SCIEX OS 2.2 Release Notes

Introduction

Thank you for choosing SCIEX to supply your system. We are pleased to bring you the SCIEX OS 2.2 software, which supports the following systems:

- ZenoTOF 7600 system
- X500R QTOF and X500B QTOF systems
- SCIEX 7500 system
- SCIEX Triple Quad 4500, 5500, 5500+, 6500, and 6500+ systems

  Note: QTRAP systems are not supported.

- Echo MS system, which includes a SCIEX Triple Quad 6500+ system and the Echo MS module

SCIEX OS 2.2 also allows the user to process data acquired from triple quadrupole, QTRAP, and TripleTOF systems operating the Analyst software, version 1.6.2 or higher, or the Analyst TF software, version 1.7.1 or higher.

This document describes features in the software. We recommend that users keep these release notes for reference as they become familiar with the software.

New in Version 2.2

This section describes the enhancements and fixes in SCIEX OS 2.2. 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.

New Features and Enhancements in Version 2.2

- **Support for SCIEX Triple Quad Systems:** The software supports SCIEX Triple Quad 4500, 5500, 5500+, 6500, and 6500+ systems.

- **Export and Import of User Management Settings:** The SCIEX OS user database can be exported on one SCIEX computer, and then imported on a different computer. This feature allows configuration changes to be made on one computer, and then populated to the other computers in the laboratory.

  Note: (Regulated customers) If user management settings are imported after software validation, then we recommend that customers document the configuration changes following their internal change control process.

- **Multiple MS Methods:** Users can open multiple MS methods in the MS Method workspace.
- **Custom columns in the Batch workspace:** Users can create custom columns in the Batch workspace, so that they can be used in processing, for example, in formulas and calculated columns.

  Note: Data cannot be imported from a laboratory information management system (LIMS) into a batch with custom columns.

- **Fragmentation mode in the Data Acquisition window**: When SCIEX OS acquires data from a ZenoTOF 7600 system, the graph title in the Data Acquisition pane shows the fragmentation mode configured in the method.
- **Import of Variable SWATH windows:** Users can now import variable SWATH windows from a text file.
- **Save results for Automation Batch**: This new permission allows Results Tables created automatically in the Batch workspace to be saved.
- **QJet RF amplitude for X500 QTOF systems:** The user can manually override the **QJet RF amplitude** parameter for X500 QTOF systems.

  Note: When the user opens an MS method that was created in a previous version of SCIEX OS, the **Override QJet RF** value and **QJet RF amplitude** parameters are exposed. The parameters are set to the default value. (ONYX-15939)

- **New Reporter software fields:** These new fields are available in the Reporter software templates:
  - StdAdd_ActualConcentration
  - StdAddn_CalculatedConcentration
  - StdAddn_Accuracy
  - StdAddn_CalibrationCurve
  - Report_Created_By
  - ISMSMSPeak

Fixed Issues in Version 2.2

MS Method Workspace

- When the user was editing the Mass Table for an MS method, the **Delete** key did not work. (ONYX-7384)

Batch Workspace

- Users were unable to import batch files from a network location. (BLT-3147)
- In the Decision Rule Configuration dialog, when a processing method was selected, the list in the **Flagging Rules** field might include Combined flagging rules that were defined in the processing method, but not applied. That is, the **Apply Rule** check box was not selected. (ONYX-8352)

Queue Workspace

- SCIEX OS might be unable to append data to a wiff file on a network resource. (ONYX-11437)

MS Tune Workspace

- Users could not restore instrument settings saved in a previous version of SCIEX OS. (BLT-2722)

Analytics Workspace

- An error was shown when the user configured the table settings on the Components page of the processing method to show **Mass (Da) and Width (ppm)**. (MQ-7709)
- When a table display settings (cset) file was imported, the **Component Name** column was moved to near the right side of the table. (BLT-2564)
- The formula editor did not identify syntax errors that followed a boolean operator.
- When a Results Table was exported to a text file, the date format was not in the selected regional format. (BLT-2314)
- The **Comment** column has been added to the component table on the Components page in the Processing Method Editor. (BLT-2726)
- Multiply charged species could not be imported from a text method into Components page in the Processing Method Editor. (BLT-2745)
- Metric plots did not automatically refresh after manual integration if the column used was a calculated column. (BLT-2822)
- The **Sample Name** column in the Results Table could not be moved to accommodate exports to a LIS. (BLT-2852)

- Only the currently visible **XIC Width** column was exported. (BLT-2874)
- For Formula Finder and ChemSpider workflows, the incorrect polarity was used in processing of negatively charged compounds. (BLT-2963)
- SCIEX OS closed unexpectedly during review of components for which a peak was not found. (BLT-2976)
- Formulas could not be saved if they contained column names or cell values that were not present in the current data. (BLT-2991)
- SCIEX OS closed unexpectedly when the user opened the Peak Review pane for a highly charged ion with a formula. (BLT-2998)
- For ion ratios with a variable tolerance, the flagging rule failed to flag the value correctly. (BLT-3052)

Reporter

- A new tag, Report_Created_By, shows the name of the user who created the report. (BLT-1818)
- MS/MS peaks were not shown for the internal standards of an analyte. (BLT-2123)
- Reports created for individual samples only included information about QC samples. (BLT-2661)
- Metric plots were not generated if they were inside a control, such as an IF statement. (BLT-2901)
- Component group names and sample ID columns inside IF statements were not processed in reports. (BLT-2904)
- Sample serial numbers were not included in reports. (BLT-2931)
- After an upgrade from Microsoft Office 365 to Microsoft 365 Apps, or from Microsoft Word 2016 to Microsoft Word 2019, some of the chromatograms on the generated reports were empty. (BLT-3080)

Explorer Workspace

- XICs copied with the **Copy Graph** command were low resolution. (BLT-2869)
- The commands to export to the Analyst software have been removed from the Explorer workspace. (BLT-2974)

Audit Map

- SCIEX OS did not apply the default audit map to a project created with the Analyst software. (BLT-2833)
- User login failures were not recorded in the audit trail when the audit trail was configured to record them. (BLT-2995)

Devices

- In the Detailed Status dialog for the diverter valve, the **Time** value was incorrect while the system was in the equilibration and loading states. (ONYX-7831)
- (Shimadzu LC-40 systems) The injection volume could not be set to 50 µL for a 50 µL loop. (BLT-3024)
- (Agilent LC systems) In the pump section of the Detailed Status dialog, the A and B solvent bottles were not shown. The user could not see which solvents were being used. (BLT-2319)
- (Agilent G7167A multisampler) SCIEX OS did not support customized well plates defined for the G7167A multisampler. Two new plate layouts have been added, to support row and column layouts for the 54 vial plate. (BLT-2389, BLT-2401)
- The firmware version shown in the Event Log was incorrect for some mass spectrometers. (BLT-2625)
- A slow performance issue occurred during device activation and opening of the MS Tune workspace. The problem occurred primarily with the Waters Acquity LC, but could also be observed with other LC devices. This fix was also included in the SCIEX OS 2.1.6 Patch for Slowness Issue. (BLT-2957)
- Users could not activate the mass spectrometer device when the acquisition computer was connected to a customer LAN. This fix was also included in the SCIEX OS 2.1.6 Patch for Communication Issue. (BLT-3007, BLT-3028, BLT-3066)
- The **Plate Layout** feature was disabled in the Batch workspace for an ExionLC system with a multiplate sampler. This fix was also included in the SCIEX OS 2.0.1 Patch for Shimadzu Plate Layout. (BLT-3061)

SCIEX 7500 System

- The collision energy (CE) parameter was shown incorrectly in IDA experiments with Negative polarity. (ONYX-8566)
- An error was shown during step 5 (Optimize Collision Energiy) if the user did not complete all of the preceding steps, in order. (ONYX-8568)

Echo MS System

- Issues could occur when the column-serpentine sampling sequence is used:
  - The drop-out rate for droplet capture might be higher, resulting in poorer reproducibility.
  - The additional load resulting from prolonged back-and-forth movement along the Y-axis might cause stress on the motion mechanism over time.

Notes on Use and Known Issues

Notes on Use

- (Regulated customers) We recommend that, if user management settings are imported after software validation, then customers follow their internal change control process to document the configuration changes.
- For ExionLC 2.0 systems:
  - If solvent level monitoring is used, then make sure that the current volume is correct, and that the proper warning level and shutdown level are set in the Device Control or Device Details dialog before each batch acquisition. If the current volume must be updated during sample acquisition because the mobile phase is being topped up, then use the solvent levels panel for the pump in the Device Details dialog.
  - When loading samples in the sample trays, make sure to follow the plate layout in the software. Refer to the document: *ExionLC 2.0 System Hardware User Guide*.
  - A Diode Array Detector (DAD or DAD-HS) cannot be used for data acquisition at the same time as a Multiwavelength detector (MWD). Do not configure the LC system with both a DAD and an MWD.
  - A sampling rate of only 10 Hz or lower is supported for the ExionLC 2.0 DAD (DAD or DAD-HS), and MWD. An LC method with a sampling rate greater than 10 Hz is not saved.
  - When creating a DAD method, make sure that the wavelength for 2D data channels and for the wavelength program are within the wavelength range defined for 3D data mode, even if the 3D data mode is not selected.
- When a batch starts, SCIEX OS stops the installation of Windows Updates, Windows Defender virus scans (Windows 10), and Symantec Endpoint virus scans (Windows 7). Schedule updates and virus scans to occur at times when data acquisition is not occurring.
- To avoid performance issues or data corruption, the user should not perform any computer maintenance procedures, such as defragmentation or disk cleanup, during sample acquisition.

- For Echo MS systems:
  - When an MS method is created, the **Spray Voltage** defaults to 4500 V.

    Note: We recommend that a value of 5000 V or less be used, to maximize the life span of the open port interface (OPI) electrode assembly.

  - Because the peaks are narrow, we recommend that the number of transitions be minimized. We recommend that four to six transitions be used.
  - The user must not use the same data or results file name in multiple batches. Always use a new data and results file in each new batch.
  - Values entered in the **Injection Volume** column in the Batch workspace do not replace the ejection volume specified in the AE method.
- If the ClearCore2 service is interrupted during network acquisition, then the partial sample data for the sample under acquisition at the time of the interruption is not written to the data file. If the service is interrupted during local acquisition, then the partial sample data is written to the data file but is marked as corrupted. Any auto-triggered processing and decision rule processing also fails if the ClearCore2 services is interrupted.
- The following methods allow the user to view data in real time in the Explorer workspace while acquiring to a network resource:
  - Open the Data Acquisition panel at the bottom of the SCIEX OS window.
  - In the Queue workspace, open the sample being acquired by double-clicking it.

  (DS-1873)

  Note: If the sample is left open in the Explorer workspace, a "File not found message" is shown after the sample has been moved to the network resource.
- Data files created in the SCIEX OS 2.2 cannot be appended to data files acquired in SCIEX OS version 1.3.1 or earlier. (DS-1931)
- Data containing custom columns cannot be appended to data files acquired in SCIEX OS version 2.1.6 or earlier.
- MultiQuant software files (qmethod, qsession, and cset) cannot be opened or used in the Analytics workspace of SCIEX OS. However, MultiQuant software methods that have been exported to a text file can be imported into the Analytics workspace.
- For non-targeted workflows, Results Tables should be limited to 150,000 rows. SCIEX OS performance degrades significantly when Results Tables exceed this size.

- If the AutoPeak integration algorithm is used, then the user must consider all calculated parameters in the context of a component within the specific Results Table. The software creates an AutoPeak model for each component and this model is used for all samples for the component. The AutoPeak Asymmetry calculated parameter shows the ratio of the skew of the particular to the skew of the AutoPeak model for the component. (BLT-2030)
- When transferring data to the Watson LIMS, the user must wait for the transfer to complete successfully before clicking **Confirm** in SCIEX OS. If the user clicks **Confirm** before the transfer is complete, then the transfer status is shown as Failed.
- The default value for **XIC width** on the Integration page of the processing method is 0.02. For processing of nominal mass data, a value of 0.1 or higher is recommended, to maximize the quality of library searches. (MQ-7810)
- When transferring instrument settings from the Analyst software to SCIEX OS 2.2, make sure to use the Instrument Settings Converter that is included in the SCIEX OS 2.2 installation package.
- When converting methods, make sure to use the version of the SCIEX OS to Analyst Software Method Converter that is included in the SCIEX OS 2.2 installation package.

General Issues

Issue	Notes
The user cannot open report (xps) files created during tuning in the MS Tune workspace or in the MS Method workspace with Guided MRM. Windows reports that it cannot open files of this type.	This issue occurs if the Microsoft XPS Viewer is not installed on the computer. The viewer is included in the SCIEX OS installation package. To install it follow these steps: 1. Run a Command Prompt as administrator: a. In the **Type here to search** field in the Windows Taskbar, type **cmd**. b. Right-click **Command Prompt** and click **Run as administrator**. 2. In the Administrator: Command Prompt window, type the following command, and then press **Enter**: **dism /online /norestart /add-package /packagepath:"C:\Program Files\SCIEX\SCIEX OS\Microsoft-Windows-Xps-Xps-Viewer-Opt-Package~31bf3856ad364e35~amd64~~.cab"** **Note:** Type the whole command on a single line. A progress bar is shown as the XPS Viewer is installed. 3. When the installation is complete, close the Command Prompt window.
(SCIEX 7500 systems) Data with a long file path (129 or more characters) cannot be processed using the Analyst 1.7.2 or Analyst 1.6.3 software with HotFix 5. In addition, the file information for such a data file cannot be fully displayed in the Analyst 1.7.2 or the Analyst 1.6.3 software with HotFix 5. (BLT-2246/AN-2250)	To avoid this issue, use the Analytics workspace in SCIEX OS to process the data, or make sure to use a shorter file path.

Issue	Notes
The content pane of the Help is blank. (BLT-2497)	The Help file is blocked. To resolve the issue, follow these steps: 1. Browse to the Help file, in the folder C:\Program Files\SCIEX\SCIEX OS\Documentation, right-click it, and then click **Properties**. 2. In the Properties dialog, select **Unblock**. 3. Click **OK**. **Note:** If the Properties dialog does not contain this check box, then the Help file is not blocked.

Devices Issues

Issue	Notes
When one, two, or three rinse solvents are selected, then rinsing does not occur. (BLT-1212)	Add a fourth rinse solvent, and reduce the volume of each rinse to reduce the rinsing time.
The user cannot start the syringe pump when the mass spectrometer is in Standby state because the **Direct device control** button for the syringe pump is not active. (BLT-2698)	Start data acquisition or a tuning procedure to make the **Direct device control** button active.
The following error message is shown: "Failed to write LC data in wiff file." (BLT-2960)	The error message can be shown under these conditions: • If an LC method is configured without a detector. The message can be ignored. • If the LC method is configured with a detector. The message indicates an issue with the acquisition of the LC data for the sample.
The system does not activate the **Standby** button on the right status panel when a device, such as the CDS, goes to fault, preventing the user from clearing the error. (MSCS-1314)	If this issue occurs, then click **Start** in Direct Control to change the CDS state from Fault to Running to clear the Fault state of the CDS.

Issue	Notes
Information is missing on the Device Details dialog for the LC system. (ON-2069)	This issue occurs if the Windows region settings are set to a format other than **English (United States)**. To avoid this error, configure Windows following the instructions in the document *Software Installation Guide*.
When the Remote Desktop application is used to access the acquisition computer, the following issues might occur: • In the LC Method workspace, some parameters are not visible. • On the Detailed Status dialog for an LC system, some LC parameters are not visible. (ONYX-7153/ONYX-8185)	This issue occurs when the user disconnects and reconnects the Remote Desktop session without logging off the acquisition computer. To avoid this issue, use one of these methods: • Log off of the acquisition computer and then log on again. • Use Full Screen mode in the Remote Desktop application. • Correct the resolution on the acquisition computer. • View the detailed status on the acquisition computer directly.
SCIEX OS does not automatically start and stop an external syringe pump during tuning. (ONYX-8459)	Start the syringe pump manually before beginning the tuning procedure.
After changing any parameter in the solvent levels panel, wait 5 seconds for the status to be updated, before making additional changes. (ONYX-9093)	N/A
(Waters LC) LC device properties and method information are missing from the Sample Information shown in the Explorer workspace. (ONYX-11604)	N/A

Agilent LC System Issues

Issue	Notes
High throughput settings are not supported in the autosampler. (ACQ-529)	The high throughput settings are not currently supported.
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.

Issue	Notes
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.
Real-time DAD data from the Agilent G7121B 1260 Infinity II FLD Spectra module is not recorded when spectrum mode is set to Apex or All in Peak. (ONYX-4998)	Apex and All in Peak spectrum mode are not supported. Use a different mode.
The system remains in Loading or Equilibrating state when a Agilent G7121B 1260 Infinity II FLD Spectra module is being used if the Signal A Excitation is set to Zero Order and the photo-multiplier (PMT) Gain is set to greater than 6. (ONYX-4999)	If Signal A Excitation is set to Zero Order, then set the PMT Gain to 6 or less.

ExionLC 2.0 System Issues

Issue	Notes
The **Rack Type** is not updated in the Plate Layout window if the user changes the **Rack Type** in the Batch workspace when the Plate Layout dialog is open. (ONYX-8760)	If the user changes the **Rack Type** in the batch grid while the Plate Layout dialog is open in the Batch workspace, then the visual representation of the vial layout in the Plate Layout is updated, but the **Rack Type** field is not updated. However, all of the information in the batch, including **Rack Type** and **Vial Position**, is correct. To avoid this issue, change the **Rack Type** in the Plate Layout dialog or close the Plate Layout dialog before changing the **Rack Type** in the batch grid.
Multiple instances of the Device Details dialog can be open at the same time. (ONYX-9049)	If the Device Details dialog is open when the user changes the device configuration, then the Device Details dialog for the older configuration stays open, even after another instance of the Device Details dialog is opened for the new configuration. This issue does not affect usability. However, to avoid confusion, make sure to close any open Device Details dialogs before changing the device configuration.

ExionLC AC, ExionLC AD, and Shimadzu LC System Issues

Issue	Notes
Injection begins before the column reaches the set temperature.	If the **WAIT TIME** for the column oven is manually set to 0, then make sure to equilibrate the system and wait for 10 to 15 minutes after the column oven has reached the set temperature before submitting any samples. Alternatively, set the **WAIT TIME** to a value equal to any integer from 1 to 10 and then select **Wait for temperature equilibration before run** in the LC method. If this option is selected, then, after the column oven reaches the set temperature, the software will wait the amount of time specified in the **WAIT TIME** before the beginning injection.
When a hardware profile with a PDA detector is activated, the detector defaults in the LC method are different between a newly created LC method and an opened LC method that was previously created with the same LC but without a PDA detector activated. (ACQ-2176)	To avoid any issues, make sure that the correct parameters are used for the PDA device.
After the system goes to Standby state, or after it is deactivated, the temperature reverts to the temperature that was set in the last equilibration procedure or LC method. (BLT-2300)	N/A
(Shimadzu LC-40 systems) Content in fields in LC methods that are automatically populated does not print in reports. (BLT-2850)	Replace the automatically populated content by typing in values.
The Nexera Mikros LC pump does not go into fault state when the maximum pressure limit is reached. (ONYX-7794)	N/A
The Nexera Mikros LC pump is incorrectly identified as an LC-20AB pump in the device configuration. (ONYX-8030)	The LC system performance is not affected, but the pump is incorrectly identified in data files, logs, and audit trails.

Issue	Notes
(Shimadzu LC-40) In the Plate Layout dialog, if the user is configuring a rack type with multiple plates, then when the user finishes configuring a plate and selects the next plate, the name of the configured plate changes to **<Unassigned>**. (ONYX-8441)	Save the batch and open it again, to show the plate names correctly in the Plate Layout dialog.
(Shimadzu LC-20 systems) Equilibration stops before the column reaches the set temperature. (ONYX-14932)	N/A

Acquisition Issues

Issue	Notes
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.
(X500 QTOF and ZenoTOF 7600 systems) For *Scheduled* MRM^{HR} methods, the mass table columns do not print. (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 HR 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.

Issue	Notes
(X500 QTOF systems) In manual tune, if the user submits a batch without a calibration sample (that is, no CDS- or LC-autocal), then 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 the one submitted in the batch, then inter-sample calibration will fail due to mass accuracy drift for all the samples in the batch. (ACQ-2834)	To avoid any issues users can do one of the following: • If the user submits a batch without a calibration sample after finishing manual acquisition in the MS Method workspace, then inter-sample calibration behaves as expected. The first sample in the batch is used to generate the reference list to calibrate subsequent samples. • 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.
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.
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.
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.
(SCIEX 7500 systems) When an IDA experiment with an MRM survey scan is looped with another experiment that uses the *Scheduled* MRM algorithm with sMRM triggering applied, the trigger threshold specified in the **Intensity threshold exceeds** field in the IDA criteria is not applied to the candidate masses in the MRM survey scan. (MSCS-2283)	• Turn off sMRM triggering in the looped *Scheduled* MRM algorithm experiment. The IDA intensity threshold will be applied to the candidate masses in the MRM survey scan. • Change the MRM survey scan to use the *Scheduled* MRM algorithm instead, and set the retention time of the compounds of interest to 0. The IDA intensity threshold will be applied to the candidate masses in the survey scan.
(ZenoTOF 7600 systems) No data is acquired in EAD fragmentation mode. (MSCS-2527)	If EAD fragmentation is used, then the accumulation time must be at least three times the reaction time. If it is not, then no data is acquired. To resolve the issue, increase the accumulation time.

Issue	Notes
(X500 QTOF and ZenoTOF 7600 systems) Negative mass defect values are shown with the incorrect sign in the Mass Defect IDA criteria. (MSCS-2537)	The algorithm selects the correct precursors, so the acquired data is correct.
(ZenoTOF 7600 systems) The wiff data files acquired with SCIEX OS version 2.1.6 or earlier might show an incorrect fragmentation mode in the graph title when opened with later versions of the software. (MSCS-2945)	This issue occurs for wiff data files that use MRM^{HR} or *Scheduled* MRM^{HR} algorithm methods with mixed fragmentation mode (EAD/CID).
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.
When the prints a batch to PDF, any numeric values, in either column headings or body cells, are missing from the document. (ONYX-2236)	N/A
When a row is copied from a file, such as an Excel spreadsheet, and then pasted in the grid in the Batch workspace, some components are not added to the grid. (ONYX-6068)	Add missing components to the batch manually.
When the user pastes a row over an existing row in the Batch workspace, the content is not pasted correctly. (ONYX-6083)	To avoid this issue, instead of pasting over an existing row, insert an empty row and paste the new content in it. Then delete the existing row.
When the Acquisition Methods folder contains a corrupt MS method, then no MS methods are available for selection in the **MS Method** column in the Batch workspace. (ONYX-6795)	If the list of MS methods in empty, then find and delete the corrupt method.
When the user stops the queue with the option **Stop after the current tasks are completed**, acquisition completes, but processing does not start. (ONYX-6802)	N/A

Issue	Notes
In the Queue workspace, samples that are re-injected as the result of decision rule processing show ***Embedded Method*** in the **Processing Method** column, instead of the name of the processing method associated with the original sample. (ONYX-6896)	When the first sample is processed, the Results file is created and the processing method specified in the **Processing Method** column is embedded in the new Results file. Therefore, the embedded method specified for the reinjected sample is the same as the processing method specified for the first sample.
If the acquisition computer is being controlled by Windows Remote Desktop while acquiring IDA data, then acquisition performance might be slow, resulting in loss of data points. (ONYX-7491)	Do not use Remote Desktop to control the acquisition computer while acquiring IDA data.
When wiff data acquired in SCIEX OS is opened in the Analyst software, the **MRM detection window** in the Analyst software does not match the **Retention time tolerance** in SCIEX OS. (ONYX-7602)	The **Retention time tolerance** value is used to calculate the **MRM window**. This value is not the same as the **MRM detection window**, which shows the default value for the detection window.
An error occurs when the user attempts to print a method to a PDF file that is currently open. (ONYX-7813)	Close the PDF file before printing the method, or save with a different file name.
(QTRAP systems) A default value for AF2 cannot be set for MS^3 experiments in Negative polarity. (ONYX-8041)	When the user sets a default value for AF2 for MS^3 experiments in Negative polarity, the default value is not saved. To save a default value for AF2 in Negative polarity, first configure Positive polarity with the AF2 value required for Negative polarity. Then change to negative Polarity and save the default values.
An MS method that uses the *Scheduled* MRM algorithm can be saved with an invalid method duration. (ONXY-8443)	The **Duration** for an MS method that uses the *Scheduled* MRM algorithm might become invalid if the scan time is too large. If the user attempts to save the method, an error message is shown, and the **Duration** field contains an error icon. If the user specifies a valid method duration, changes the duration back to the incorrect method duration, and then saves the method, the method is saved successfully. Make sure to determine the correct method duration before saving the method.

Issue	Notes
(ZenoTOF 7600 systems) The number of cycles and cycle time shown in the Sample Information for a sample in the PeakView software is incorrect for a wiff file acquired with the *Scheduled* MRM^{HR} algorithm. (ONYX-10623)	N/A
(ZenoTOF 7600 systems) TOF Mass Calibration parameters shown for the sample in the wiff file do not match the parameters shown in the wiff2 file. (ONYX-11356)	Calibration parameters are recorded differently by the Analyst TF software and SCIEX OS. The wiff file follows the Analyst TF software model.
(X500 QTOF and ZenoTOF 7600 systems) When a looped experiment is created with complex scans, IDA, SWATH, MRMHR, the looped experiment is shown as a scheduled experiment, even though user did not specify experiment scheduling. (ONYX-11359)	1. Save and close the method. 2. Open the method. 3. Clear **Experiment scheduling** on the Advanced tab. The looped experiment shows as unscheduled.
(X500 QTOF and ZenoTOF 7600 systems) The user can enter non-integer values in the **For** field for **Exclude former candidate ions**. (ONYX-11383)	Non-integer values are replaced by "0" on saving and reopening of the method, but the data is acquired correctly, with the non-integer value taken into account.
(SCIEX Triple Quad 7500 systems) The user can convert a method created for a QTRAP system in the Analyst software for use with a system that does not have a QTRAP license. (ONYX-14104)	N/A
In **Guided MRM > MRM Infusion** , the source and gas parameters on the Set Initial Conditions page revert to the default values when the user clicks **Start**. (ONYX-15218)	Set the parameters again.
Settling time cannot be set to 15 ms in a Q1-IDA looped experiment. (ONYX-15511)	N/A

Issue	Notes
(ZenoTOF 7600 systems) In the MS Method workspace, the user can define up to 2500 transitions for an MRM^{HR} experiment, which can result in slowness of acquisition. (ONYX-16282)	A maximum of 548 concurrent transitions can be defined for a *Scheduled* MRM^{HR} experiment.
When the user opens or imports a batch that contains manually added components, the manually added components might be lost for samples that are not standards or QCs. (ONYX-16474, ONYX-16466, ONYX-16467)	After opening or importing a batch with manually added components, review it carefully to make sure that all components are present.
(ZenoTOF 7600 systems) The **Zeno threshold** parameter is active for experiment and fragmentation types for which it is not applicable. (ONYX-16556)	The **Zeno threshold** parameter is used for IDA experiments, with both EAD and CID fragmentation, and for MRM HR and MSMS experiments, with CID fragmentation only. However, the **Zeno threshold** field is active all experiment types, for both EAD and CID fragmentation. The parameter is also shown in the Sample Information for MRM HR and MSMS experiments with EAD fragmentation. For MRM^{HR} experiments, the Zeno threshold field name is incorrect. It should be **Zeno threshold (CID)**.
When the user closes the active method, the adjacent method does not become active. (ONYX-16704)	Because no methods are active, controls, such as the **Start** button are not active. Select a method to make it active.
When the user creates multiple guided MS3 infusion methods, the methods have the same name. (ONYX-16740)	Because the methods have the same name, the **Views** menu only has one of them. To resolve the issue, save one of the methods with a new name: **Save > Save as** .

Echo MS System Issues

Issue	Notes
When entries are deleted in the Plate Layout dialog, the rows are not deleted from the Batch workspace, and some fields remain.	To delete the rows, select them, and then right-click and click **Delete Rows**.
When consecutive batches save data to the same data file, peak splitting is unsuccessful, and automatic processing fails. (ONYX-6904)	Peak splitting is performed after data is acquired. If a subsequent batch is acquiring data to a file while the system is splitting peaks written to that file during the previous acquisition, then a resource conflict occurs. To avoid this issue, write data from each batch to a separate data file.
The following limitations apply: • Decision rules do not work properly with an Echo MS system. • An LC system cannot be used in a configuration with an Echo MS system. • The MS Tune workspace cannot be used if an Echo MS system is configured. (ONYX-10636)	• Do not use decision rules when an Echo MS system is configured in SCIEX OS. • Do not activate an LC system when an Echo MS system is active. • Do not do tuning in the MS Tune workspace when an Echo MS system is active. Tuning of the SCIEX 6500+ system is performed using the IonDrive Turbo V ion source and the associated probe.
When the user uses the Plate Layout dialog to populate **Well Positions** in the Batch workspace, sometimes the **Well Positions** are not populated. This issue might occur under these conditions: • When the user opens the Batch workspace for the first time after opening SCIEX OS. • When the user tries to populate **Well Positions** in an empty batch. (ONYX-12525)	If the issue occurs, then do one of the following: • Close the software and then open it again. • Open a saved batch then use the Plate Layout dialog to update the **Well Positions** in that batch.
When the user clicks **Remove All** on the Plate Layout dialog, the software responds very slowly. (ONYX-12726)	For better performance, remove the wells in the Batch workspace grid. Select the wells in the grid, and then right-click and select **Cut**.

Issue	Notes
(Echo MS systems) When a mobile phase low warning is triggered during acquisition, the acquisition fails. (OPP-288)	Before starting acquisition, make sure that the mobile phase bottle contains enough mobile phase to complete the planned acquisitions.
(Echo MS systems) When the user uses the Plate Layout dialog to add sample wells to the grid in the Batch workspace, the selected wells cannot be added. (OPP-365)	Select a different column in the target row and try again.
(Echo MS systems) The **Est. Start Time** in the Queue workspace is not updated for AE samples. (OPP-421)	This is a user interface issue only. System functionality is not affected

Analytics Workspace Issues

Issue	Notes
None of the Results Tables in a project root directory will open.	This error occurs if the root directory for a project has been used as a root directory for the Analyst software. The Analyst software creates one or more of the following files in the Default/Project Information folder in the root directory: • ProjectSettings.atd • Default Audit Map.cam • Project.atd If these files exist in the Project Information folder, then delete them.
No reports can be created from the Results Table after a custom template that contains both picture elements and a query is used to create a csv report. (BLT-1507)	To avoid issues, use one of the supported templates. Refer to the document: *Software User Guide*.
SCIEX OS becomes unresponsive when processing a wiff file on a network location while the Analyst software, running on a different computer, is acquiring data to that file across a network. (BLT-2873)	SCIEX OS does not support this workflow.

Issue	Notes
For Analyst software data, Q3 Resolution is reported as Maximum for LIT scans. (DS-2220)	Open the data in Explore mode in the Analyst software.
The csv report does not support graphics or logos. (MQ-1361)	The csv report is only supported if the report does not contain any graphics.
The software seems unresponsive when PDFactory is used to create a protected PDF report from a Results Table that contains more than 2,500 rows using the Positive Hit template. (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.
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.
When the AutoPeak integration algorithm is used on UV, DAD, or ADC data, the model can take a very long time to build before processing. (MQ-4421)	Do not use the AutoPeak integration algorithm for UV/DAD/ADC data that has poor peak shape.
In the Mass Reconstruction workflow, signal-to-noise (S/N) values reported in the Results Table are not calculated correctly for reconstructed peaks. (MQ-7073)	To calculate S/N, open the average *m/z* spectrum in the Explorer workspace, perform manual reconstruction, and then calculate S/N on the target peak. **Note:** This workaround requires Biotool Kit License. 1. Select the Average spectrum in the Peak Review pane. 2. Click **Open data exploration** ( ). 3. Click **Bio Tool Kit > Reconstruct Protein**, enter a resolution value, specify the reconstruction parameters, and then perform reconstruction. 4. Calculate S/N manually. Refer to "Show the Graph Selection Information" in the document: *Software User Guide*.
Names of calculated columns cannot be the same as function names. (MQ-8087)	Assign a name that does not match a function name.

Issue	Notes
The **Percent CV** shown in the Statistics pane is different than the percent CV calculated with the **GETSTAT** function. (MQ-8211)	The **GETSTAT** function uses the **Actual Concentration** values to identify replicates, but the Statistics pane uses the **Actual Concentration** values after the user-specified **Number format** is applied. If the **Number format** is set to 0.00, for example, a concentration of 5.001 will be treated as 5.00 in the Statistics pane.
The software does not support flagging rules based on the **Outlier Reasons** column or on calculated columns based on the **Outlier Reasons** column. (MQ-8295/MQ-8381)	Do not create flagging rules that use the **Outlier Reasons** column.
When a metric plot is applied to a column based on a custom formula, changes to any input of the formula are not reflected in the Metric Plot immediately. (MQ-8524)	To refresh the metric plot, select a different component in the Results Table, and then select the original component again.
The **Acquisition Date & Time** column is not processed properly in formulas. (MQ-8662)	Do not use the **Acquisition Date & Time** column in formulas.
The formula editor does not identify incorrect use of the ampersand (&) and bar (|) characters in formulas. (MQ-8837)	To represent the boolean AND, use "&&". To represent the boolean OR, use "||".
The calibration curve in the Calibration Curve report is in log-log plot format when **Log-log plot** is not selected in the Calibration Curve pane. (MQ-9424)	Close the Results Table, open it, and then create the report again.
Data cannot be imported from an LIMS into a Results Table with custom columns, and data cannot be exported from a Results Table with custom columns to a LIMS. (ONYX-15730)	N/A
The ChemSpider database cannot be accessed with a proxy server. (PV-632)	N/A

Explorer Workspace Issues

Issue	Notes
When a user acquires large numbers of *Scheduled* MRM^{HR} algorithm transitions (up to 2500 transitions), short delays might be observed during real time data collection. (Onyx-17742)	To avoid other data file issues, do the following: • Do not open data exploration to view real time data for the current sample. • Acquire only one sample per data file.
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. (BLT-719)	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.
The error "The requested action could not be completed. Make sure your data is complete and all fields contain appropriate values" is shown in the Formula Finder. (BLT-1423)	This error occurs if the structure for the selected ion, as predicted by Formula Finder, is not included in the list of positive ions on the Elemental Composition tab of the Formula Finder Settings dialog. For example, for the ion at *m/z* 1004, Formula Finder matches to (M+NH4)+. If this ion is not included in the list of positive ions to search for, then an error occurs when no matches are found.
The following issues can occur when the user explores data during acquisition: • 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) • If the user toggles between MS experiments using **Move to next** or **Move to previous** in the Explorer workspace to show an extracted ion chromatogram (XIC) or base peak chromatogram (BPC) generated in real time, then only one point is shown in the XIC/BPC pane.	To avoid this issue, do the following: • Generate XICs for the required experiment by clicking **File > Show XIC** • Generate the XIC/BPC post-acquisition. • Close the XIC pane and reopen it.

Issue	Notes
Detector optimization data is not shown correctly in the Explorer workspace. (DS-1044)	The Z-axis (Detector Voltage) is labeled 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.
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. Click **Fill Peaks** to open 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 occurs, then wait for the acquisition to complete before exploring the data.

MS Tune Workspace Issues

Issue	Notes
(X500 QTOF systems) During manual tuning, the optimized parameter value is not saved to instrument definition file after the user clicks **Save Settings**. (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.
(ZenoTOF 7600 systems) If the mass spectrometer is turned off within about five minutes after calibration is completed in the MS Tune workspace, then the calibration settings are lost and the previously saved calibration settings are restored. (MSCS-2627)	Perform the tuning procedure again.
(SCIEX 4500, 5500, 5500+, 6500, 6500+, and 7500 systems) In the MS Tune workspace, during automatic calibration for the 10 Da/s scan rate, the wrong isotope might be selected. (TUN-7245)	After automatic calibration is complete, review the Instrument Tuning report to make sure that the correct isotope was used for all masses. In Positive polarity, make sure that the correct (second) isotope is used for mass 1952. In Negative polarity, make sure that the correct (second) isotope is used for masses 1863 and 1979. For all other masses, make sure that the first isotope is used.

Issue	Notes
(SCIEX Triple Quad 4500, 5500, 5500+, 6500, and 6500+ systems) In high resolution mode, only the 10 Da/s scan rate is tuned. (TUN-7292)	The resolution offset for 10 Da/s is copied to the other scan rates.
The user cannot open the Explorer workspace to show data acquired with the **Advanced Troubleshooting** command in the MS Tune workspace. (ONYX-16557)	N/A

Reporter Issues

Issue	Notes
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)	To avoid any issues, print using the XPS option instead of the PDFactory option.
If the **For Each Sample** tag is removed from a report template, then it cannot be added back. (RPT-21)	Create the report again.

MS FW Updater Issues

Issue	Description
The MS FW Updater utility cannot be run from 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.

SCIEX OS to Analyst Software Method Converter Issues

Issue	Description
A method cannot be converted from SCIEX OS if the method contains an EMS scan. (ONYX-12112)	This issue occurs if an earlier version of the Method Converter is used. Make sure to use the version of the Method Converter included in the installation package for SCIEX OS 2.2.
The SCIEX OS to Analyst Software Method Converter cannot be opened in the Analyst software if the Analyst software is installed after the SCIEX OS to Analyst Software Method Converter. (ONYX-14031)	Install the Analyst software before the SCIEX OS to Analyst Software Method Converter.

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Documentation

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To find software product documentation, refer to the release notes or software installation guide that comes with the software.

To find hardware product documentation, refer to the *Customer Reference* DVD that comes with the system or component.

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