of the appropriate Role. 3. On the General tab, verify that the following Privileges are <i>not</i> selected: • Instrument Configuration • Modify List of Custom Formulas (under Data Vault Basics) • Export Raw File (under Reporting) • Modify Custom Formulas (under Reporting) • Archive • Administration

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