

SII for Xcalibur

Installation Guide

Software Version 1.8 • March 2024

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Document history

Revision: 1.0, P/N 065607

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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

Thermo Scientific™ Standard Instrument Integration (SII) for Xcalibur™ software is used to configure and control supported instruments from Thermo Scientific™ Xcalibur™ software. SII for Xcalibur is based on the Thermo Scientific™ Dionex™ Chromeleon™ 7 Chromatography Data System. Chromeleon is automatically installed during the SII for Xcalibur installation process. This guide describes how to install the software and configure your chromatography system.

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 installation guide, Thermo Fisher Scientific provides the following documentation:

- *SII for Xcalibur Quick Start Guide*

- *SII for Xcalibur Release Notes*
- *SII for Xcalibur List of Supported Instruments*
- Application-specific Help available from within Chromeleon and Xcalibur

Access manuals as PDF files

To access the *SII for Xcalibur Quick Start Guide*:

In the Thermo Xcalibur Instrument Setup window, select  on the toolbar.

–or–

In the Thermo Xcalibur Instrument Setup window, select **Help > Thermo Scientific SII for Xcalibur Help** or **Help > Help on Current Item**.

To access the Chromeleon manuals:

Select **Start > All Programs > Thermo Chromeleon 7 > Documents** from the Windows® taskbar.

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.

Install the software

You can install SII for Xcalibur software and configure your chromatography system in Thermo™ Foundation™ for use with the Xcalibur data system.

Computer requirements

SII for Xcalibur runs under the following operating systems: Microsoft® Windows® 10 Enterprise 2019 LTSC or Microsoft® Windows® 10 Enterprise 2016 LTSC (64-bit U.S. English version only). The PC hardware required for SII for Xcalibur is determined by the requirements for Chromeleon and Xcalibur:

- For Chromeleon system specifications, refer to the Thermo Fisher Scientific Web site.
- For Xcalibur system specifications, refer to the installation documentation provided with Xcalibur.

SQL Express 2014 SP3 has been validated with SII for Xcalibur 1.8. To install, execute the package located in Tools\Microsoft SQL Server 2014 SP3 Express.

Windows user management



CAUTION: The person installing SII for Xcalibur must be logged on as a Windows user with local administrator privileges.

Supported software

Refer to the *SII for Xcalibur List of Supported Instruments* for full details about various software versions and compatibility with SII for Xcalibur.

Supported chromatography systems

Refer to the *SII for Xcalibur List of Supported Instruments* for a list of HPLC and IC modules supported for use with the software.

Supported mass spectrometers

Refer to the *SII for Xcalibur List of Supported Instruments* for a list of mass spectrometers supported for use with the software.

TIP: It is possible to operate the liquid chromatography (LC) front-end system without a mass spectrometer. This is useful, for example, when you need to test the LC system but a properly configured mass spectrometer is not available, or when the LC system is in stand-alone operation. To operate without a mass spectrometer, make sure the Xcalibur Instrument Configuration does not include a mass spectrometer and that the Instrument Setup does not include a mass spectrometer part.

Verify prerequisites for installation

Existing SII for Xcalibur configurations

Follow the instructions in this section if:

- SII for Xcalibur 1.1, 1.2, 1.3, 1.4, 1.5, 1.5.1, 1.6, or 1.7 is installed on the PC.

–or–

- The installed version of any Thermo Scientific mass spectrometer software is not compatible with SII for Xcalibur 1.8. For details about the supported software versions and configurations, refer to the *SII for Xcalibur List of Supported Instruments*.

Upgrade the prerequisite software for SII for Xcalibur

Procedure

1. (If applicable) In the Thermo Foundation Instrument Configuration window, remove **SII for Xcalibur** from the Configured Devices list.
2. (If applicable) From the Windows Control Panel, uninstall SII for Xcalibur.

3. Upgrade the mass spectrometer software driver, Foundation, Xcalibur, and TraceFinder, as applicable, to the required version. For installation instructions, including the correct order of installation, refer to the appropriate software manual.



CAUTION: If Xcalibur 4.0 and the Exactive Series driver are installed on the PC and if SII for Xcalibur 1.1 was previously installed, you must uninstall Xcalibur 4.0 and then install Xcalibur 4.5 SP1. If you upgrade SII for Xcalibur directly from version 1.1 to 1.8 on a PC that is running Xcalibur 4.0, the Exactive Series instrument method editor may stop functioning.

4. (Optional) Uninstall DCMS^{Link} for Xcalibur (see [Uninstall DCMSLink \(for Xcalibur users only\)](#)).
5. Install SII for Xcalibur 1.8 (see [Install SII for Xcalibur](#)).

New SII for Xcalibur configurations

Before installing SII for Xcalibur for the first time, check that the following tasks have been completed, in the order listed here:

- Foundation is installed
- The software driver for the mass spectrometer is installed
- Xcalibur is installed

NOTE: Do not install SII for Xcalibur 1.8 on a computer with Chromeleon already installed. The required version of Chromeleon will be installed automatically when SII for Xcalibur 1.8 is installed.

Uninstall DCMSLink (for Xcalibur users only)

If DCMS^{Link} for Xcalibur is currently installed on the PC, decide which of the following options to pursue:

- Uninstall DCMS^{Link} now, before installing SII for Xcalibur.
—or—
- It is possible to operate SII for Xcalibur while DCMS^{Link} is installed on the PC, and then uninstall DCMS^{Link} later. However, after doing so, SII for Xcalibur must be reinstalled.



CAUTION: Failure to correctly follow one of the options will prevent proper operation of SII for Xcalibur.

Install SII for Xcalibur

Use the following instructions to perform the initial SII for Xcalibur installation or to upgrade the software from an earlier version. When you install SII for Xcalibur 1.8 on a PC on which an earlier version of SII for Xcalibur is installed, the earlier version will be upgraded.



CAUTION: The person installing SII for Xcalibur must be logged on as a Windows user with local administrator privileges.



CAUTION: Do not connect any analytical instruments to the PC until after you finish the software installation.



CAUTION: To avoid station IQ errors and other possible issues, you must install and activate Microsoft IIS (Internet Information Services) before installing SII for Xcalibur.

Procedure

1. Check that the prerequisites for installation (see [Verify prerequisites for installation](#)) have been met.
2. Log onto Windows as a user with local administrator privileges.



CAUTION: Installation of SII for Xcalibur without the required privileges can cause problems with the underlying Chromeleon 7.3.2 installation.

3. Double-click the **Install.exe** application from the installation medium to start the installation procedure.

The SII for Xcalibur Setup window appears.

4. Select the **I agree to the license terms and conditions** checkbox.
5. Select **Install**.

TIP: The Windows User Account Control (UAC) dialog box will appear shortly after selecting **Install**. If the UAC prompt is not acknowledged within 2 minutes, it times out and the installation is interrupted. To avoid this, do not leave the installation unattended until after the UAC dialog box appears.

6. The setup now guides you through the installation procedure; follow the on-screen instructions as they appear.

NOTE: Installation of the USB instrument drivers package triggers a Windows security warning. It is safe to dismiss the warning and continue the installation.

At the end of the installation process, Chromeleon will automatically run an Installation Qualification (IQ) and generate a report with the results.

7. To finalize Almanac installer, execute **Thermo.Chromeleon.Almanac.Service.msi** located in the /Tools/Almanac/ folder on the image.

NOTE: In order for SII for Xcalibur 1.8 to work with Xcalibur versions 4.5 or 4.6, refer to the **readme.txt** file located on the installation medium under Tools > Configuration.

Activate a third-party license

You can use any one of the following methods to activate the third-party license initialization codes which are in the Pending Activation, Grace Period Expired, Subscription Pending Activation, or Subscription License Expired state:

- Web activation
- Manual activation

Procedure

1. Select **Start > Thermo Chromeleon 7 > License Manager**.
2. If the license code has not been previously added, select **Add**, enter the **License Initialization Code (LIC)**, then select **Add** again.
3. Select the license initialization code to be activated.
4. Select **Activate** (or right-click on the selected code and select **Activate**).

The License Activation dialog box is displayed with an auto-generated License Request Code (LRC) and a QR code.

5. Perform one of the following to activate the third-party license:
 - Select **Web Activation**, to automatically activate the third-party license. For more details, see [Activate a license automatically](#).
 - Select **Manual Activation**, to manually activate the third-party license. For more details, see [Activate a license manually](#).

Activate a license automatically

You can activate licenses automatically using the web activation method. This is the easier and quickest option if your computer is connected to the internet and can communicate directly with Thermo Fisher servers. The License Activation Code (LAC) is auto-generated and the licenses are activated automatically on successful validation of license codes with the Thermo Fisher license server.

Procedure

- On the License Activation dialog box, select **Web Activation**.

The license is activated.

Activate a license manually

You can activate licenses manually using the QR code or by browsing to the web address displayed on the License Activation dialog box. If the LRC is valid and can be activated, the website will supply a LAC to enter in the dialog box to complete the activation process.

Procedure

1. On the License Activation dialog box, select the hyperlink, or scan the QR code using your mobile phone.

The License Activation Web Portal is displayed on your default browser.

2. Enter the **License Request Code** which is displayed on the License Activation dialog box.
3. Select **Activate License**.

The web portal generates the License Activation Code. Use this code to activate the third-party license.

4. On the License Activation dialog box, enter the **License Activation Code** in the LAC text box.
5. Select **Manual Activation**.

The license is activated.

NOTE: The license activation status is displayed on the log area of the License Activation dialog box.

Start the Chromeleon Instrument Controller Service

The Instrument Controller Service controls the exchange of data between Chromeleon and the analytical system. For example, acquisition data is received from the Instrument Controller and forwarded to Xcalibur.

Use one of the following procedures to start the Instrument Controller Service:

- Right-click the Chromeleon tray icon  in the notification area of the Windows taskbar and select **Start Chromeleon Instrument Controller**. The icon changes to gold  to indicate that the service is starting, and then changes to gray  when the service is running (idle).
—or—
- If the Chromeleon tray icon is not on the Windows taskbar, select **Start > All Programs > Chromeleon > Services Manager** and then select **Start Instrument Controller**.

Enable automatic server start

Procedure

1. Right-click the Chromeleon tray icon and select **Show Chromeleon Services Manager**.

The Chromeleon Services Manager dialog box appears.
2. Select the **Start Service on System Start** checkbox.

NOTE: To enhance system performance, Thermo Fisher Scientific recommends having Chromeleon automatically start the Instrument Controller each time the PC is turned on.

Install the hardware

Connect a chromatography system

Connect the chromatography system to the PC as described in the installation instructions for the system.

Connect an external autosampler

Install the external autosampler according to the instructions in the autosampler manual. When controlled by Xcalibur, the following connections are required:

- The autosampler must be connected to the mass spectrometer to allow hardware synchronization between the instruments.
- The autosampler must be connected to a digital input device to establish a connection with SII for Xcalibur. When an injection occurs, the autosampler sends a signal to SII for Xcalibur, which then starts the sample run for instruments controlled by SII for Xcalibur. A proxy autosampler driver, such as a remote inject driver or an analog-to-digital driver, must be added to the Chromeleon instrument configuration.

Connect a mass spectrometer

Connect the mass spectrometer to the PC as described in the installation instructions for the system.

NOTE: In order to start MS data acquisition, the start input on the mass spectrometer must be connected to a relay output on another module (for example, an autosampler or pump). For details, refer to the installation instructions for the mass spectrometer.

Configure instruments in the software

Before you can control a chromatography instrument, that instrument and all its modules must be defined in the instrument configuration. The key steps include:

- Adding SII for Xcalibur to the Configured Devices list in the Thermo Foundation Instrument Configuration window
- Adding each instrument driver to the Chromeleon configuration

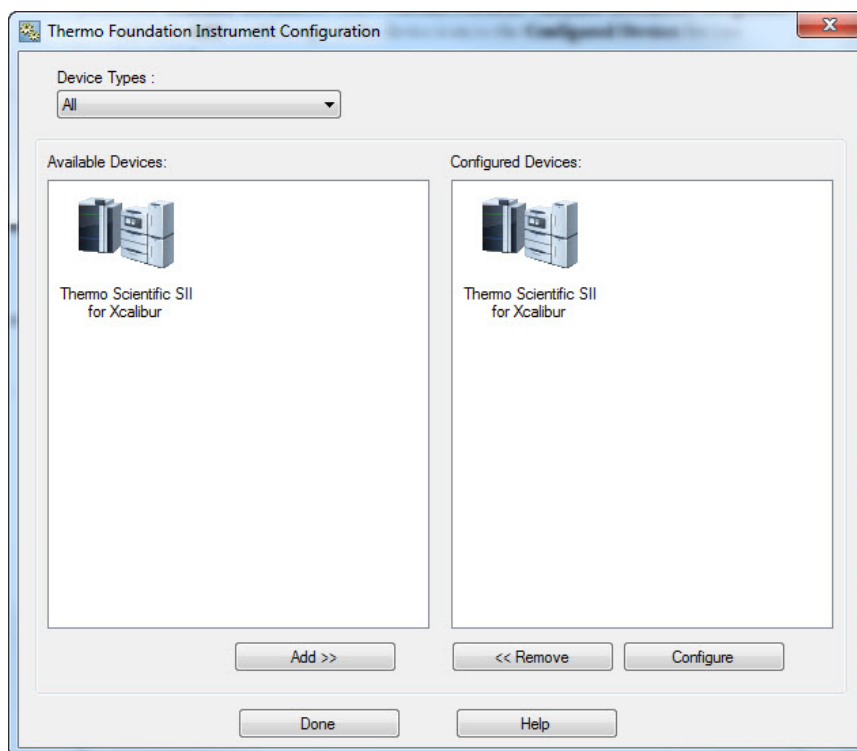
Add SII for Xcalibur to the Configured Devices list

Procedure

1. Check that Xcalibur is not running. If it is running, stop any sequences on the Xcalibur Home page, delete any samples from the Acquisition Queue, and close Xcalibur.
2. Select **Start > All Programs > Thermo Foundation x.x > Instrument Configuration**, where x.x is the Foundation version currently in use.
The Thermo Foundation Instrument Configuration window appears.
3. Under Device Types, select **All** to display all the installed device drivers in the Available Devices list.

4. In the Available Devices list, select **Thermo Scientific SII for Xcalibur** and select **Add** to add a copy of the device icon to the Configured Devices list.

Figure 1 Thermo Foundation Instrument Configuration window



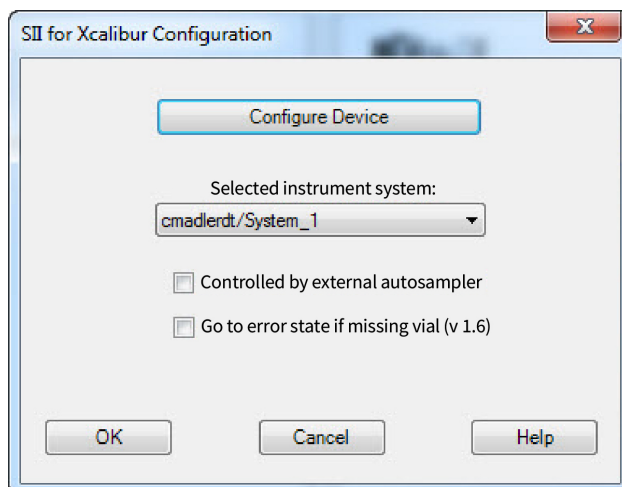
CAUTION : Before uninstalling Chromeleon and SII for Xcalibur (for example, before installing a software update), you must first remove the SII for Xcalibur device from the instrument configuration.

5. In the Configured Devices list, select **Thermo Scientific SII for Xcalibur** and select **Configure**.

If Chromeleon User Management is enabled, the SII for Xcalibur Login dialog box might appear now. Enter your username and password, and then select **OK**. The dialog box will not appear in the future.

6. In the SII for Xcalibur Configuration dialog box, select **Configure Device** to launch the Chromeleon Instrument Configuration Manager.

Figure 2 SII for Xcalibur Configuration dialog box



Create a Chromeleon instrument

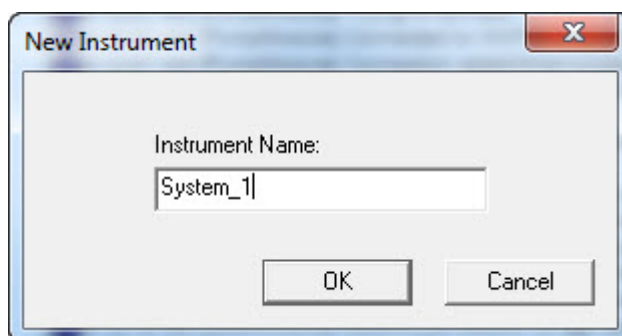
NOTE: In Chromeleon, all modules that are combined in a chromatography system to enable chromatographic separations make up an *instrument*. For example, an instrument might consist of two pumps, one autosampler, one column oven, and two non-MS detectors that are switched in series. (The mass spectrometer is not considered part of the Chromeleon instrument.)

Procedure

1. In the Instrument Configuration Manager left pane, right-click the name of the PC on which the software is installed (see [Figure 6: Instrument Configuration Manager](#)) and select **Add Instrument**.

The New Instrument dialog box appears.

Figure 3 New Instrument dialog box



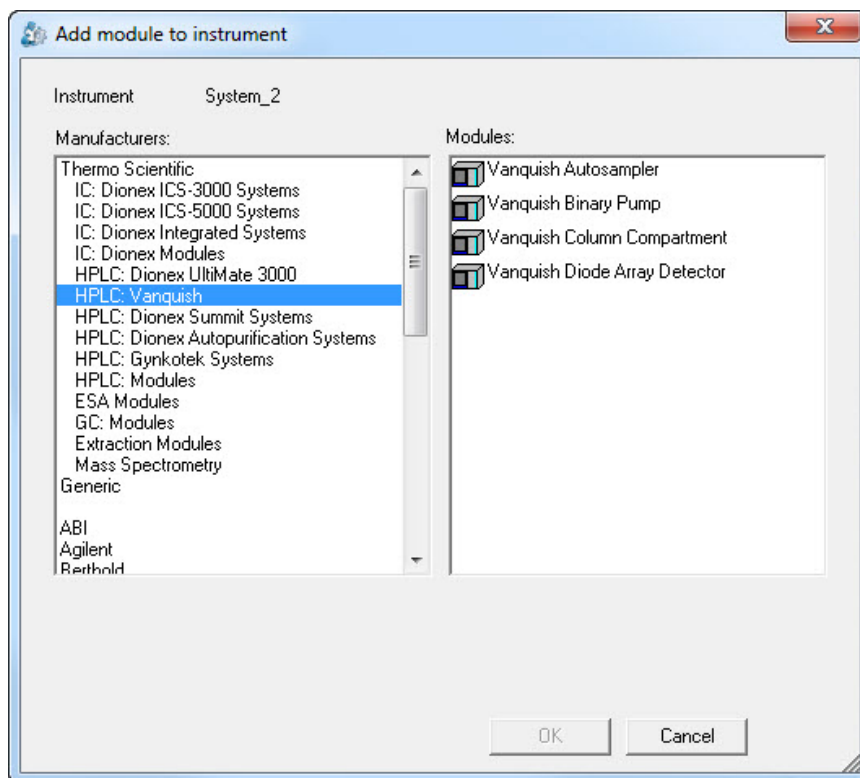
2. (Optional) Edit the proposed instrument name.
3. Select **OK** to close the dialog box.

The instrument name is now displayed in the Instrument Configuration Manager left pane (see [Figure 6: Instrument Configuration Manager](#)).

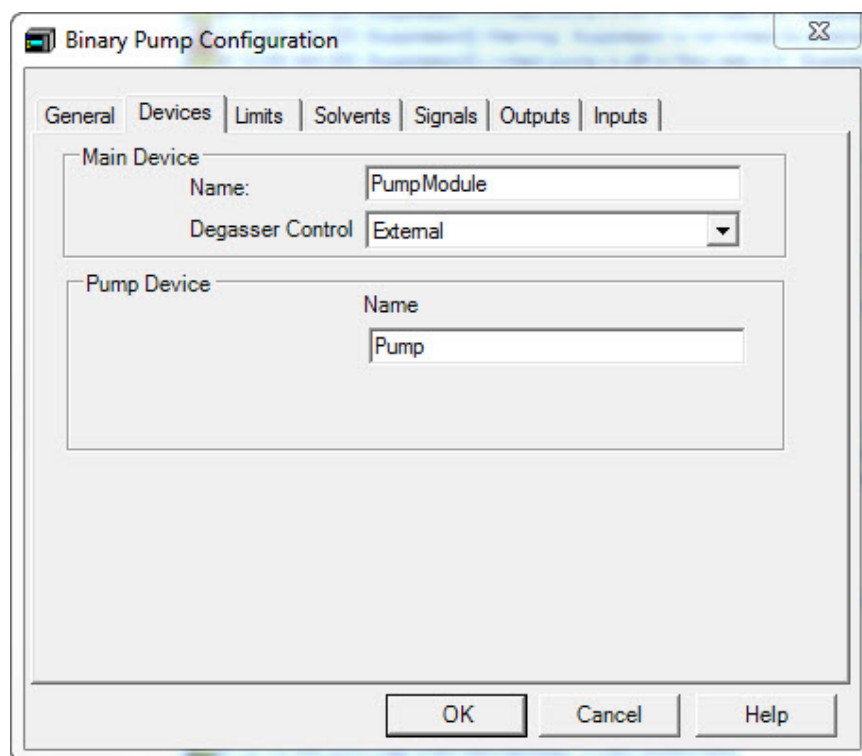
4. Begin adding modules to the Chromeleon instrument:

- a. Right-click the instrument name and select **Add Module**.
The Add Module to Instrument dialog box appears.
- b. Select the manufacturer from the **Manufacturers** list and the name of the driver from the **Modules** list.

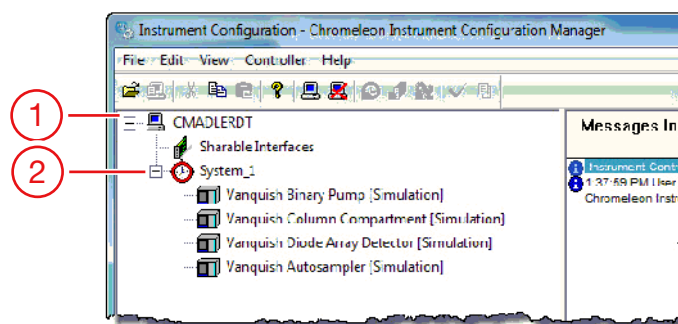
Figure 4 Add module to Instrument dialog box



- c. Select **OK**.
The properties dialog box for the selected device appears. (At least one page of options is available for each module.)
- d. Specify properties for the module in the dialog box.

Figure 5 Example of the properties dialog box for a pump

5. Continue adding modules to the instrument and specifying module properties.

Figure 6 Instrument Configuration Manager

No.	Description	No.	Description
1	PC name	2	Instrument name

6. When an external autosampler is installed, it can be controlled via a Chromeleon driver or a TTL input.
 - For driver control: Add the driver to the instrument configuration and specify the driver properties. For example, select Generic (from the Manufacturers list) and Remote Inject (from the Modules list) or Thermo Scientific (from the Manufacturers list) and A2D Analog to USB Adapter (from the Modules list).

- For TTL control: Open the properties dialog box for the pump (or other device) that is providing the input signal and enable the appropriate input.
7. When you have finished adding modules to the instrument, select **File > Save Installation**.
 8. Select **File > Exit**.

The name of the new instrument is displayed in the SII for Xcalibur Configuration dialog box (see [Figure 2: SII for Xcalibur Configuration dialog box](#)), under Selected Instrument System.

When SII for Xcalibur is installed, up to four Chromeleon instruments can be configured. You can change the instrument that is under SII for Xcalibur control at any time. To do so, select the down arrow next to Selected Instrument System and select a different instrument.

9. Select the **Controlled by External Autosampler** checkbox if the instrument configuration includes an external autosampler.



CAUTION : Before running any sequences, the external autosampler (not SII for Xcalibur) must be specified as the Start Instrument in the Xcalibur Run Sequence dialog box. For details, refer to the *SII for Xcalibur Quick Start Guide*.

10. (Optional) Select the **Go to Error State if Missing Vial (v 1.6)** checkbox if you want a missing vial to trigger an error state.
11. Select **OK** to save your changes and close the dialog box.
12. In the Thermo Foundation Instrument Configuration window, select **Done**.
13. Select **OK** to save the selected configuration.

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