

# **SCIEX OS 1.3.1**

## **Release Notes**



RUO-IDV-03-1821-F January 2018

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AB Sciex Pte. Ltd. Blk 33, #04-06 Marsiling Ind Estate Road 3 Woodlands Central Indus. Estate. SINGAPORE 739256

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Introduction 1

Thank you for choosing SCIEX to supply your system. We are pleased to give you SCIEX OS 1.3.1 that supports both the SCIEX X500R QTOF and the SCIEX X500B QTOF systems, which provide liquid chromatography-time-of-flight mass spectrometry functions.

This document contains instructions for installing the software, describes features in the software, and provides troubleshooting guidelines. Keep these release notes for your reference as you become familiar with the software.

## **Technical Support**

SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the system or any technical issues that might arise. For more information, visit the website at <a href="sciex.com">sciex.com</a>.

## **Contact Us**

#### **SCIEX Support**

- sciex.com/contact-us
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#### **Customer Training**

- In North America: NA.CustomerTraining@sciex.com
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Requirements

# **Required Software**

Microsoft Word 2013 is required for the report functionality in the Analytics workspace.

# **Operating System Requirements**

- Microsoft Windows 7 64-Bit, SP1
- English (Language and Keyboard settings)

## **Computer Requirements**

Dell OptiPlex XE2 computer, with:

- An Intel Core I5-4570S processor (Quad core, 2.90 GHz, 6 MB with HD Graphics 4600)
- 32 GB DDR3 1600 Mhz SDRAM
- 2\*2 TB HDD (RAID1)
- DVD+-RW
- Computer specification required for acquisition computers: Two single-port Broadcom Ethernet cards

Installation Instructions

## **Install the Software**

If the software must be installed from a DVD, then always install the software from the official DVD and confirm after the installation that the correct version is installed.

- 1. Log on to the computer as a Microsoft Windows user with Administrator privileges.
- 2. Do one of the following:
  - If the software is being installed from a DVD, then load the DVD in the DVD drive and continue with step 5.
  - If the software is being installed from a downloaded file, then continue with step 3.
- 3. Download the required .zip file from the SCIEX website.

**Tip!** To prevent potential installation issues, save the file to the D drive.

- 4. After the download is complete, right-click the downloaded file and then click **Extract All**.
- 5. Browse to the extracted files or the DVD and then double-click **Setup.exe**.
- 6. Follow the on-screen instructions.

The initial setup might take several minutes as the SQL server must be installed.

**Note:** To avoid installation issues, make sure that the path to the installation folder is not too long. If the path is longer than 118 characters, then installation will not proceed.

- 7. After the software is installed, restart the computer.
- 8. Start the software.
- 9. Type the license key in the appropriate field.

The license key comes with the system. If a license key is not available, then contact sciex.com/request-support

10. Complete the software activation screen.

Licenses are required for the Bio Tool Kit and ChemSpider features. Make sure to obtain licenses before attempting to use the features in the Explorer workspace.

11. For acquisition computers, run the MS FW Updater Utility. Refer to the MS FW Updater Utility READ ME file that comes with the software installation package.

## **Upgrade from SCIEX OS 1.2 or Later**

A new software license is required to upgrade from SCIEX OS 1.2. Upgrades from SCIEX OS 1.3 do not require a new software license.

**Note:** To upgrade from versions of SCIEX OS earlier than version 1.2, uninstall SCIEX OS and then install SCIEX OS 1.3.1. Also upgrade any vertical applications. Refer to Install Optional Vertical Applications on page 8 for information about upgrading the vertical applications.

**Note:** Some of the steps might take some time to complete.

- 1. Log on to the computer as a Microsoft Windows user with Administrator privileges.
- 2. For acquisition computers perform these steps:
  - a. Open the currently installed SCIEX OS.
  - b. Open the MS Tune workspace.
  - c. Click Positive MS Tuning.
  - d. Click **Save Tuning Settings** in the left panel and then click **Save Settings**.
- 3. Back up the SCIEX OS data folder.
- 4. Do one of the following:
  - If the software is being installed from a DVD, then load the DVD in the DVD drive and continue with step 7.
  - If the software is being installed from a downloaded file, then continue with step 5.
- 5. Download the required .zip file from the SCIEX Web site.

**Tip!** To prevent potential installation issues, save the file to the D drive.

- 6. After the download is complete, right-click the downloaded file and then click Extract All.
- 7. Browse to the extracted files or the DVD and then double-click **Setup.exe**.
- 8. Follow the on-screen instructions.

The initial setup might take several minutes as the SQL server must be installed.

9. After the software is installed, restart the computer.

10. For acquisition computers, run the MS FW Updater Utility. Refer to the MS FW Updater Utility READ ME file that comes with the software installation package.

## **Install Optional Vertical Applications**

The following optional applications must be installed after the SCIEX OS is installed:

- BioPharmaView<sup>™</sup> software version 2.1
- MarkerView<sup>™</sup> software version 1.3.1
- LibraryView<sup>TM</sup> software version 1.2

If the application is not installed, then the software tile will not be shown on the home page.

When upgrading from SCIEX OS 1.2 or later, it is not necessary to upgrade the optional applications. When upgrading from earlier versions, these optional applications must be upgraded.

**Note:** If newer versions of the applications are available, then contact sciex.com/request-support to verify software compatibility.

- 1. Install SCIEX OS.
- 2. Make sure that SCIEX OS is closed, and then install the BioPharmaView<sup>™</sup>, MarkerView<sup>™</sup>, or LibraryView<sup>™</sup> software.
- 3. Refer to the respective release notes for more information about installing the applications.

# **Downgrade to Previous Versions of the Software**

Contact sciex.com/request-support for help on downgrading from the current version of the software.

Fixes in Version 1.3.1 4

This section describes the enhancements and fixes in SCIEX OS 1.3.1. To view the enhancements and fixes for a previous release of SCIEX OS, refer to the *Release Notes* that came with that version of the software.

- When processing *Scheduled* MRM<sup>HR</sup> data the user might rarely see an exception message, **The results table cannot be created because more than ten samples could not be integrated**. The user was not able to finish processing data and generate results. (MQ-3496)
- TDC sync errors occurred during batch execution after the diverter valve position was switched. This error caused the batch to stop. (MSCS-1404)
- The wrong sample might be injected from a Shimadzu or ExionLC<sup>™</sup> autosampler. This error occurred if another sample or batch of samples was submitted to the queue while a sample was waiting to be injected. (ACQ-3182)
- MS Tune specifications have been updated to be consistent with the Service installation specifications. The previous MS Tune specifications were too restrictive, causing the MS Tune procedure to fail. (ACQ-3205)
- Rarely, a large data file could not be opened or processed in the Analytics workspace. The following error was shown: Non-negative number required. (DS-2133)

#### **Notes on Use**

**Note:** The numbers in parentheses are reference numbers that identify issues in our internal tracking system.

- For optimal performance, at least 20 GB of free disk space is required on drive D. Batches might not be acquired successfully if there is insufficient disk space. (DS-870)
- All default Ion Reference tables installed by SCIEX OS will be upgraded and any modifications made by the
  user will be lost if they were saved to the default filenames. We recommend saving the modified tables under
  different names. User-created custom tables will not be modified. When performing Auto-calibration in the
  Batch workspace using the CDS, the user must make sure to select the correct Ion Reference table for the
  corresponding CDS solution (that is, the names on the CDS bottles must match those of the Ion Reference
  tables). (BLT-441, ACQ-2527/2627, ONYX-1975)
- The following table shows the calibration solutions required for SCIEX X500R QTOF and the SCIEX X500B QTOF systems before upgrading to SCIEX OS 1.3 or later.

**Table 5-1 Calibration Solutions** 

Solution	Part Number
FG*ESI POSITIVE CALIBRATION SOLUTION X500B	5049910
<b>Note:</b> This solution is used for both X500R and X500B systems, for positive and negative TOF MS and TOF MSMS optimization.	
PTO* CALIBRATION SOLUTION SUITE FOR X500B SYSTEM	5033025
Note: This kit contains:	
FG, ESI NEGATIVE CALIBRATION SOLUTION X500	
FG, APCI POSITIVE CALIBRATION SOLUTION X500	
FG, APCI NEGATIVE CALIBRATION SOLUTION X500	
FG, ESI POSITIVE CALIBRATION SOLUTION X500B	
PTO* ESI POSITIVE CALIBRATION SOLUTION X500B 5 PACK	5032735

- Data files created in SCIEX OS version 1.2 or earlier cannot be appended to data files acquired in SCIEX OS 1.3 or later. (DS-1931)
- Acquisition methods, batch files, data files, processing methods, and Results Tables or qsessions created or saved in SCIEX OS 1.3 or later cannot be opened in SCIEX OS version 1.2 or earlier. (MQ-2321)
- In the Analytics workspace, users must open and then save methods created in SCIEX OS 1.1 or earlier to
  implement the updated isotopic abundance table. If an existing method is used without first opening the
  method, then the precursor mass calculation will not be updated and the results will be incorrect. To avoid
  any issues, do the following:
  - 1. Open the method. The precursor masses update automatically.
  - 2. Save the method using the same or new name. If the user clicks **Close**, then a message is shown, indicating that the method has been changed and that the user must save the method. (MQ-2183)
- To avoid performance issues or data corruption, do not perform any computer maintenance procedures, such as defragmentation or disk cleanup, during sample acquisition.
- The latest version of the isotopic abundance table has been implemented in SCIEX OS version 1.2 and later.
   Any tables that use the atomic masses and isotopic abundances have been updated and, therefore, the average molecular mass calculation might change based on the revised calculation. (PV-1075)
- Set the anti-virus software to not scan during sample acquisition to avoid affecting system performance.
- When performing Windows updates, do not install optional updates because they might impact functionality
  in the software. Only install required updates, and schedule installation of updates when the system is not
  acquiring data.

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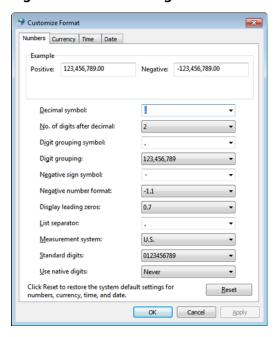
SCIEX OS 1.3.1

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## **Known Issues**

The local settings shown in Figure 5-1 are supported.

**Figure 5-1 Local Settings** 



Label	Supported in SCIEX OS
Decimal symbol	Either '.' or ',' is supported.
No. of digits after decimal	Controlled by the number format in SCIEX OS.
Digit grouping symbol	Not supported.
Digit grouping	Not supported.
Negative sign symbol	Controlled by SCIEX OS.
Negative number format	Not supported.
Display leading zeros	Not supported.
List separator	Not supported.
Measurement system	Not supported.
Standard digits	Not supported.
Use native digits	Not supported.

**Table 5-2 General Issues** 

Issue	Description
In some rare instances, keyboard input is not accepted. (BLT-350)	If this issue occurs, then start SCIEX OS again. Starting the software does not impact any ongoing data acquisition.
	<b>Tip!</b> Users can copy and paste information in the fields, if required.
Microsoft Office cannot be installed after SCIEX OS is installed. (BLT-353)	To avoid this issue, do the following:  1. Install SCIEX OS.
	2. Remove Microsoft Access.
	3. Install Microsoft Office (32-bit).
	4. Install Microsoft Access.
SCIEX OS 1.3 or later is not removed when a user tries to remove it using Setup.exe. (ONYX-2124)	If a user tries to remove SCIEX OS 1.3 or later using Setup.exe, the entry from Windows Programs and Features for SCIEX OS is removed. However, the program remains and can still be opened. To remove SCIEX OS, run Setup.exe from SCIEX OS folder and then follow the on-screen instructions to install the software. This process will add the entry for SCIEX OS back to the Windows Programs and Features list. Use the Programs and Features list to remove SCIEX OS 1.3 or later.
The correct status of a program that has been removed is only shown in the service package after the service package has been generated twice. (ACQ-2516)	To avoid any issues, generate the service package twice after a program is removed.

**Table 5-3 Devices** 

Issue	Description
Agilent LC: An error occurs if the device configuration in the method does not match the configuration of the active device (ONYX-2652)	If the user opens an LC method that was created using a different sampler or pump than the one that is currently active, then the LC method window is blank. An error occurs when the user attempts to switch between modules. If this error occurs, then either change the device configuration to the configuration that was active when the LC method was created, or create a new LC method with the currently active device configuration.
In some cases, devices cannot be added manually. (ACQ-3014)	In some cases, when devices are added manually, the <b>Test device</b> function fails. To avoid this issue, use <b>Autoconfig</b> to add devices.
The system remains in Run state after recovery from MS communication loss during acquisition. (MSCS-432)	If the Ethernet cable is disconnected during acquisition, then the acquisition stops and the system goes to Fault state. After the Ethernet cable is connected again, if the user attempts to run another acquisition, then the acquisition completes and the real time display stops updating, but the system remains in Run state. If this issue occurs, then reactivate the device profile.
Agilent LC: High throughput settings are not supported in the autosampler. (ACQ-529)	The high throughput settings are not currently supported.
Shimadzu LC: Incorrect device status is shown when the device is recovering. (ACQ-1410)	If a sub-device is turned off prior to sample submission, then the Shimadzu LC goes to Standby state even though the status should be Fault. If the user attempts to submit the batch to the queue again, then the first sample is submitted but fails immediately because the LC goes to Fault state and the sample becomes corrupted. If this issue occurs, then reset the computer and restart the software.
Shimadzu LC: The device traffic light does not update from Fault state when an error is recovered through Direct Control. (ACQ-1420)	If the user opens the Direct Control device and then clicks <b>Clear Error</b> when the LC is in Fault state, then the device recovers but the status in the software still indicates a fault. To clear this error, click <b>Standby</b> in the status panel.
The LC method does not run correctly if the devices that are turned on and connected do not match the devices in the activated device list. (ACQ-1716/2062)	To make sure that the system works correctly, either turn off the devices or turn on the devices to match the activated devices list.

**Table 5-3 Devices (continued)** 

Issue	Description
Shimadzu LC: A performance issue is observed during running of a long batch using the Shimadzu PDA at sampling rates higher than 12.5 Hz. (ACQ-2037)	The expected duration of the batch might be longer than anticipated. To avoid any issues, use a sampling rate lower than 12.5 Hz.
Shimadzu LC: Inverted UV data is acquired during acquisition with two UV channels. (ACQ-2042)	This occurs when polarity is set to negative in the LC method UV detector section. To avoid any issues, use the positive setting for the polarity field.
Agilent LC: During equilibration, if the user aborts the sample, then the Agilent LC might go to a Fault state. (ACQ-2142)	If this issue occurs, then click <b>Standby</b> to recover the device.
Agilent LC: Agilent LC shows a Fault state even when the sub-devices have recovered from a fault and are in Ready state. (ACQ-2144)	If this issue occurs, then click <b>Standby</b> to return the LC to Ready state.
When the duration of a gradient table for an LC pump or column oven temperature table in an LC method is longer than the duration of the MS method, then the LC devices will stop running when the MS method duration expires. (ACQ-2167/2088)	To avoid this issue, make sure that the value in the <b>Stop Time</b> field for the LC method duration is the longest time that the LC method must run.
Shimadzu and ExionLC LCs: The PDA default parameters are different depending on how the LC method is accessed. (ACQ-2176)	To avoid any issues, make sure that the correct parameters are used for the PDA device.
Agilent LC: The comma is ignored as a decimal separator when the flow rate in the LC gradient grid is copied. (ACQ-2191)	This is an issue with the Agilent LC. To avoid this issue, manually type the flow rate, using a comma as the decimal separator.
Agilent LC: The Fault state is not reflected correctly if the devices are in Fault state during device activation. (ACQ-2195)	To avoid this issue, clear the fault in the device, then deactivate and reactivate the Agilent devices.
A system error is shown when there is a communication error between the devices and the mass spectrometer. (ACQ-2663)	If the batch is stopped, but the HPLC system continues to run, then the error message: CBM Disconnected is shown. This error might be caused by a communication error in the Shimadzu system. To avoid this issue, verify and set the IP address of the CBM to a unique ID and then inspect for any loose cable connections.

#### **Table 5-3 Devices (continued)**

Issue	Description
If the devices list contains a diverter valve and the user tries to acquire data using a method that does not contain a second step, then the acquisition stops. (MSCS-1284)	To avoid any issues, either make sure that the method has a switching step for the diverter or do not include a diverter valve in the devices list.
The system does not activate the <b>Standby</b> button on the right status panel when a subdevice, such as the CDS, goes to fault, preventing the user from clearing the error. (MSCS-1314)	If this issue occurs, then the user must go to CDS direct control and then click <b>Start</b> to change the CDS status from Fault to Running to clear the Fault status of the CDS subdevice.
The calibrant delivery system (CDS) does not stop after the user starts it from Direct Control and then starts the queue with analytical samples. (ONYX-1428)	If the calibrant runs throughout the batch, then the sample might become contaminated with the calibrant. If this issue occurs, then stop the batch, stop the CDS, and start the batch again.

#### **Table 5-4 MS Methods**

Issue	Description
By default, the Apply Scan Schedule check box is selected in the MRM method that is generated when the Guided MRM HR feature is used. (ACQ-1681)	If this option is not required, then clear the check box before acquiring data using this method.
Ion source parameters are not updated to the mass spectrometer. (ACQ-2177)	During manual acquisition using a SWATH® and MRM HR method, the ion source gas and temperature parameters are available to be edited in the user interface. Users can edit the fields. However, the changes are not updated to the mass spectrometer nor are the changes logged in the sample information for that sample.
Only the grid parameters use the regional settings character for the decimal separator. (ACQ-2190)	Regional settings are followed in the MS Method and Batch grids, but not in the other fields in the MS Method Editor or the Equilibration dialog. To avoid any issues, use a period (".") as a decimal separator in all of the fields, excluding the MS Method and Batch grids.
The Method Editor grids resize beyond the available width. (ACQ-2243)	If this issue occurs, then use the scroll bars to access sections of the user interface that are not currently visible.

**Table 5-4 MS Methods (continued)** 

Issue	Description
The software does not save the required parameters when switching from an open method to another method after the ion source or probe is changed. (ACQ-2262)	If this issue occurs, then update the parameters, as required. Some parameters become unavailable if they are not required for the new ion source or probe.
No validation message is shown for the maximum number of windows per cycle in the Autofill SWATH Windows dialog. (ACQ-2296)	The maximum number of SWATH windows per cycle for an experiment is 200. If the options selected in the Autofill SWATH Windows dialog result in more than 200 windows per cycle being calculated, then the Windows per cycle field value is NA. The method cannot be generated. To avoid this issue, reduce the number of windows per cycle by increasing the Window width or by narrowing the difference between the Precursor start mass and the Precursor stop mass.
The MS Method workspace does not update to show the correct information when running the calibrant. (ONYX-1556)	Although the user interface is not updated, the correct parameters are used and reflected in the file information.
If the user manually changes the decimal separator from period to comma in the Windows operating system and then also applies regional settings in SCIEX OS, then the following issues occur:  • The default values in the MS Method Editor numeric fields show periods as decimal separators instead of commas.	To avoid any issues, use regional settings that use commas as the decimal separator, for example German.
When the user edits the MS method, the numeric fields allow the user to type commas, but after the cursor is moved, the comma is not accepted. For example, the user types 0,25, but the value is entered as 25. (ONYX-2050)	

**Table 5-5 Acquisition** 

Issue	Description
<ul> <li>In the Batch and Queue workspaces, printouts using the PDFactory option have the following issues:</li> <li>Reports generated with PDFactory do not include any numeric values, such as method names, sample names, sample IDs, barcodes, and so on, where the names are numbers. (ONYX-2236)</li> </ul>	To avoid any issues, print using the XPS option instead of PDFactory.
<ul> <li>The date and time when other regional settings are used are not shown. (ACQ-2700)</li> </ul>	
<ul> <li>The row index is blank when only several isolated rows are printed using PDFactory. (ACQ-2701)</li> </ul>	
<ul> <li>If the Auto-Calibrate option is selected during batch creation, then the Calibration Sample Frequency, CDS Channel, and the Vial Position (if LC is selected for calibrant delivery) values are missing. (ACQ-2804)</li> </ul>	
<ul> <li>Printing reports using XPS and PDFactory in Landscape mode work as expected, but when PDFactory in Portrait mode is used, the last two columns on the first page are omitted and the time at which the batch is printed is truncated and not shown in full. (ACQ-1275)</li> </ul>	
Users can create a batch with more than 500 components. (ACQ-3073)	SCIEX OS supports a maximum of 500 components. If a user adds more than 500 components to a batch, no error is reported. However, when the user closes and then opens the batch, an error message is shown.
Inconsistent behaviour occurs during imports from an acquisition method and from a processing method, resulting in unreliable qualification results. (BLT-284)	Information imported from an acquisition method has a mass accuracy to two decimal places. Formulas used to calculate mass accuracy in a processing method produce results to four decimal places. Therefore, this might cause inconsistent results between the two methods.
The CDS remains in Wash mode after the software stops responding. (MSCS-666)	If this issue occurs, then clear the Wash mode option in the Direct Control dialog.

**Table 5-5 Acquisition (continued)** 

Issue	Description
Real time updates for the DAD panel might be slower than the response time chosen in the method (DS-853)	To avoid this issue, either reduce the frequency of the DAD acquisition or inspect the data after the acquisition has completed.
The Ion source gas 2 setting is included in a user message. (MSCS-943)	When the APCI probe is used, a user message is shown stating that the Ion source gas 2 setting should be a specific value. Ignore the Ion source gas 2 settings in the user message.
Real time sample information is only updated when the MS Method workspace is refreshed. (MSCS-968)	To avoid this issue, close the data file and then open it post-acquisition to view the Sample Information.
An incorrect message is shown when the probes are switched. (MSCS-972)	The error does not affect acquisition. Users can cancel the message and acquisition will continue.
Samples in the queue might be marked as failed even though the data is acquired successfully. (DS-1016)	During the processing of complex data during acquisition, a sample in the queue might be marked as failed even though it was acquired successfully and the queue has moved to the next sample. If this occurs, the sample and data file are not actually affected, and can be used for exploring or processing. To refresh the queue icons, restart SCIEX OS.
Acquisition is aborted when acquiring using Scheduled MRM <sup>HR</sup> and SWATH® methods or Scheduled MRM <sup>HR</sup> and IDA methods and the TOF MS method of the MRM HR method is deleted. (MSCS-1059)	To avoid this issue, do not delete the TOF MS experiment from the MRM HR method.
The CDS pump continues to run after the calibrant sample in the queue is aborted. (MSCS-1145)	If this issue occurs, then stop the CDS manually.
Peak labelling is inconsistent between XWC and TWC graphs during real time UV data acquisition. (DS-1262)	To avoid any issues, examine data post-acquisition using the Explorer workspace.
The Data Acquisition panel shows the previously acquired sample. (DS-1384)	If this issue occurs, then restart the software.
A message is shown indicating that a data file is corrupted and the batch cannot be submitted. (ONYX-1539)	Occasionally, it has been observed that a batch could not be submitted because of a corrupted file message in the Batch Editor. However, when the data file is opened in the Explorer workspace, no corruption of the data file is observed. If this issue occurs, then use a different data file name for the batch or move the affected data file using Windows Explorer.

**Table 5-5 Acquisition (continued)** 

Issue	Description
When data is ramped, the real time data stops updating before the end of acquisition. (ONYX-1682)	Real time and post-acquisition data do not match when parameters are ramped during acquisition. To avoid issues, use the post-acquisition data for any analysis.
In the Batch workspace, the list of available MS and LC methods is incomplete if the methods are copied from a different project. (ACQ-2127)	If this issue occurs, then restart the software.
An error is shown and the batch cannot be submitted if the Data File name is centered in the cell and the user presses Shift + Tab to move to the next cell. (ACQ-2135)	To avoid this issue, do not use the Tab key to move between cells. Remove the entire contents of the cell and then re-enter the required Data File name.
Changing polarity in the Ion Reference Table does not cause the fields to be validated. (ACQ-2186)	If the user creates a positive Ion Reference Table and then changes the polarity, the <b>OK</b> button is not enabled and an error is shown. If this issue occurs, then click the <b>Negative polarity</b> radio button, click the <b>Positive polarity</b> radio button, and then click the <b>Negative polarity</b> radio button again.
The Harvard syringe pump goes to Fault state when Standby is selected. (ACQ-2193)	To avoid this issue and clear the error, use the Direct Control feature to start the syringe.
The user is unable to activate the LC after it goes to Fault state. (ACQ-2207)	If this issue occurs, then clear the error on the LC, and then deactivate and activate the devices.
When a Shimadzu LC is used, the system is unable to perform an injection if there are injection events in the autosampler Time program table. (ACQ-2242)	To avoid this issue, do not add injection events to the autosampler Time program table.
Occasionally, the mass spectrometer goes to Fault state and the system cannot be recovered. (ACQ-2250)	If this issue occurs, then deactivate and reactivate the devices, and then click <b>Standby</b> .
During manual tuning, the optimized parameter value is not saved to instrument definition file after the user clicks <b>Save Settings</b> . (ACQ-2519)	During manual tuning the optimized parameter value is not saved. To avoid any issues, complete all of the tuning steps when in manual tuning mode.
Pasting data in the TOF MSMS table of an MRM HR method when the Apply Scan Schedule feature is selected hides the RT and RT Tolerance columns. (ACQ-2521)	If this issue occurs, then adjust the width of the other columns to make the two columns viewable.

**Table 5-5 Acquisition (continued)** 

Issue	Description
Not all of the columns shown in the UI are printed. (ACQ-2611)	Not all of the columns shown in the UI are shown in printouts of the method when the user does the following:  1. Creates an MRM method.
	2. Applies a scan schedule.
	3. Selects to show the advanced parameters.
	4. Saves and then prints the method.
	To avoid this issue, change the paper size to a size larger than Letter size.
In the Batch and Queue workspaces, row heights on the first and second page are not consistent when either the PDFactory or the XPS option are used to print. (ACQ-2687)	This issue does not affect the content of the reports.
The software disregards the user choice to not proceed with a batch import. (ACQ-2704/	The software disregards the user choice to not proceed with a batch import when a user does the following:
ACQ-2705)	1. Create a batch.
	Select a non-MRM MS method and then type a sample name and data file name. Do not save the batch.
	3. Click <b>Open &gt; Import from File</b> . The Import a batch file dialog opens.
	4. Browse to the applicable file, do not select to append the file, and then click <b>Import</b> .  The first Import warning message is shown. If the user selects <b>No</b> , then a second warning message is shown.
	During batch import, if the user selects <b>No</b> for the second warning message, then the progress bar does not close.  Users must click <b>Cancel</b> or import the file again to close the progress bar.
Pasted data is duplicated in the Batch grid. (ACQ-2713)	If data is copied and pasted from the Batch grid index using the right-click menu, then a duplicate is added to the end of the sample. To avoid any issues, either type the data or paste data from an Microsoft Excel file.

**Table 5-5 Acquisition (continued)** 

Issue	Description
When the software ramps the CE parameter during MRM generation in negative polarity, the real time Data Acquisition panel does not show spectral data and the x-axis scale is shown in positive mode. (ACQ-2727)	To avoid issues, use the MRM generator to view the results of the parameter ramp. Do not use the Real Time panel.
After the user changes two numbers in the Ion Reference table and then types values in the Precursor and Fragment columns, an extra zero is added in the Ion Reference tables. For example, if the user types 12, then 120 is shown in the column.	To avoid any issues, always highlight the whole number and then type the number. Do not highlight portions of the number.
If the user highlights the decimal portion of Precursor or Fragment, and then start typing, the second number is entered as a zero. For example, if the original entry is 1.1111 and the user highlights 1111 and starts typing 2222, then 20222 is shown in the column. (ACQ-2832)	

**Table 5-5 Acquisition (continued)** 

Issue	Description
In manual tune, when the user submits a batch without any calibration sample (no CDS- or LC-autocal), the ions from the manual MS method acquisition are used as the inter-sample DBC reference list for the first sample and all the subsequent samples in the batch. If there are any mismatches in the mass range, polarity, and so forth, between the MS method used for manual acquisition and that submitted in the batch, then inter-sample calibration will fail due to mass accuracy drift for all the samples in the batch. (ACQ-2834)	<ul> <li>To avoid any issues users can do one of the following:</li> <li>If the user submits a batch without any calibration sample after finishing manual acquisition in the MS Method workspace, inter-sample calibration behaves as expected. The first sample in the batch is used to generate the reference list to calibrate subsequent samples.</li> <li>If the user submits a batch with a calibration sample while manual acquisition is in progress, then inter-sample calibration behaves as expected with no mass accuracy drift observed.</li> </ul>
An error occurs if the user performs these steps, an error occurs:  1. Click <b>Auto-Calibrate</b> to configure the properties for auto-calibration in the Batch workspace.	Click <b>No</b> to dismiss the error dialog, and then click <b>New</b> to create a new batch.
2. Click <b>OK</b> to close the Batch - Automatic Calibration Editor dialog.	
3. Start to close the Batch workspace, but then click <b>Cancel</b> .	
4. Click <b>Auto-Calibrate</b> again.	
(ACQ-3016)	

## **Table 5-6 Analytics**

Issue	Description
The <b>Used</b> column becomes unavailable for selection after several filtering and sorting actions. (MQ-3275)	Close and then open the Results Table.
An error message is shown if the user clicks the header row of the Components table in the Processing Method Editor before pasting a copied components list. (MQ-3115)	Click on the first row under the column header before pasting, instead of the column header.
The software cannot perform quantitative and qualitative processing of data from Q1 scans. (MQ-2790)	N/A

**Table 5-6 Analytics (continued)** 

Issue	Description
The details in the XIC, MS, and MSMS panes in the Peak Review panel can go out of sync if the expand and collapse buttons are clicked out of order. (MQ-2510)	Click the buttons until the panes are back in sync.
Real time updates might be delayed when creating Results Tables. (DS-1042)	Delays are observed when the user runs acquisitions or processes data containing a large number of experiments. To avoid any issues, do one of the following:  Reduce the number of experiments that are being acquired.  Reduce the number of experiments used to generate the
	Results Table.     Avoid generating Results Tables and acquiring data concurrently.
CSV does not support reports that contain graphics or logos. (MQ-1361)	The .csv report is supported if the report does not contain any graphics.
Changing the regression setting for one algorithm in the Project default page updates the regression setting for the other algorithm. (MQ-1376)	The regression settings fields are not independent of the algorithm selected. If the user changes a regression setting field in one algorithm, then the corresponding field in the other algorithms is also changed. To avoid any issues, when switching between algorithms, users must update the regression settings as required for the algorithm.
An error occurs when a library without a name is imported. (MQ-1379)	To avoid this issue, assign names to libraries before importing them.
The expected retention time of an individual component that is part of a group (the <b>Update Retention Time</b> feature is set to <b>Group</b> ) can be changed, resulting in inconsistent expected retention times and retention time windows in the group. (MQ-1511)	The user can manually change the <b>Expected RT</b> for each component in the group.
The combined score is non-zero when both the Library and Search Formula Finder scores are zero or not available. (MQ-1545)	In addition to the Library Search and Formula Finder scores, the software uses the mass error, isotope, and retention time scores to calculate the combined score. To avoid including these scores, set the weighting of each to zero.
Saved Results Tables are not automatically updated when a library is added or removed from the database. (MQ-1684)	To avoid any issues, manually reprocess the results based on the updated library database.

**Table 5-6 Analytics (continued)** 

Issue	Description
The library search reports a higher-than-expected purity score from low quality spectra. (MQ-1679) (MQ-1773)	If this issue occurs, confirm retention time, peak quality, and integration to determine if the compound is a true positive.
The default CES library search selection results in missed hits in non-CES data. (MQ-1805)	If this issue occurs, then clear the Collision Energy Spread check box from the search algorithm.
Compound-specific acceptance criteria are not available. (MQ-1822)	Currently, only the global settings are available for Library Search.
Licences for licensed packages created with LibraryView Package Builder are saved to C:\Program Files\AB SCIEX\LibraryView\bin. (MQ-1847)	Licences for the licensed packages created with LibraryView Package Builder 1.0 should be manually copied to C:\Program Files\SCIEX\LibraryView\LibraryViewFramework\Server.
During any looped or combined experiments, a dual subtracted MS/MS spectrum is shown in the Peak Review pane. (MQ-1848)	This is not an issue and the software is working as designed. A single IDA experiment will have only a single subtracted spectrum range.
Incompatible components in the embedded AutoPeak method are not handled correctly. (MQ-1873)	When an existing AutoPeak method is used to process data with the option to create a model using the currently selected sample, the Results Table opens correctly. However, incompatible components are shown with a red exclamation mark in the embedded method. Users can remove the incompatible components from the method or they can modify the fragment mass retention time or experiment index to avoid this behavior.
The software stops responding when the Summation algorithm method contains incompatible components. (MQ-1888)	If an existing Summation algorithm method is used and if the method is not completely compatible with the data, then the software will stop responding. If this issue occurs, then edit the method to remove the incompatible components.
The software seems unresponsive when PDFactory is used to create a protected PDF report from a Results Table that contains more than 2500 rows using the Positive Hit template docx. (MQ-1896)	Creating the report can take some time. The PDFactory progress window, which is always shown in the background, shows that the PDF creation is in progress. Users can minimize all of the windows, including SCIEX OS, to view the PDFactory progress window.
Some chromatograms are not shown when the Peak Review pane is opened. (MQ-2070)	If this issue occurs, then click an index in the Results Table.

**Table 5-6 Analytics (continued)** 

Issue	Description
After the Analytics workspace is closed by clicking the blue X in the top right corner, the Samples pane and the Components and Groups pane are not refreshed when the workspace and Result Table are opened again. (MQ-2074)	If this issue occurs, then click anywhere on the screen to refresh the panes.
A corrupted first sample in a data file prevents sample processing. (MQ-2118)	If the first sample in a data file is corrupted, then the user is unable to process any samples in this data file and receives an informational message. A sample can become corrupted if it is aborted or fails acquisition prior to the system going to Run state during sample acquisition. If acquisition must be aborted before the system goes to Run state for the first sample, and if the data will be quantitated, then acquire the batch to a different data file. To create a Results Table using a data file that contains a corrupted sample, do the following:  1. Create a Results Table using an uncorrupted sample from an uncorrupted batch.
	2. Click Process > Add Samples.
	3. Select all of the samples for the corrupted batch except the first corrupted sample.
	4. Click <b>OK</b> .  The corrupted batch is added to the Results Table.
	5. Remove the uncorrupted sample from the original batch by clicking <b>Process &gt; Remove Selected Samples</b> .
	6. Process the batch as normal.
The IS Name cannot be pasted in the Components Table in the Method Editor. (MQ-2193)	To avoid issues, either manually select the IS Name or paste the IS column separately.
AutoPeak results generated on different computers that have different CPU architectures show a difference at the eleventh digit. (MQ-2316)	Users can customize the Results Table view. In an open Results Table, click More > Results Tables > Display settings and set the Number Format field to a value that is less than 11. Users will notice differences in their results if the value is 11 or higher.
If the user processes data while the system acquires data, then large temp files might be created that impact system performance. (MQ-2382)	If the system stops responding while acquiring and processing data on the same computer, then delete the \Update\Local\Temp file located on the C drive.

**Table 5-6 Analytics (continued)** 

Issue	Description
The user is prompted to save changes to the Results Table even if no changes were made. (MQ-2400)	If the user moves a qsession file to another folder, and then opens and closes the Results Table without making any changes, the software prompts the user to save the changes. Users can select either <b>Save</b> or <b>Cancel</b> . Data analysis is not affected.
Users are able to process and create Results Table with an invalid method. (MQ-2431)	To avoid any issues, users must open methods created in earlier versions of SCIEX OS and correct any errors. If errors are not corrected, then processing time might be impacted.
Potential extra time is added to random cycles during IDA acquisition. (ONYX-1764)	To avoid any issues, make sure that the Google update services (gupdate and gupdatem), if present on the system, as well as Windows backup, are disabled before running IDA.

**Table 5-7 Explorer** 

Issue	Description
If data from an acquisition method with ramped parameters is viewed during acquisition, then the data does not update, and the resulting spectrum is incorrect. (DS-1959)	Do not view data for an acquisition method that contains ramped parameters until after acquisition is completed.
SCIEX OS stops responding or generates an error when the user tries to simultaneously generate a DAD contour plot and XWC in a IDA+DAD datafile. This issue only occurs when the user has started to generate a DAD contour panel and while it is updating in the background, the user accesses a XWC at the same time. (BLT-498)	<ul> <li>If this issue occurs, then do one of the following:</li> <li>Generate the XWC first and then generate the DAD contour panel.</li> <li>Wait until the contour panel has finished updating before generating the XWC.</li> </ul>
<ul> <li>The following issues can occur when the user explores data during acquisition:</li> <li>Real time data does not match the post-acquisition data if the XICs and BPCs for scheduled scans are generated before the scheduled time. (DS-903/ DS-1092)</li> <li>If the user toggles between MS experiments using the Move to next or Move to previous button in Explorer to show XIC/BPC generated in real time, only one point is shown in the XIC/BPC pane.</li> </ul>	<ul> <li>Generate the XIC/BPC post-acquisition.</li> <li>Close the XIC pane and reopen it.</li> </ul>

**Table 5-7 Explorer (continued)** 

Issue	Description
Updates to the real time data spectra shown in the MS and DAD tabs in the data acquisition panel might be slower than in the Explorer workspace. (DS-934)	The x-axis (Detector Voltage) is labelled incorrectly. To avoid any issue, use the Detector Optimization Report or the Data Acquisition panel to inspect the data acquired during the detector optimization process.
A mismatch in the real time graph in the MS and DAD acquisition panels and in the Explorer workspace occurs when the LC method duration is longer than the MS method. In this scenario, both the MS and DAD acquisition panels stop updating at the end of MS method duration, even though the UV, DAD, or ADC channel continues to update in real time in the Explorer workspace until the end of the LC method acquisition time. (DS-852)	
The number label in an XIC trace is misleading in the Explorer workspace. (PV-1009)	The value shown is correct because it represents the centroid value of the peak (use the <b>Fill Peaks</b> button for a better view of the peak). The peak label is placed on the highest point of the peak in question regardless of its position. Therefore, the label might seem to be in the incorrect position, but the value is correct.
	If this issue starts to occur, then wait for the acquisition to complete before exploring the data.
Detector optimization data is not shown correctly in the Explorer workspace. (DS-1044)	Although the software generates an error, all of the samples are opened. The user can remove the corrupted sample from the batch.
Real time sample data can be used to recalibrate the sample. (DS-1094)	To avoid any issues, recalibrate the sample post-acquisition.
Incorrect precursor charge might be shown in the IDA Explorer and survey scan spectrum. (MSCS-1117)	This issue does not affect decision making during IDA acquisition.

## **Table 5-7 Explorer (continued)**

Issue	Description
The use is unable to generate a spectrum from a highlighted region in the XIC. (ONYX-1882)	An error message is shown when a user does the following:  1. Open two files in separate panes in the Explorer workspace and then generate an XIC graph for each file.
	2. Combine the XIC graphs in a single pane.
	3. In the XIC pane, highlight a region and then double-click to generate a spectrum.
	4. In the Process All Overlays? dialog that opens, click <b>All Overlaid</b> and then click <b>OK</b> .  The error message "Incorrect Argument - invalid cycle range" is shown instead of the spectrum.
	To avoid any issues, select a narrower region where the graphs are overlapped.
When a user processes large amounts of data or multiple data files in the Explorer workspace, the user interface might stop responding and there could be delay before the sample queue moves to the next sample. (ONYX-2047/DS-1688)	If this issue occurs, then wait for the software to finish processing in the Explorer workspace or avoid processing a large amount of data during data acquisition.

#### Table 5-8 MS Tune

Issue	Description
	To avoid this issue, set the start and stop masses to cover the Q1 center mass range.
An MS Tune acquisition event continues after the user navigates away from workspace. (ACQ-2113)	If this issue occurs, then stop the acquisition from the Queue workspace.

#### **Table 5-9 Software Installation**

Issue	Description
The SCIEX OS might fail to install if an incorrect user account is used. (BLT-340)	If this issue occurs, then contact sciex.com/request-support. Only Administrators should install or remove the software.
The SCIEX OS fails to install if more than one instance of the Installation Wizard is open. (BLT-341)	If two instances of the SCIEX OS Installation Wizard are opened, and the user attempts to proceed with the installation from the second instance (regardless of whether or not the first instance is closed), then the installation fails. To avoid this issue, open only a single instance of the Installation Wizard and then proceed with the installation.

## **Table 5-10 MS FW Updater**

Issue	Description
the DVD. (BLT-597)	To update the mass spectrometer firmware, copy the FirmwareUpdater folder to the D:\ drive and then run the utility from that location.

# **Mass Spectrometer Firmware Versions**

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Device	Firmware	
Mass spectrometer	ATLAS_QTOF_ICX_v0_r04	

Device	Instrument Configuration Table	
Mass spectrometer	X500R CONFIG_X500R_v0_r04	
	X500B CONFIG_X500B_v0_r03	

# **Peripheral Devices and Firmware**



SCIEX OS 1.3.1 supports the devices listed in the following table.

In most cases, more recent firmware versions from the device manufacturer will work with SCIEX OS 1.3.1. If issues occur, then change the device firmware to the version listed in this table. For information on checking and upgrading firmware, refer to the documentation provided by the device manufacturer. For information on installation and configuration of devices, refer to the *Devices Guide*.

Table A-1 ExionLC<sup>™</sup> Series of Devices

Peripheral Device	Tested Firmware (and other firmware)	Communication Cable Required
ExionLC <sup>™</sup> Controller	2.0, 3.01	Ethernet
ExionLC <sup>™</sup> AC Pump	2.04	Optic
ExionLC <sup>™</sup> AC Autosampler	2.05, 3.12	Optic
ExionLC <sup>™</sup> AC Column Oven	(2.03)	Optic
ExionLC <sup>™</sup> AD Pump	2.04, 3.11	Optic
ExionLC <sup>™</sup> AD Autosampler	(3.12)	Optic
ExionLC <sup>™</sup> PDA Detector	(3.11)	Ethernet
		Note: The PDA Detector requires a switching hub to connect to the system controller and the acquisition computer. Refer to the ExionLC <sup>TM</sup> PDA Detector Operator Guide.
ExionLC <sup>™</sup> UV Detector	2.03	Optic
ExionLC <sup>™</sup> Rack Changer	(2.0)	Optic
ExionLC Degasser	_	N/A

Table A-2 Agilent 1290 Infinity and Infinity II Series of Devices

Peripheral Device	Model	Tested Firmware (and other firmware)	Communication Cable Required
Binary Pump	G4220A	A.06.73, B.07.01	Ethernet or CAN
Standard Autosampler	G4226A	A.06.54, A.07.01	Ethernet or, if the system contains a DAD, then CAN
Column compartment	G1316C	A.06.53	CAN
DAD	G4212A	A.06.73, B.06.30	Ethernet
Infinity II High-speed Pump	G7120A	(B.07.10)	CAN
Infinity II Flexible Pump	G7104A	B.07.10	CAN
Infinity II Multisampler	G7167B	D.07.17	CAN
Infinity II Multicolumn Thermostat	G7116B	D.07.10	CAN
Infinity II DAD	G7117B	(D.07.10)	Ethernet

Table A-3 Agilent 1260 Infinity and Infinity II Series of Devices

Peripheral Device	Model	Tested Firmware (and other firmware)	Communication Cable Required
Infinity II Binary Pump	G7112B		CAN
Infinity II Quarternary Pump	G7111B	D.07.13	CAN
Infinity II Bio-Inert Pump	G5654A	D.07.13	CAN
Infinity II Multisampler	G7167A	D.07.16	Ethernet or, if the system contains a DAD, then CAN
Infinity II Bio-Inert Multisampler	G5668A	D.07.16	Ethernet or, if the system contains a DAD, then CAN
Infinity II Multicolumn Thermostat	G7116A	D.07.13, D.07.16	CAN
Infinity II DAD	G7117C	D.07.10	Ethernet

#### **Table A-4 Shimadzu**

Peripheral Device	Tested Firmware (and other firmware)	Communication Cable Required
SIL-20ACXR Autosampler	3.12	Optic
SIL-30AC Autosampler	3.12	Optic
LC-20ADXR Pump	3.11	Optic
LC-30AD Pump	3.11	Optic
CTO-20AC Column Oven	2.03	Optic
SPD-20A UV-VIS Detector	1.04	Optic
SPD-M30A UV Detector	3.11	Ethernet
		Note: The Detector requires a switching hub to connect to the system controller and the acquisition computer.
FCV-12AH Valve	N/A	N/A
FCV-13AL Valve	N/A	N/A
CBM-20 A with Ethernet Switch (system controller with 8 fiber optic ports)	2.81, 3.01, 3.11	Ethernet
Rack Changer II	2.0	Optic