

Thermo Scientific SII for Xcalibur Quick Start Guide

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.

Contents

- [Overview](#)
- [Starting the Software](#)
- [Equilibrating the System](#)
- [Direct Control of the System](#)
- [Automated Control of the System](#)
- [Viewing Chromatographic Data](#)
- [Troubleshooting](#)

Overview

Instrument Control

For a list of instruments supported by SII for Xcalibur, refer to *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.

Data Acquisition and Storage

- 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.

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.

Starting the Software

These 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 *SII for Xcalibur Installation Guide*; the Chromeleon, Xcalibur, and Thermo Scientific™ Foundation™ manuals; and the hardware manuals.

❖ To start Xcalibur and SII for Xcalibur

1. If it is not already running, start the Chromeleon Instrument Controller Service (refer to *SII for Xcalibur Installation Guide* for details).
2. Click **Start > All Programs > Thermo Xcalibur > Xcalibur**. The Roadmap View of the Home Page window appears.
3. On the **Status** page of the Information view, click **Thermo Scientific SII for Xcalibur**. A simplified version of a Chromeleon ePanel appears in the SII for Xcalibur status pane (see [Figure 1](#)).

Use this ePanel to monitor basic operating parameters (pump flow rate, autosampler status, and so on). Clicking the **Direct Control** button below the ePanel opens a standard Chromeleon ePanel Set, which allows direct control and in-depth monitoring of the HPLC or IC system.

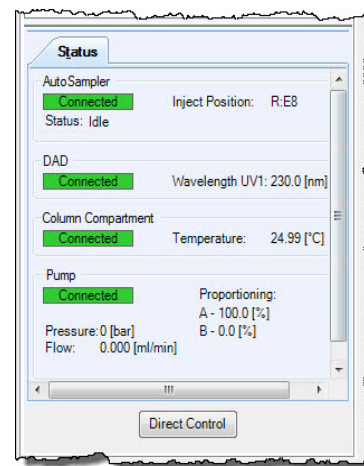


Figure 1. SII for Xcalibur status pane

Equilibrating 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.

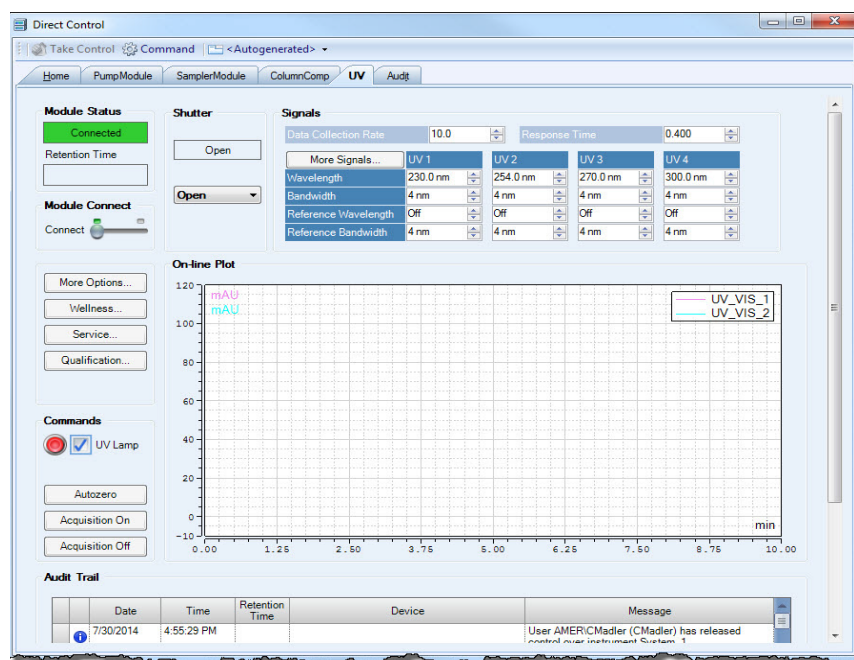
Direct Control Window

❖ To open the Direct Control window

Click **Direct Control** in the SII for Xcalibur status pane (see [Figure 1](#)). By default, the Chromeleon ePanel Set appears in a maximized window (see [Figure 2](#)).

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 Direct Control window toolbar provides access to the following commands:

- **Take Control and Release Control**

The instrument is usually controlled by Xcalibur. Clicking **Take Control** places the instrument under user control. This is required in order to perform manual actions from an ePanel or to take over control of the system from either Xcalibur or another user. Clicking **Release Control** 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.

IMPORTANT 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 from the Command Window” on page 4.

- **<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, click the down arrow on the <Autogenerated> button, click **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, click the down arrow on the <Autogenerated> button, click **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 from the ePanel Set

- ❖ **To control an instrument from the ePanel Set**

1. If necessary, open the Direct Control window (see [Figure 2](#)).
2. To access module-specific properties, click the corresponding tab on the ePanel Set. For example, if you want to change the pump flow rate, click the pump tab.
3. 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. Click the button or enter the preferred property value.
4. After you click a command button 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.

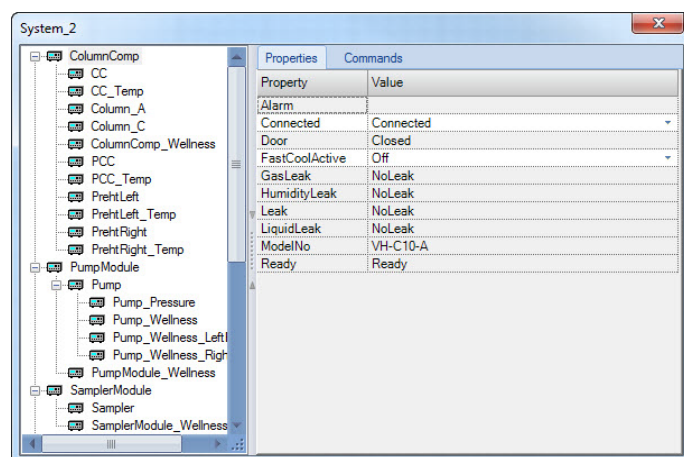
Note Changes to commands and properties are recorded in the Instrument Audit Trail. To view the Instrument Audit Trail, click the **Audit** tab on the ePanel Set.

Control from the Command Window

- ❖ **To control an instrument from the Command window**

1. If necessary, open the Direct Control window (see [Figure 2](#)).
2. Click the **Command** toolbar button to display the Command window (see [Figure 3](#)).

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. Click 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. Click the **Properties** tab.
- b. Click the property value and type a new value. If only predefined values are allowed, click the arrow and select a value from the list.

5. To execute a command:

- a. Click the **Commands** tab.
- b. If the command does not require any parameters, click the button next to the command name.
- c. If the command includes parameters, click the down arrow in the **Parameters** cell, enter values for the parameters, and click **OK**. Then, click 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, click the **Audit** tab on the ePanel Set.

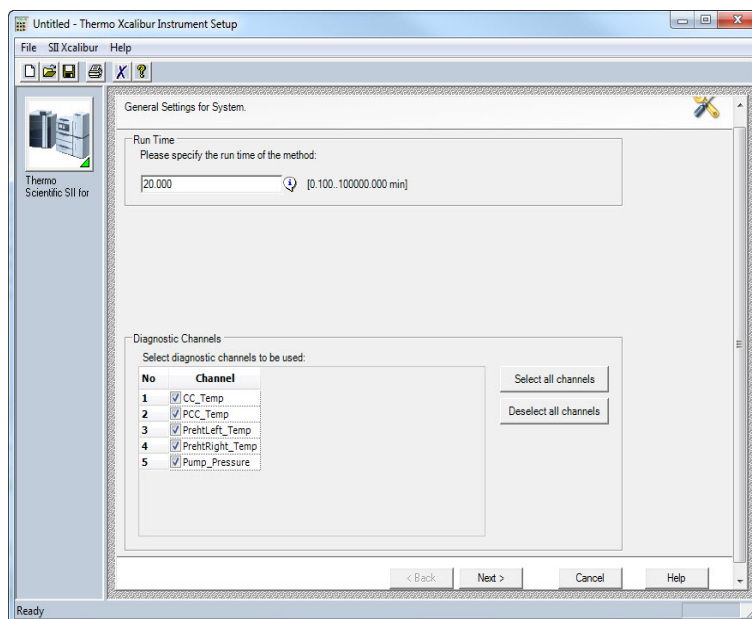
Follow the instructions here to create and edit the part of the instrument method with HPLC or IC instrument parameters. Create and edit mass spectrometer parameters in the Xcalibur Instrument Setup as usual. For details, refer to the Xcalibur Help.

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.

❖ **To create an instrument method**

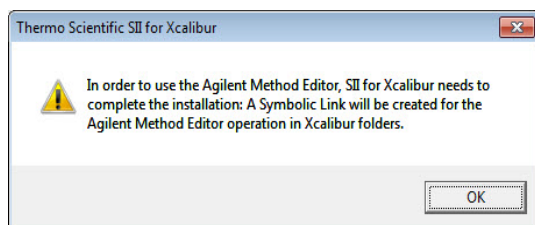
- From the Xcalibur Home Page window, click **GoTo > Open Instrument Setup**. The Instrument Setup window appears. By default, the first page of the SII for Xcalibur Instrument Method Wizard is displayed (see [Figure 4](#)).

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 message box appears (see [Figure 5](#)).

Figure 5. Thermo Scientific SII for Xcalibur message box

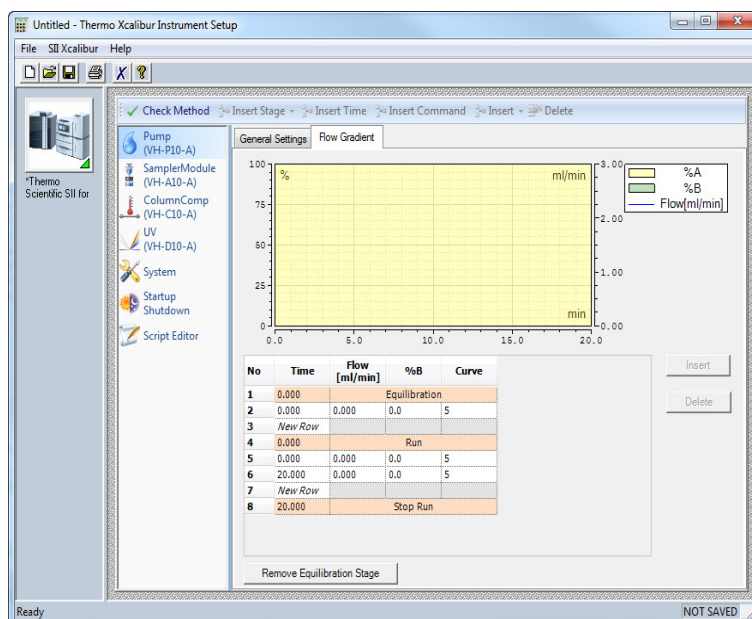


- a. Click **OK**. The Windows User Account Control dialog box appears.
 - b. Click **Yes**. This enables proper operation of the Agilent Method Editor.
3. Follow the instructions on the Instrument Method Wizard pages to select the method parameters. Be sure to select the acquisition channels that you want to acquire and store in Xcalibur.

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

4. When you finish selecting parameters, click **Finish**. The module view of the wizard appears (see [Figure 6](#)).

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 [“Editing an Instrument Method”](#) on [page 8](#).
- The left pane contains two additional icons:
 - Click the Startup/Shutdown icon to view and customize parameters for standby and shutdown modes for supported instruments. For details, see [“Editing On/Off/Standby States”](#) on [page 11](#).

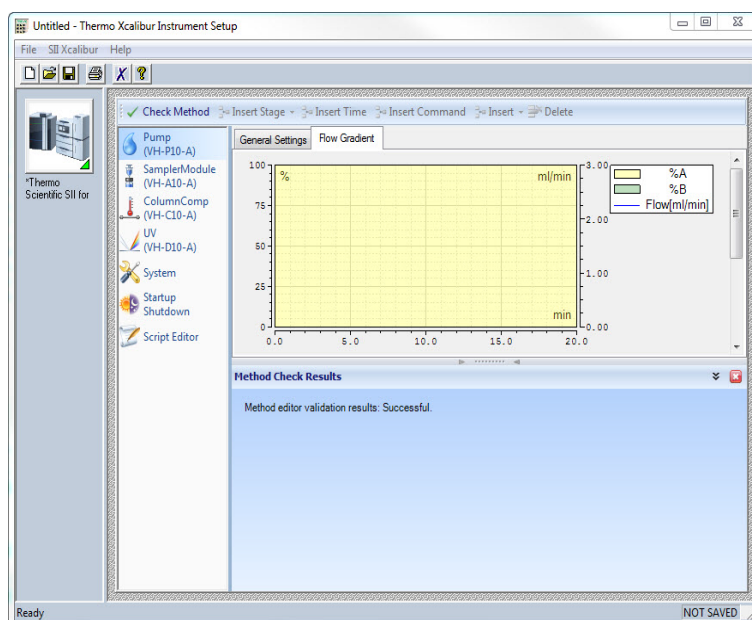
- Click the Script Editor icon to display a chronological list of all steps defined in the Instrument Method Wizard. You can review and customize method parameters, line-by-line. For details, see “Editing an Instrument Method” on page 8.



5. Click **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 (see Figure 7).

The window identifies any problems that were detected. Serious problems must be resolved before Chromeleon will execute the method.

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

Figure 7. SII for Xcalibur Method Check Results window



6. Correct the problems as necessary.
7. To temporarily hide the Method Check Results window, click  on the title bar of the window. Click the button again to display the window.
–or–
To close the Method Check Results window, click  on the title bar.
8. Click **File > Save** and enter a method name. Also enter any comments that you wish to save with the method.

Note Methods created by following the procedure above can be used as acquisition methods, Xcalibur **Start Up** methods, or Xcalibur **Shut Down** methods.

Editing an Instrument Method

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

- 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.

Opening the Instrument Method

❖ To open the instrument method

1. From the Xcalibur Home Page window, click **GoTo > Open Instrument Setup**. The SII for Xcalibur Instrument Method Wizard appears.
2. Click **File > Open** and select the method to edit.
3. Click **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.)


Editing the Instrument Method in the Module View

❖ To edit an instrument method in the module view

1. Click the appropriate module icon in the left pane of the SII for Xcalibur Method Wizard (see [Figure 7](#)).
2. On each page, modify parameters as needed.
3. When you finish editing, check the file for errors (see [Step 4 on page 4](#)).
4. Click **File > Save**.

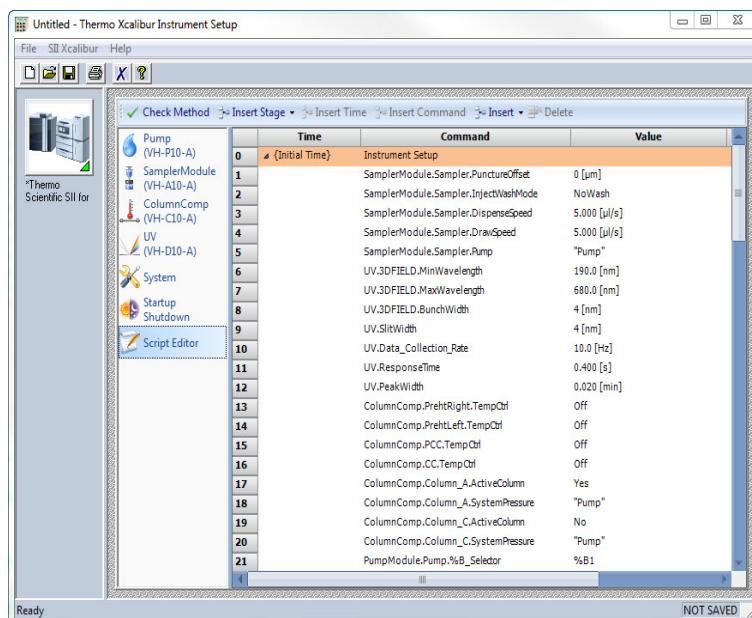
Editing the Instrument Method in the Script Editor View

❖ To edit an instrument method in the Script Editor view

1. Click  **Script Editor** in the left pane of the SII for Xcalibur Method Wizard (see [Figure 8](#)) 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. The sections below describe common changes; 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 finish editing, check the file for errors (see [Step 4 on page 4](#)).
4. Click **File > Save**.

To edit the value and/or property of a command

1. Click the **Value** column.
2. Type a value in the box.

—or—

Click the arrow and select (click) a value from the list.

To insert a new command

1. Click the line where you want to insert the new command.
2. Click the **Insert Command** toolbar button.
3. Click the down arrow in the **Command** column of the new line to display a list of available commands.
4. Click the required command to insert it into the table.
5. Click the **Value** column. To enter a value for the new command:

Type a value in the box.

—or—

Click the arrow and select (click) a value from the list.

To delete a command

1. Click the line with the command that you want to remove.
2. Click the **Delete** toolbar button.

To add a comment

1. On the toolbar, click the down arrow on the **Insert** button and click **Comment**.
2. Enter your comment in the **Comment** column.

To delete a comment

On the toolbar, click the down arrow on the **Delete** button and click **Comment**.

To 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.

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

To delete a time step

1. Click the time step.
2. Click **Delete Time** on the toolbar.

To insert a new stage

1. Click the line where you want to insert the new stage.
2. On the toolbar, click the down arrow on the **Insert Stage** button and select an option.
3. Insert the commands required for the new stage.

To delete a stage

1. Click the line with the stage that you want to remove.
2. Click **Delete** on the toolbar.

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 SmartShutdown method) runs between the last injection and the start of the On/Off/Standby state (see “[Specifying the Post-Sequence State](#)” on page 13). 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.

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

❖ **To edit a Standby (Smart Standby) or Off (Smart Shutdown) state**


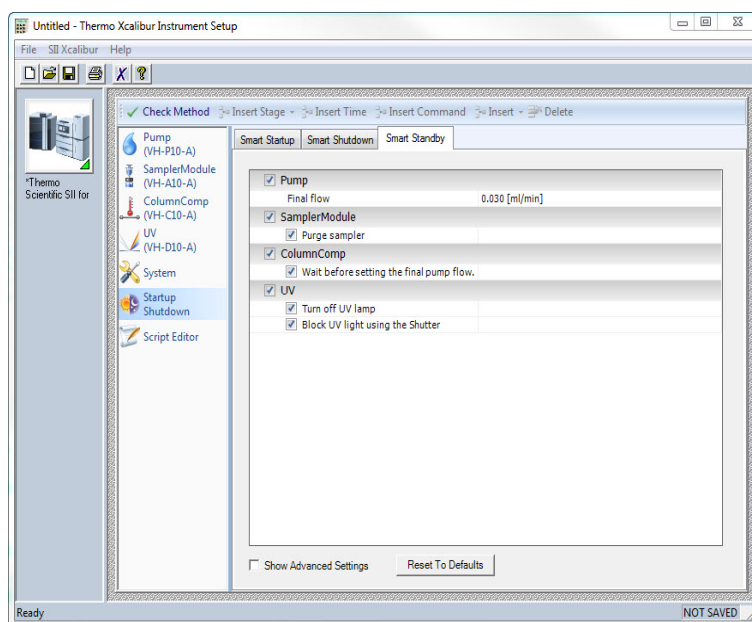
1. Open the instrument method that will run last.
2. In the left pane of the SII for Xcalibur Instrument Method Wizard, click  Startup Shutdown.
3. Click the **Smart Standby** or **Smart Shutdown** tab to display the corresponding tab page (see [Figure 9](#)).

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, click 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 click **Reset to default** on the context menu.

5. Click **File > Save**.

Running a Sequence

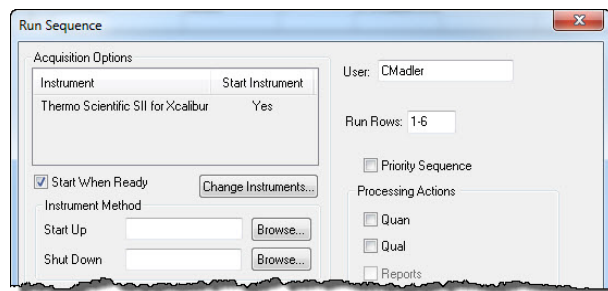
When SII for Xcalibur is installed, create and edit sequences in Xcalibur as usual.

❖ **To 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.

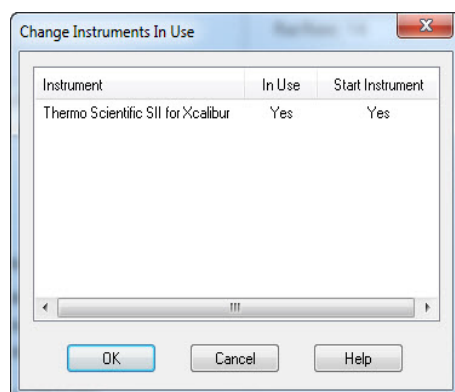
1. From the Sequence Setup view of the Home Page window, click **Actions > Run This Sample** or **Actions > Run Sequence** to open the Run Sequence dialog box (see [Figure 10](#)).

Figure 10. Xcalibur Run Sequence dialog box: Start Instrument parameter



2. Click the **Change Instruments** button to open the Change Instruments in Use dialog box (see [Figure 11](#)).

Figure 11. Xcalibur Change Instruments in Use dialog box



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

❖ To 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. Click **Direct Control** in the SII for Xcalibur status pane (see [Figure 1](#)) 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.

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.

Specifying the Post-Sequence State

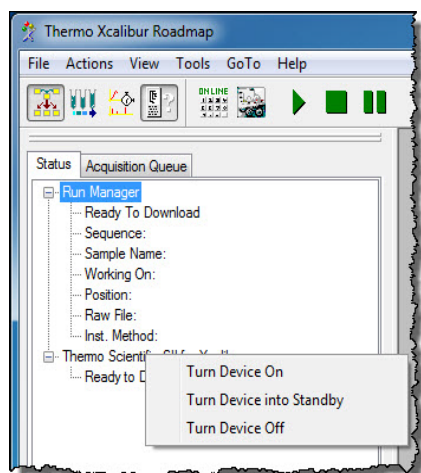
- **Standby:** Select the Standby option to place the system in the Standby state when the current sequence is completed. After the last injection or the shutdown method (whichever occurs later), SII for Xcalibur will execute the SmartStandby portion of the last instrument method that was used. Select 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.

❖ **To manually implement the On/Standby/Off state**

On the Status page of the Xcalibur Information view, right-click **Thermo Scientific SII for Xcalibur** and select either **Turn Device into Standby** or **Turn Device Off** on the context menu (see [Figure 12](#)).

Note The **Turn Device On** command is currently reserved for error recovery.

Figure 12. SII for Xcalibur Device commands context menu



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

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

- After creating or editing an instrument method, you can immediately check the method for possible errors in the syntax or semantics, using the **Check Method** toolbar button 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 Xcalibur message box is displayed.
- If a preflight error related to an LC device driver occurs, an Xcalibur message box is displayed and the message is logged in the Chromeleon audit trail. To view the audit trail, click 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 Xcalibur message box is displayed and the sequence is aborted.

Table 1. Error messages

| Error message | Remedy |
|---|--|
| Preflight check failed: <Description of error.> | <ol style="list-style-type: none"> 1. Click OK on the SII for Xcalibur message bar to dismiss the message. 2. Click Actions > Stop Analysis in Xcalibur. 3. Click Actions > Start Analysis in Xcalibur. <p>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.</p> |
| Method validation failed Row <row number>. | <ol style="list-style-type: none"> 1. Edit the method in the SII for Xcalibur Method Wizard. 2. Click Check Method to validate the method. <p>Note: The sequence may contain more than one problem; only the first failed method is reported.</p> |
| Device abort. | <ol style="list-style-type: none"> 1. Click OK to close the Xcalibur message box. 2. Check 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 click Turn Device On. This restores the software to the Ready to Download state. 5. Click Actions > Start Analysis in Xcalibur. |

Table 1. Error messages, continued

| Error message | Remedy |
|--|--|
| 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: <ol style="list-style-type: none">1. Click Start and type <i>services.msc</i> in the search box. In the search results, click <i>services.msc</i>.2. In the list on the right side of the Services window, right-click the name of each Chromeleon service and then click Start. Enable the SII for Xcalibur license: <ol style="list-style-type: none">1. Click Start > All Programs > Thermo Chromeleon 7 > Administration Console.2. Click User Database, and then click the Roles folder. Expand the name of the appropriate Role.3. On the License tab, select the Standard Instrument Integration License check box. |
| <i>(Continued from previous page)</i> 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. | Specify the required access privileges: <ol style="list-style-type: none">1. Click Start > All Programs > Thermo Chromeleon 7 > Administration Console.2. Click User Database, and then click the Roles folder. Expand the name of the appropriate Role.3. On the General tab, verify that these 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, and Administration. |

Related Documentation

- For detailed information about the Chromeleon data system, refer to the Chromeleon Help:
Click **Help > Thermo Scientific SII for Xcalibur Contents and Index** from the Thermo Xcalibur Instrument Setup window.
—or—
Press **F1** from the Direct Control window.
- For detailed information about the Xcalibur data system, refer to the Xcalibur Help.

Contacting Us

❖ To contact 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.

Trademarks

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