SCIEX OS 2.0.1 Release Notes

Introduction

Thank you for choosing SCIEX to supply your system. We are pleased to bring you the SCIEX OS 2.0.1 Software, which supports the SCIEX X500R QTOF and SCIEX X500B QTOF Systems, which provide liquid chromatography-time-of-flight mass spectrometry functions, and the SCIEX Triple Quad™ 7500 LC-MS/MS System – QTRAP® Ready. SCIEX OS 2.0.1 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 2.0.1

This section describes the enhancements and fixes in SCIEX OS 2.0.1. 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.

Fixed Issues in Version 2.0.1

- The component name was changed with an appended _sum for non-internal standard (IS) components and _IS for summed IS when summing multiple ions in the Results Table. Because the component names and IS names did not match the names in the LIMS, the import to LIMS was unsuccessful. (BLT-2171)
- Retention time Confidence Flag was not Updated for samples with manual Integration in the Results Tables. It works properly when peaks are integrated using the integration algorithm parameters. (BLT-2207)
- Fields in the Batch workspace might be slow to populate. (BLT-2216)
- Copying of information from Microsoft Excel to the Batch workspace in SCIEX OS might be slow. (BLT-2227)
- Data acquired by a SCIEX 7500 System on a network could not be processed using the Analyst® 1.7.2 Software. (BLT-2240)

- It was not possible to limit the transfer of results to the Watson LIMS to only those rows that are visible in the Results Table. The user now has the option to transfer all results or only visible results. Note that transfer of visible results is only supported if all visible samples have the same number of components. (MQ-7898)
- It was not possible to transfer internal standards to the Watson LIMS. The user now has the option to transfer only analytes or analytes and internal standards. (MQ-7937)
- Occasionally, the incorrect error message was shown when the user clicked **Test Device** when configuring an LC system in the Configuration workspace. Now, the failure message sent by the LC system driver is also shown. (ONYX-8875)
- The injection volume in a batch was not updated based on the injection volume defined in the selected LC method except on the initial draw of the row. (ONYX-9055)

Notes on Use and Known Issues

Notes on Use

- When performing Windows Updates, users should not install optional updates, because they might impact functionality in the software. Only install the required updates. Schedule the installation of updates to occur when the system is not acquiring data.
- If users do not have read permissions for the Default project, then an error might occur when they try to open SCIEX OS. (ONYX-3131)
- System performance might be slower when many workspaces are open, or when large numbers of transitions are being processed. (ONYX-2321)
- When the user opens a batch that was created in an earlier version of SCIEX OS, the **Injection Volume** field is not automatically populated. The user must click each **LC Method** field in the batch. (ONYX-2967)
- 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.
- 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 will not be written to the data file. If the service is interrupted during local acquisition, then the partial sample data will be written to the data file but will be marked as corrupted. Any auto-triggered processing and decision rule processing will also fail 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 2.0.1 cannot be appended to data files acquired in SCIEX OS version 1.3.1 or earlier. (DS-1931)
- When specifying a new Results file for a sample in the Batch workspace, the user must also specify a processing method. If no processing method is specified, then the **Processing Method** column in the Queue workspace will contain ***Embedded Method*** and automatic processing fails. (ONYX-4864)
- When specifying a Results file in an Analyst Data path, the user cannot create a subfolder. The user must select an existing folder. (ONYX-4962)
- If a user does not have permissions to access the Explorer workspace, then the user cannot open the Calibration report from the Queue workspace. (ONYX-3401)
- 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.
- The software does not use the selected regression parameter (Area or Height) to calculate the ion ratio for a component. The software uses the regression parameter defined for the first component in the Results Table to calculate the ion ratio for all of the components in the Results Table. (MQ-5546)
- 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)
- The **Apply to Workstation** button is active even though the current audit map template is applied to the workstation. To determine which audit map template is currently applied to the workstation, open the Audit Trail workspace. (ONYX-3400)

General Issues

Issue	Notes
The user cannot open report (xps) files created during in the MS Tune workspace, during tuning, 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 adminstrator: 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.
If SCIEX OS is installed on a computer configured for a language other than English, then an error is shown the first time that SCIEX OS is opened. (BLT-892)	Open SCIEX OS again.
SCIEX 7500 System data with a long file path cannot be processed in the Analyst® Software. Some sections in the file information for such data files are also not displayed. (ONYX-9408)	To avoid the issue, make sure to use a shorter file path.

Devices 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.
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 LC system 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 system goes to Fault state and the sample becomes corrupted. If this issue occurs, then restart the computer and open the software again.
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 **Clear Error** 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 **Standby** in the status panel.
Agilent LC: 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.
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.

Issue	Notes
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.
After processing several samples, the pressure graph shows the pressure dropping to zero briefly, before returning to its original pressure. (ACQ-2043)	The pressure drop occurs when the injection loop is switched in to the flow path. The pressure is sampled every 5 seconds, so the pressure drop might not be shown every time the injection loop is switched. This issue does not impact performance.
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 **Standby** 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 **Standby** 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 **Stop Time** field for the LC method duration is the longest time that the LC method must run.
Shimadzu and ExionLC™ AC/ExionLC™ AD 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.
In some cases, devices cannot be added manually. (ACQ-3014)	In some cases, when devices are added manually, the **Test device** function fails. To avoid this issue, use **Autoconfig** to add devices.

Issue	Notes
The user can configure unsupported devices and options. (BLT-1740)	The SCIEX Triple Quad™ 7500 System – QTRAP® Ready does not support the calibrant delivery system and contact closure options.
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.
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.
The mass spectrometer mass mode is not shown if the mass spectrometer fails to activate, or if it activates while it is in Fault state. (MSCS-2065)	Activate the device again when the mass spectrometer is in the Ready or Idle state.
The user is unable to configure an X500 QTOF System in the Devices workspace after downgrading from SCIEX OS 2.0 to SCIEX OS 1.7. (MSCS-2286)	After installing SCIEX OS 1.7, stop the ClearCore2 service and then install the C++ redistributables (vc_redis*.exe) from the Install folder in the SCIEX OS 2.0 installation package.
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 *Software Installation Guide*.
Agilent LC: If a sample vial is missing, then the system fails to acknowledge the missing vial and injects air. (ONYX-4849)	This issue occurs when a sample vial is missing if one or both of the following options is selected: • **If a sample is missing, then proceed to the next sample** on the Queue Settings page. • **Ignore missing vessel** on the Direct Control dialog. If neither of these options is selected, then the system goes to Fault state and the sample fails. To avoid this error, clear both of these options, and then make sure that all vials are present.

Issue	Notes
Agilent LC: 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.
Agilent LC: 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.
When the user presses **F1** in the LC Method workspace, both the SCIEX OS *Help System* and the Help for the LC system open. (ONYX-7149)	N/A
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-8048/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.
Shimadzu LC-40: The **Purge**, **Rinse**, and **Cooler** buttons on the Device Control dialog are not active. (ONYX-7702)	Use the keypad controls on the autosampler, or include these functions in the LC method.
The Shimadzu Nexera Mikros LC pump does not go into fault state when the maximum pressure limit is reached. (ONYX-7794)	N/A

Issue	Notes
In the Detailed Status dialog for the diverter valve, the **Time** value is incorrect while the system is in the equilibration and loading states. (ONYX-7831)	Wait for the next sample to start running, and then open the Detailed Status dialog again to view the **Time**.
The Shimadzu 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.
When an Agilent DAD is connected to a Shimadzu LC stack, there is a delay of 0.2 minutes between the DAD trace and the MS trace. (ONYX-8120)	When processing data acquired with this configuration in the Explorer workspace, use the **Process > Offset Chromatogram** command to set the total offset to 0.2 minutes.
If the device configuration includes a detector configured to acquire data in channel mode, and the acquired data contains duplicate wavelengths, then the wavelength data shown in the Data Acquisition panel and the Explorer workspace is incorrect. (ONYX-8382)	Data is shown properly in the Analytics workspace.
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.
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.

Acquisition Issues

Issue	Notes
Auto-triggered processing of samples might be interrupted if the active Results Table file is opened during acquisition or processing. This occurs only when the MS Method contains a large number of compounds, that is, more than 500 compounds. If this occurs, then any Decision Rules that have been implemented will also be disrupted. (ONYX-8733)	To avoid this issue, do not open an active Results Table file from the queue if data is acquired using MS Methods that contain a large number of compounds (<500).

Issue	Notes
In the Batch and Queue workspaces, printouts using the PDFactory option have the following issues: • 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) • The date and time when other regional settings are used are not shown. (ACQ-2700) • The row index is blank when only several isolated rows are printed using PDFactory. (ACQ-2701) • (X500 QTOF Systems) 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) • Printing reports using XPS and PDFactory in landscape mode works as expected, but when PDFactory is used in portrait mode, the last two columns on the first page are omitted, and the time at which the batch is printed is truncated. (ACQ-1275)	To avoid any issues, print using the XPS option instead of the PDFactory option.
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** 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 type the **Data File** again.

Issue	Notes
(X500 QTOF Systems) 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. However, changes made by the user are not updated to the mass spectrometer nor are the changes logged in the sample information for that sample.
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.
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 **Standby**.
The software does not save the required parameters when switching from an open method to another method in the MS Method workspace 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.
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 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.
When the software ramps the CE parameter during MRM HR 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 HR generator to view the results of the parameter ramp. Do not use the Data Acquisition panel.

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.
(X500 QTOF Systems) 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.
When the user opens an MS method, the **Print** button is not available. (ACQ-3301)	Close the method and then open it again.
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.
(X500 QTOF Systems) For MRM HR methods, retention time is not validated when the Method duration is changed in the MS Method workspace. (BLT-961)	Save, close, and open the method again.
Batches fail when acquiring data with a DAD in Spectrum mode. (BLT-978)	For enhanced batch stability, use the DAD in Signal mode.
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.

Issue	Notes
Samples in the queue might be marked as failed even though the data was 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, then the sample and data file are not affected, and they can be used for exploring or processing. To refresh the queue icons, restart the software.
Real time updates might be delayed when Results Tables are being created. (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.
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.
Agilent LC: When a batch created with SCIEX OS 1.2 or earlier is opened, LC information, such as **Rack code**, **Rack position**, and **Plate code**, is missing. (DS-2186)	These fields have been redefined in this version of the software. Populate them again.
(X500 QTOF Systems) 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.
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.
An incorrect message is shown when the probe is changed. (MSCS-972)	The error does not affect acquisition. Users can cancel the message and acquisition will continue.

Issue	Notes
(X500 QTOF Systems) Acquisition is aborted if the TOF MS experiment is deleted while data is being acquired with MRM HR and SWATH® methods or MRM HR and IDA methods. (MSCS-1059)	To avoid this issue, do not delete the TOF MS experiment from the MRM HR method.
In an IDA method with a survey scan that uses the *Scheduled* MRM™ Algorithm with sMRM triggering, the **Inclusion list** is not used. (MSCS-2270)	Do not use an inclusion list with IDA survey scans that use the *Scheduled* MRM™ Algorithm with sMRM triggering.
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.
(X500 QTOF Systems) 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.
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.
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.
In the MS Method and LC Method workspaces, the Print dialog does not open, or there is a delay before it opens. (ONYX-3412)	Wait approximately 1 minute for the Print dialog to open.

Issue	Notes
User interface issues occur when a Results file is being specified. The **Results File** cell is not shown correctly. (ONYX-4790)	Resize the column or click in another cell.
Automatic processing fails if the file path specified for the **Results File** in the batch is too long. (ONYX-4827)	In the batch, limit the length of the **Results File** path to 300 characters or less.
The message "The path name is too long" is shown when a root directory is defined, but the path is less than 247 characters. (ONYX-4981)	This message is also shown if the logged-on user does not have write access to the network resource.
When rows are pasted in the Batch workspace, if the **Results File** in the copied row does not contain a value, then the name of the MS Method is inserted in the **Results File** column of the pasted row. (ONYX-5029)	Edit the batch to correct the **Results File** column contents for the affected rows.
When a csv file is imported in the Mass Table of an MS method, no error message is shown if the number of columns in the import file is greater than the number of columns in the Mass Table. (ONYX-5216)	This issue occurs if a text editor is used to add a column, delimited by a comma (,), to a row in the csv file, and the comma and column text are not added to the other rows. 1. Export the Mass Table to a csv file. 2. Open the exported file in Microsoft Excel. 3. Edit the Mass Table. 4. Save the updated csv file. 5. Import the file again.
In the MS Method workspace, when the user is editing the Mass Table for an MS method, the **Delete** key does not work. (ONYX-5467/ONYX-7384)	To delete content in the Mass Table, use one of the following methods: • Use the **Backspace** key to delete the text. • Double-click the cell to enter Edit mode, and then use the **Delete** key. Then type new text, if required.

Issue	Notes
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.
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.
An error occurs when the user selects a row in the Mass Table and then uses the **Fill Down** command. (ONYX-7225/ONYX-7461)	Select the column at the cell to be copied, and then use the **Fill Down** command. Do not select the row.
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 the user changes the polarity of an LIT method, **Dynamic fill time** is turned on. (ONYX-7740)	Turn off the **Dynamic fill time**.

Issue	Notes
Dwell time is not updated correctly when the user changes the polarity multiple times in a method that contains an experiment that uses the *Scheduled* MRM™ Algorithm looped with one or more other types of experiments. (ONYX-7841)	The calculated dwell time for the transitions in the experiment that uses the *Scheduled* MRM™ Algorithm will vary by a few ms from the correct dwell time.
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.
The user cannot specify decimal values in the **Start at** and **Stop at** fields for AF2 ramping. (ONYX-8318)	Stop ramping manually when the required stop value is reached.
The **CE spread** field is active for ER scans. (ONYX-8328)	The **CE spread** parameter is not used in ER scans. Any values entered in this field are ignored.
The software stops responding when second-level IDA criteria are added to an MS method with multiple IDA experiments if the survey scan uses the *Scheduled* MRM™ Algorithm. (ONYX-8333)	Survey scans that use the *Scheduled* MRM™ Algorithm to trigger an MS^3 experiment are not supported in looped IDA methods.
In the Decision Rule Configuration dialog, when a processing method is selected, the list in the **Flagging Rules** field might include Combined flagging rules that are defined in the processing method, but not applied. That is, the **Apply Rule** check box is not selected. (ONYX-8352)	If the user selects a Combined flagging rule that is not applied in the processing method, then no decision rule processing is performed in the queue.

Issue	Notes
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.
An error dialog is shown when the user clicks **Open data exploration to view real-time data** ( ) while acquiring IDA data in the MS Method workspace. (ONYX-8446)	If the user collapses the IDA experiment, submits the IDA method, and then clicks , an error dialog is shown. Click **OK** to open the Explorer workspace. To avoid this issue, do not collapse the IDA experiment.
When the user prints a method with multiple experiments, only the **Nebulizer current** for the first experiment is printed. (ONYX-8462)	N/A
The wiff files written by SCIEX OS contain less detailed MS method information than the wiff files created by the Analyst® Software. (ONYX-8546)	N/A
(X500 QTOF Systems) When a *Scheduled* MRM^{HR} method is printed, the report does not contain all of the columns in the Mass Table. (ONYX-8563)	Change the document orientation to landscape in the Print dialog before printing.
The polarity of the collision energy (CE) parameter is shown incorrectly in Negative IDA experiments polarity. (ONYX-8566)	The correct value for CE is used for acquisition.
An error is shown during step 5 (Optimize Collision Energies) if the user does not complete all of the preceding steps, in order. (ONYX-8568)	Click **OK**.

Issue	Notes
When the (s)MRM Plots dialog is open, it is in front of all other dialogs. It the dialog is expanded, the user might be unable to view other dialogs, such as the Save dialog. (ONYX-8601)	Use one of the following workarounds: • Press **Alt+Esc** to cycle through the open dialogs, until the required dialog is visible. • Press **Alt+F4** to close the underlying dialog and return the focus to the (s)MRM Plots dialog. • Press **Alt+Space** to open the context menu for the underlying dialog.
If multiple transitions have the same retention and dwell time, then only the last one is shown in the tooltip in the Dwell Time graph in the (s)MRM Plots dialog. (ONYX-8621)	N/A
If the scheduled ionization feature is used with a device configured with contact closure, then ionization might begin before the device controlled through contact closure begins injecting sample. (ONYX-8626)	Increase the ionization start time to allow contact closure signals to be sent and sample injection to begin.
(SCIEX Triple Quad™ 7500 Systems) Information Dependent Acquisition (IDA) might trigger dependent scans for the same ion more often than specified by the criteria if both **Exclude former candidate ions** and **Exclude isotopes +/-** are selected. (ONYX-8947)	If an EMS, Neutral Loss, Precursor Ion, or Q3 is selected as the survey scan for an IDA method, then dependent scans for the same ion might be triggered more often than the number of occurrences specified for **Exclude former candidate ions** if the **Exclude isotopes +/-** check box is also selected. To avoid the issue, optimize the gradient with an increased LC run time to prevent compounds from co-eluting. Alternatively, use an IDA method with the **Dynamic Background Subtraction** and **Exclude Isotopes** options selected.

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 Default Templates.
SCIEX OS stops responding during processing when a non-targeted workflow is being used. (BLT-2069)	For non-targeted workflows, limit processing to 20 samples at a time.
Ion summation parameters are not preserved for MultiQuant™ Software quantitation methods imported to SCIEX OS. (BLT-2172)	Configure the ion sum parameters in the processing method in SCIEX OS.
Data with a long file path that was generated by a SCIEX 7500 System cannot be processed using the Analyst® 1.7.2 Software. In addition, the file information for such a data file cannot be fully displayed in the Analyst® 1.7.2 Software. (BLT-2246)	To avoid this issue, use the Analytics workspace in SCIEX OS to process the data.
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.

Issue	Notes
Changing the regression setting for one algorithm in the Project default page updates the regression setting for the other algorithms. (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 **Update Retention Time** feature is set to **Group**) can be changed, resulting in inconsistent expected retention times and retention time windows in the group. (MQ-1511)	The user can manually change the **Expected RT** 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.
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.
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.

Issue	Notes
Incompatible components in the embedded processing method are not handled correctly if the processing method uses the AutoPeak integration algorithm. (MQ-1873)	When an existing processing method that uses the AutoPeak integration algorithm 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 processing method that uses the Summation integration algorithm contains incompatible components. (MQ-1888)	If an existing processing method that uses the Summation integration algorithm 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 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.
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.
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.
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.

Issue	Notes
If the user processes data while the system is acquiring data, then large temporary files might be created. Large temporary files can 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.
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 **Save** or **Cancel**. Data analysis is not affected.
Users are able to process data and create a Results Table using 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.
The software cannot perform quantitative and qualitative processing of data from Q1 scans for SCIEX X500 QTOF systems. (MQ-2790)	Q1 data from SCIEX X500 QTOF systems cannot be processed in the Analytics workspace.
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.
Filtering is incorrectly applied. The appropriate rows are not shown. (MQ-4823)	If the **Text Filters** are selected before the Filter By Flag filter, then the Filter By Flag filter is not applied correctly. Always select the Filter By Flag filter first.
The Results Table pane becomes read-only after the embedded processing method is edited. (MQ-5082)	Close the Results Table and then open it again.
An error occurs when the user attempts to copy values in the **Upper Limit** column of the Concentration Acceptance or Values per component type tables in the Flagging Rules. (MQ-5599)	Type the values in the table.

Issue	Notes
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 *Software User Guide*.
An error is shown when the user configures the table settings on the Components page of the processing method to show **Mass (Da) and Width (ppm)**. (MQ-7709)	For nominal mass systems, such as the SCIEX Triple Quad™ 7500 System – QTRAP® Ready, XIC width (ppm) is not supported. Use XIC width (Da).
When the user clicks **Open data exploration** in the Peak Review pane to a data file that contains UV data in the Explorer workspace, the XIC UV graph is not shown. (MQ-7723)	Open the data file in the Explorer workspace.

Explorer Workspace Issues

Issue	Notes
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)	If this issue occurs, then do one of the following: • Generate the XWC first and then generate the DAD contour panel. • Wait until the contour panel has finished updating before generating the XWC.
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/ DS-1092) • 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
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) A mismatch in the real time graph in the MS and DAD Data 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 Data 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)	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)	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.
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.
Intermittently, the message, "This sample is corrupted" is shown the first time a sample is acquired in the MS Method workspace, or when a newly-acquired sample is opened in the Explorer workspace. (DS-2281)	Click **OK** to acknowledge the message. The sample can be processed as normal.

Issue	Notes
The user 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 **All Overlaid** and then click **OK**. 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.
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.
Sample information for IDA experiments is not shown when the users opens a *Scheduled* MRM™ data file, selects and loads a sample, and then clicks **Show Sample Information**. (PV-1330)	This issue does not affect the workflow.

MS Tune Workspace Issues

Issue	Notes
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.
When the Q1 center mass is selected, the mass range of the real-time spectrum is not updated correctly. (DS-915)	To avoid this issue, set the start and stop masses to cover the Q1 center mass range.
If the user tunes the mass spectrometer, saves the new instrument settings, and then restores the previously saved instrument settings, then the audit record is incomplete. (ONYX-8392)	N/A

Reporter Issues

Issue	Notes
A Microsoft Office Document Customization error occurs when the user tries to edit a report template.	This error occurs because the TemplateContentControlManager is not installed. Follow these steps: 1. Navigate to C:/Program Files/AB Sciex/ReporterOfficeAddins/ TemplateContentControlManager. 2. Double-click **TemplateContentControlManager.vsto**. 3. If the TemplateContentControlManager is installed, then click **Close**. Otherwise, click **Install** and then follow the onscreen instructions.

Software Installation and Activation Issues

Issue	Notes
SCIEX OS might fail to install if an incorrect user account is used. (BLT-340)	Contact sciex.com/request-support. Only Administrators should install or remove the software.
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 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.
If the ChemSpider license has expired, and the user installs a new license, when the user attempts to start a ChemSpider session, a message is shown warning that ChemSpider is not licensed. (BLT-985)	Close and then open SCIEX OS, and then start ChemSpider again.
SCIEX OS cannot be uninstalled. (BLT-1024)	If SCIEX OS cannot be uninstalled, then make sure that Microsoft .NET 2.0 is activated. Refer to the Microsoft Help for detailed instructions. Then try again.
When the software is downgraded from version 2.0 to version 1.3, the Batch, Queue, and User workspaces are missing. (OFX-489)	If a backup of the SCIEX OS 1.3 installation is not available, then: 1. Remove SCIEX OS 2.0. 2. Remove the LibraryView™ Framework. 3. Rename the C:\Program Data\SCIEX\ folder. 4. Rename the C:\Program Files\SCIEX\ folder. 5. Rename the D:\SCIEX OS Data\ folder. 6. Install SCIEX OS 1.3. SCIEX OS must be reconfigured and all methods, settings, users, and so on must be recreated.

Issue	Notes
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 the 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.
Occasionally, SCIEX OS might fail to install because of an issue with SQL server or because of an issue with the LibraryView™ Framework. (ONYX-2987)	If this issue occurs, then: 1. Remove LibraryView™ Software, if installed. 2. Remove the LibraryView™ Framework, if installed. 3. Remove all of the Microsoft SQL Server 2008 components. 4. Shut down and then start the computer again. 5. Install SCIEX OS. If the installation issue persists, it might be necessary to remove the LibraryView.mdf and the LibraryView_log.mdf files from the C:\Program Files\Microsoft SQL Servier\MSSQL10_50.SQLEXPRESS \MSSQL\DATA folder. **Note:** Because the libraries are stored in the mdf files, any existing libraries will be removed if these files are deleted and will have to be installed again.
An error is shown when SCIEX OS is installed on a computer without .NET Framework 4.x. (ONYX-8028)	If this issue occurs, then install it with Install/NDP472-KB4054530-x86-x64-AllOS-ENU.exe, located in the installation package.

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.

Default Templates

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
All Peaks Qual	A report showing, for each sample, a section including the File Information, Sample Information, Analyte Results Table, and overlaid chromatograms of all of the analytes and internal standard. The Analyte Results Table is printed as shown in the Results Table. All the qualitative confidence traffic lights are listed at the beginning of the table.	N/A
Analyte 20 percent Report	A report showing, for each analyte, a section including File Information, and an XIC table for each Blank, Standard, QC, and 20% of all Unknowns.	This is an example report template that has a Query attached - Analyte20percent.Query.
Analyte Summary	Table of results showing Sample Name, Calculated Concentrations and Outliers for all samples in the batch for the specific analyte and the associated Internal Standard.	N/A
Calibration Curve	A report showing the File Information, Statistics Table (standards), and Calibration Curve for analytes, one page per analyte.	• Standards for which the Reportable check box is cleared will not be reported in the data table. Statistics will not be affected by the Reportable status. • The report will show the regression equation and graph, as shown and calculated in the Calibration Curve pane in the Analytics workspace, based on the status of the **Used** column.

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
Intact Quant All Peaks and Graphs	A report showing the Results Table entries for each sample. All columns visible in the Results Table are shown in the report. The report also includes the XIC chromatograph, average spectrum, and reconstruction spectrum, for each sample and analyte.	• This report is specific to the Mass Reconstruction workflow.
Intact Quant Analyte Summary and Calibration Curve	A report showing the Results Table entries, the calibration curve, and the statistics data for each analyte. The Results Table includes Sample Name, Sample Type, Analyte name, Actual Concentration, Area, Height, Expected MW, MW, MW Delta, Calculated Concentration, and Accuracy.	• This report is specific to the Mass Reconstruction workflow.
Intact Quant Sample Summary	A report showing Results Table entries for all samples. The Results Table includes Sample Name, Sample Type, Analyte Name, Actual Concentration, Area, Height, Expected MW, MW, MW Delta, Calculated Concentration, Accuracy and Accuracy acceptance.	• This report is specific to the Mass Reconstruction workflow.
Metric Plot	A report showing, for each analyte, a section including the File Information and a metric plot of the analyte peak area.	• The state of the **Reportable** check box does not affect the report content. All data points are included even if the check boxes are cleared.
MQ Analyte Report 1	A report showing, for each analyte, a section including File Information, Sample Results Table, and XIC table for each sample - WILL GENERALLY PRINT 2 PAGES PER ANALYTE FOR < 8 SAMPLES	N/A

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
MQ Analyte Report 2	A report showing, for each analyte, a section including File Information and XIC table for each unknown sample - WILL GENERALLY PRINT 2 PAGES PER ANALYTE FOR < 8 SAMPLES	• Only unknowns are reported.
MQ Analyte Report 3	A report showing, for each analyte, a section including File Information, and Unknown Samples Summary Table.	• Only unknowns are reported.
MQ Analyte Report condensed table	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. The table is shown as 2 columns to fit more samples per page.	• Only unknowns are reported.
MQ Analyte Report with chromatograms	A report showing, for each analyte, a section including File Information, Sample Results Table, and a small chromatogram for each sample.	• Only unknowns are reported.
MQ Blank Template	N/A	• Only header information, the logo, and page numbers are shown in the report
MQ Pep Quant	N/A	• For use with the Peptide Quantitation dataset. Refer to the the second example, the absolute quantitation example, in the *User Guide* for the MultiQuant™ Software.
MQ QC Summary 1 with flags	A report showing File Information, QC Summary Table per analyte (values with a CV higher than 20% are highlighted), and QC Detailed Results Table (values with an accuracy outside of 80-120% are highlighted).	• Quality Controls that have the **Reportable** check box cleared will not be included in the report, nor will they be used in the calculations

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
MQ Sample Report 1	A report showing, for each sample, a section including File Information, Sample info, IS info, Analyte Results Table, XIC table including IS and each analyte - WILL GENERALLY PRINT 2 PAGES PER SAMPLE FOR < 8 SAMPLES	N/A
MQ Sample Report 2	A report showing, for each unknown sample, a section including File Information, TIC, Sample Details, Analyte XIC, and results in table form - WILL GENERALLY PRINT 2 PAGES PER SAMPLE FOR < 8 SAMPLES	• Only unknowns are reported.
MQ Sample Report 3	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table.	• Only unknowns are reported.
MQ Sample Report condensed table	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. The table is shown as 2 columns to fit more analytes per page.	• Only unknowns are reported.
MQ Sample Report with chromatograms	A report showing, for each sample, a section including File Information, Sample info, Analyte Results Table, and a small chromatogram for each analyte.	• Only unknowns are reported.

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
MQ Sample Report with Concentration Threshold	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Sum	• The associated query file is Sample Report with Concentration Threshold.query. • Components must be named "Cmpd *X* #", where *X* is any character from A to F, and # is any numerical value. **Example:** In the report, a component named "Cmpd A 1" will be shown under the heading **Compound Group A**; a component named "Cmpd B 1" will be shown under **Compound Group B**, and so on. • If components are in the same group, then only the first component, alphabetically, in the group will be included in the report. **Example 1:** If "Cmpd B 25" and "Cmpd C 1" both belong to the group "Grp", then "Cmpd C 1" will not be in the report. **Example 2:** If "Cmpd A 1", "Cmpd A 2", and Cmpd A 3" are not assigned to groups, then "Cmpd A 2" and "Cmpd A 3" will not be in the report. **Example 3:** If "Cmpd A 1", "Cmpd A 2", and Cmpd A 3" are assigned to groups 1, 2, and 3, respectively, then all 3 components will be in the report under the heading **Compound Group A**.

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
MQ Sample Report with MRM ratios 2	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table, overlay of all XIC. Expected Ion ratios are calculated automatically using any available standards. Ratio values are placed in custom columns within the Results Table. Any values outside 20% of expected are flagged. Quantifier analyte names must end in a blank space followed by the number 1. Ratio ion analyte names must end in a blank space followed a number between 2 and 9.	N/A
MQ Sample Report with MRM ratios EU	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. Expected Ion ratios are calculated automatically using any available standards. Ratio values are placed in custom columns within the Results Table. Any values outside of expected are flagged (using EU guidelines for ratio tolerances). Quantifier analyte names must end in a blank space followed by the number 1. Ratio ion analyte names must end in a blank space followed a number between 2 and 9.	• The associated query file is MRM ratios EU.query.

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
MQ Sample Report with MRM ratios MQ EFAB 03	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. Expected Ion ratios are calculated automatically using any available standards. Ratio values are placed in custom columns within the Results Table. Any values outside 20% of expected are flagged. Quantifier analyte names must end in a blank space followed by the number 1. Ratio ion analyte names must end in a blank space followed a number between 2 and 9.	N/A
MQ Sample Report with MRM ratios	A report showing, for each unknown sample, a section including File Information, Sample info, and Results Summary Table. Expected Ion ratios are calculated automatically using any available standards. Ratio values are placed in custom columns within the Results Table. Any values outside 20% of expected are flagged. Quantifier analyte names must end in a blank space followed by the number 1. Ratio ion analyte names must end in a blank space followed a number between 2 and 9.	• The associated query file is MRM ratios.query.
MQ Sample Report with standards, QC, and blanks	A report showing, for each sample, a section including File Information, Standards Summary Table, QC Summary Table, Blanks Results Table; then for each unknown sample a section including File Information, Sample info, IS info, Analyte Results Table, XIC table including IS and each analyte - WILL GENERALLY PRINT 2 PAGES PER SAMPLE FOR < 8 ANALYTES.	• Standards and Quality Controls that have the **Reportable** check box cleared will not be shown in their respective summary tables in the report, nor will they be used in the statistical calculations.

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
MQ Tutorial Dataset Heavy Light	N/A	• This report is intended for use with the Tutorial Dataset Heavy Light dataset. Refer to the second example, the relative quantitation example, in the *User Guide* for the MultiQuant™ Software.
Per Sample Quant-Qual	A report showing, for each selected sample, a section including the File Information, Sample Information, and Analyte Results Table for the selected analytes. The Analyte Results Table is printed as shown in the Results Table. All the qualitative confidence traffic lights are listed at the beginning of the table.	N/A
Per Sample Quant-Qual Visible Rows Using Visible Analyte	A report showing, for each selected sample, a section including the File Information, Sample Information, and Analyte Results Table for the selected analytes. The Analyte Results Table is printed as shown in the Results Table. All the qualitative confidence traffic lights are listed at the beginning of the table.	• The hidden state of a row takes precedence over the state of the **Reportable** check box. If the **Reportable** check box is selected but the row is hidden, then the row is not reported.

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
Per sample Quant-Qual with statistics	A report showing components for each sample with a WYSIWYG table. XIC, MS, and MS/MS are shown. A statistics summary table for area is shown at the end of the report.	• If the component table has UV components, then the UV trace is reported under XIC graph in the report. **Note:** If the name of the UV component is in the format [compound_nameuv] or [uv], then no UV traces are reported, because the uv suffix is associated with the UV MS Qual report. • If a sample is labeled as a QC and there are 2 or more samples, then the mean, STDEV, and %CV will be calculated and included in a QC summary table at the end of the report. • If the **Reportable** check box is cleared for a QC row, then that row will not be used for any calculations in the QC summary table.
Per Analyte Quant-Qual	A report showing, for each analyte, a section including the File Information, Results Table, Calibration Curves, and chromatograms including the internal standard and each analyte. This template is suitable for a Results Table with a group defined in it.	N/A

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
Positive Hits Qual	A report showing, for each selected sample, a section including the File Information; Sample Information; Analyte Results Table for the selected analytes; overlaid chromatograms of all of the analytes, internal standard, and the XIC; the Acquired/Theoretical MS spectra; and the Acquired/Library MS/MS spectra for each selected analyte. The Analyte Results Table is printed as shown in the Results Table. All the qualitative confidence traffic lights are listed at the beginning of the table.	N/A
Qual CSV report	A report in a csv format showing, for each sample, a section including the File Information, Sample Information, and Analyte Results Table.	• Recommended to use CSV option for Report format.

Template	Template Description (as shown in the Create Report dialog)	Additional Notes
Sample Summary	A report showing, for each sample, a section of Analytes Summary Table. This report template is suitable for a Results Table with groups.	N/A
UV MS Qual report	A report showing, for each sample, the components of that sample and their corresponding UV component with a WYSIWYG table. XIC, MS, and MS/MS are shown along with UV data. A statistics summary table for area is shown at the end of the report.	• UVMS data should be processed with the naming convention *compound 1* (any string) for the mass spectrometer (MS) component and *compound 1*uv (any string plus uv) for the corresponding UV component. • Only the Mass error, Fragment Mass Error, RT confidence, Istotope confidence and Library confidence traffic lights are shown. • A graph table is created to shown the individual components of the Results Table, including the XIC, MS1 trace, MS/MS trace, and header information from compound 1, and the UV trace from compound 1uv. Refer to Figure 1. • Analyte graphs are only repeated for the MS experiments, not for the not the UV experiments. • If a sample is labeled as a QC and there are 2 or more samples, then the mean, STDEV, and %CV are calculated and included in a QC summary table at the end of the report. Refer to Figure 1. • If the **Reportable** check box is cleared for a QC row, then that row in not used for any calculations in the QC summary table.

Figure 1 Graph Table

Analyte Name: 1

(Mass/FragMass/RT/Isotope/Library)

Retention Time	4.13	Isotope Ratio Difference	5.1
Expected RT	4.12	Library Result	No Match
Precursor m/z	433.879	Library Score(%)	0.0

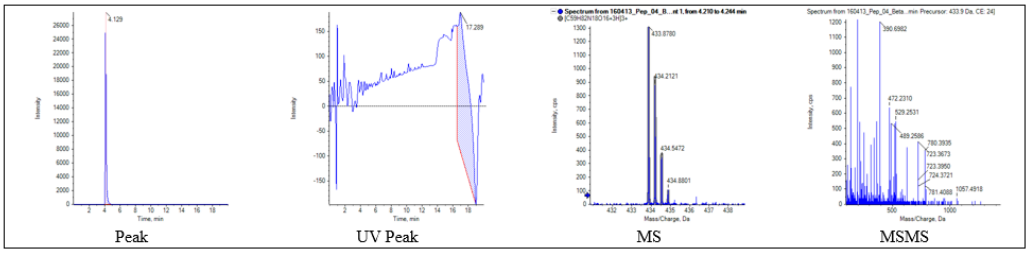

Figure 2 Statistics Table

Statistics (Grouped by Concentration for QCs - Area)

Analyte Peak Name (MRM Transition)	Mean	Std. Deviation	% CV	Number of Values Used
1 (723.3573 - 723.3773)	1.062e4	7.367e2	6.93	2 of 2
2 (753.3091 - 753.3291)	2.215e4	6.858e2	3.10	2 of 2
3 (760.3353 - 760.3553)	9.332e3	1.955e1	0.21	2 of 2
4 (631.3450 - 631.3650)	3.244e4	1.110e3	3.42	2 of 2
5 (636.3373 - 636.3573)	1.144e5	3.962e2	0.35	2 of 2
6 (871.4354 - 871.4554)	6.479e4	1.198e3	1.85	2 of 2
7 (932.4493 - 932.4693)	2.183e4	7.301e2	3.34	2 of 2
8 (1000.5743 - 1000.5943)	2.553e4	5.007e2	1.96	2 of 2
9 (755.4352 - 755.4552)	1.127e5	8.422e3	7.48	2 of 2
10 (1184.5929 - 1184.6129)	3.576e4	7.231e2	2.02	2 of 2
11 (884.4871 - 884.5071)	5.183e4	1.512e3	2.92	2 of 2
12 (1176.5468 - 1176.5668)	1.670e4	1.848e2	1.11	2 of 2
13 (871.9418 - 871.9618)	1.597e5	5.501e2	0.34	2 of 2
14 (879.4236 - 879.4436)	1.868e5	5.182e3	2.77	2 of 2

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