SCIEX OS Software 4.0 Release Notes

Introduction

Thank you for choosing SCIEX to supply your system. We are pleased to bring you the SCIEX OS software 4.0, which supports the following systems:

- ZenoTOF 8600 systems
- ZenoTOF 7600+ systems and ZenoTOF 7600 systems
- X500R QTOF and X500B QTOF systems
- SCIEX 7500+ systems, SCIEX 7500 systems, SCIEX 6500+ systems, SCIEX 6500 systems, SCIEX 5500+ systems, SCIEX 5500 systems, and SCIEX 4500 systems
- Echo® MS system, which includes a SCIEX Triple Quad 6500+ system and the Echo® MS module
- Echo® MS+ system with the SCIEX Triple Quad 6500+ system
- Echo® MS+ system with the ZenoTOF 7600 system or the ZenoTOF 7600+ system
- ExionLC 2.0 systems, ExionLC AE systems, and M5 MicroLC systems, and select other LC systems, when purchased from SCIEX

The SCIEX OS software 4.0 also lets the user process data that is acquired from triple quadrupole, QTRAP, and TripleTOF systems that operate with the Analyst software 1.6.2 or later, or the Analyst TF software 1.7.1 or later.

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

Note: The numbers in parentheses are reference numbers for each issue or feature in the SCIEX internal tracking system.

New in Version 4.0

This section gives a description of the changes in the SCIEX OS software 4.0. To see the enhancements and corrected issues for an earlier version of the SCIEX OS software, refer to the document: *Release Notes* that came with that version of the software.

New Features

- Support has been added for the ZenoTOF 8600 system.

Enhancements

- The software supports the Windows 11 LTSC 2024 operating system on these computers:
  - SCIEX Workstation - 5860 or SCIEX Workstation Plus - 5860
  - SCIEX Workstation or SCIEX Workstation+

  New acquisition computers have this version of the operating system installed.

  Note: An upgrade service is available for computers with Windows 10 installed.

Analytics Workspace

- A new tool is available to automate and optimize fragment selection for quantitative workflows. To use the tool, the user selects the **Results** > **New with optimized fragments** command. This tool can be used with full-scan and MRM^{HR} acquisition data that was acquired with an accurate mass system.
- Qualitative analysis, which includes confirmation with library matches, is added for electron-activated dissociation (EAD) data:
  - A new **MSMS Fragmentation** field is available in the Results Table and on the Components page of the processing method.
  - Library matches can be filtered on fragmentation mode.

    Note: The organization of parameters on the Library Search page has been made more logical.
  - For EAD spectra, the kinetic energy (KE) is shown in the titles of spectra in the Peak Review pane.
  - When components are imported from a library database, the user can select the fragmentation mode to import.
- Users can set a different level of precision for the **Retention Time** for an analyte and the **Retention Time** for an internal standard, which will be shown in the Results Table, chromatograms, and reports. (BLT-5701)
- When the user prints the Peak Review pane, the integration parameters are included in the report. (BLT-5753)
- Text in printouts of windows, panes, and reports is selectable. (BLT-5509)
- Data that is exported to a Watson laboratory information management system (LIMS) can use the precision settings that are configured for the Results Table. (BLT-3182)

Batch Workspace

- The submission status can be shown for the samples in a batch.

- A new customized method batch feature is available for the ZenoTOF 8600 system. With this feature, users can use a template MS method and optimize selected parameters in the Batch workspace.
- Enhancements to the decision rule functionality supply more options for automatic processing:
  - Inject a different sample before the next sample that is waiting. This option helps to decrease carryover.
  - Inject the flagged sample again with a different injection volume. This option is useful for highly concentrated samples.
- Customized column widths are used in printouts of the Batch workspace. (BLT-5765)
- When a different autosampler is selected, only the values in the LC columns that are not valid for the new autosampler are cleared. (ONYX-55523)

Configuration Workspace

- Enhancements were made to print templates:
  - The software version that is included on report templates now includes the software name. (BLT-5662)
  - The user can set a page size for a print template. (BLT-5801)
  - **Batch Name** can be included in print templates for the Analytics workspace. (BLT-5931)
  - The user can select to use shading to show confidence levels for data in the report. (BLT-5100)

Explorer Workspace

- The **Noise multiplier for S/N** field is now a text field. The user can type a number from 0.01 to 10.00.

Library Workspace

- When a spectrum is added, the user can identify the fragmentation mode for the spectrum as EAD or collision-induced dissociation (CID).
- When libraries that were created with earlier versions of the SCIEX OS software or the LibraryView software 1.7 or earlier are imported, a fragmentation mode of CID is automatically assigned to all MSMS spectra.

Metrics Tracker Workspace

- The Metrics Tracker workspace supports the tracking of instrument, sample, and auto-calibration data for ZenoTOF 8600 systems.

- Users can create rules and set notification options for when a rule is triggered.
- Users can add a comment for a specified date and time on the chart, for example, to record a power failure.
- Overlays can be used with all of the chart types for the same instrument. Instrument charts can be overlaid on instrument charts, sample charts can be overlaid on sample charts, and sample charts can be overlaid on instrument charts.

MS Method Workspace

- ZenoTOF systems: New parameters give the user more control over ZT Scan experiments.
- SCIEX Triple Quad systems and QTRAP systems: A new **Guided Optimization** > **MRM Automated** command helps users to automatically optimize for a compound. It enables high-throughput optimization of compound-dependent and source-dependent parameters for quantitation of MRM data in positive and negative polarity and ESI and APCI ionization modes. Optimization is done with sample introduction from an LC system. This feature includes these functions:
  - Automatic identification of MRM fragments and optimization of parameters.
  - Support for user-specified number of fragments per compound.
  - Saving of optimized parameters in a database for review, editing, and export to a `csv` file.
  - Ability to import the optimized parameters from the database into the MS Method or Batch workspace for method creation and acquisition.

Reporter

- New tags are added to the Reporter schema: **MSMS Fragmentation** and **KE**.

Corrections

This version includes corrections for these issues:

- The software becomes unresponsive during acquisition when the Data Acquisition pane is open. (BLT-6279)
- When the language is set to German, French, or Italian, changes to the flow rate for the syringe pump do not take effect. (BLT-6498)
- ZenoTOF systems: Over time, the software response becomes slower. (BLT-6041)

Issues in the Analytics Workspace

- The **Group peaks by adduct or charge** check box is available to users in roles that do not have the **Enable grouping by adducts functionality** permission. (BLT-6713)

- When changes are made in the Peak Review pane, calculated columns in the Results Table are not updated. (BLT-6926)
- Issues related to permissions occurred. (BLT-6581, BLT-6589).

  The information in the documentation was updated for the correct implementation.
- If a non-targeted screening workflow uses the **Standard Deviation** or **Peak to Peak** signal-to-noise algorithm, then occasionally the noise region overlaps the peak. (BLT-6506)
- An error is shown when a user adds more samples to the Results Table. (BLT-6460)
- When the AutoPeak integration algorithm is used, peaks are not integrated with Low or Medium smoothing. (BLT-6378)
- The peak-to-peak signal-to-noise values that are calculated in the Analytics and Explorer workspace are different. (BLT-6240)
- The keyboard copy command (**Ctrl+C**) copies all of the content in a Results Table cell, not only the selected text. (BLT-6205)

Issues in the Batch Workspace

- After the user changes to a different project, subfolders are not shown in the **Data File** column. (BLT-6837)
- Intermittently, the fill down function does not operate correctly in the **MS Method** or **LC Method** column. (BLT-6061/BLT-6119)

Issues in the Explorer Workspace

- The serial number of the Agilent system that is shown in the Sample Information pane is the serial number of the system that was used to create the LC method, not the serial number of the system that acquired the data. (BLT-6590)
- During TOFMS acquisition, a TIC signal is shown. But, when the user double-clicks the TIC, a spectrum is not shown. (BLT-6788/BLT-6772)
- When a `wiff` file is opened in the Explorer workspace in the SCIEX OS software, the **Dwell Weight** that is shown in the Sample Information pane is not the same as the **Dwell Weight** that is shown in the File Info pane in the Analyst software. (BLT-6392)

Issues in the MS Method Workspace

- SCIEX 7500 systems and SCIEX 7500+ systems: An error occurs when the user selects the **MRM Infusion** command. (BLT-6877)

Issues in the MS Tune Workspace

- SCIEX 7500+ systems: During tuning in Enhanced and MS^3 mode, calibration is done on five points. Only two points should be calibrated. (BLT-6761)

- Because the threshold value in SCIEX OS software is not the same as in the Tuning Tools tuning tools software, the **Enhanced Resolution (ER)** scan type cannot be used for calibration. (BLT-6363)

Issues with the Audit Trail

- On the User Management page, the incorrect user role is updated if the **Active user or group** check box is cleared for an active user. (BLT-6373)

Issues with Conversion

- If a method that uses the Scheduled MRM (sMRM) algorithm without triggering is converted from the SCIEX OS software to the Analyst software, then triggering properties are added. (ONYX-35443)
- Data that is acquired in the SCIEX OS software shows incorrect information in the File Info pane when the data is opened in the Analyst software. (BLT-5981)

Issues with Agilent devices

- The **Overlap Injection Cycle** cannot be configured for Agilent autosamplers in the LC Method workspace. (BLT-4714)

SCIEX OS 3.4.5 Module Update for Agilent Systems

The SCIEX OS software 4.0 includes the corrections that are included in this software:

- **Better visibility and tracking of the sample plate orientation**: The Agilent device driver supports front-to-back and back-to-front plate orientations for the top and bottom plates. Visual tips are supplied in the well plate assignment list. Changes that were made to the rotation of the sample plates are recorded in a log.
- **Draw from seat**: In the custom injection, the draw function is updated with an option to let the user draw from the seat. This function is not available for multisamplers with a multiwash module or dual-needle option installed.
- **Early fetch integration**: The Agilent 1260, 1290 Infinity II, and 1290 Infinity III vialsamplers with firmware version D.07.30 and later support prefetch vial options. If this feature is configured, then the autosampler gets the next sample during acquisition of the active sample. In the **Overlapped Injection Mode** list in the method file, the user can set the high throughput method parameter for the vialsampler to **Prefetch Vial**. This enhancement decreases overall LC cycle time.
- **Overlapped injection mode**: The overlapped injection mode is integrated into the SCIEX OS software 3.4.5 and labeled as **Load-Ahead**. This feature lets the user do an injection overlap in high-throughput workflows. After the sample goes into the column, the injection valve goes back to the bypass position, and the next injection cycle starts. The injection valve waits to change to the main pass until the active operation is completed. This enhancement decreases overall LC cycle time.

- **InfinityLab Assist Hub**: The InfinityLab Assist Hub supports the Infinity II and Infinity III modules. Users can see the system status, get notifications, and schedule tasks to save time and samples. The control is available through the LC method user interface and on a local tablet interface. Some features are only available in the Agilent CDS software.
- **Steady Inject Mode**: The Agilent device driver supports steady injection for multisamplers with the multiwash feature. The Steady Inject mode pressurizes the sample loop before injection to decrease the effect of pressure fluctuations on chromatographic results.
- **Collect Support Information**: The Device Control workspace is updated to include **Collect Support Info**. Users can select the information that follows, which will be saved in a `zip` file that can be sent to SCIEX support for troubleshooting:
  - ICF and driver log files: Continuously written log files. This option cannot be cleared.
  - System information: Configuration of the system and the active method.
  - Windows system information: Information about the computer hardware and the Windows operating system.
  - Windows event logs: Application and system event logs.
  - Agilent installed programs: The Agilent programs that are installed on the computer.
  - Other installed programs: All of the other programs that are installed on the computer.
  - Other files: Option to include more files in the support information `zip` file.
- **Maximum flow gradient adjustment**: The Agilent device driver supports a maximum flow gradient of 0.1 mL/min² for 1290 Infinity II pumps.
- **Thermal equilibration device for multicolumn thermostats**: The Agilent device driver is compatible with the thermal equilibration device. This device makes column temperatures stable before and during analysis for better accuracy and reproducibility.
- **Export and import functions in custom injection**: The Custom Injection tab is updated to include the **Export** and **Import** options to let the user easily import or export different pretreament files.
- **InfinityLab Sample Thermostat**: The Agilent device driver supports the InfinityLab Sample Thermostat feature. This feature lets the user set the temperature condition for the sample. In the Enable Analysis option, set the temperature to **With any temperature** or **Temperature within ± 2° C** to start the analysis for each acquisition.
- **Pump seal wash run mode**: The Agilent device driver supports the seal wash run mode for some Infinity II and Infinity III pumps.
- **Pressure Control**: The Pressure Control section is updated with **Slow**, **Medium**, and **Fast** options that let the user control the rate at which the pressure increases during manual acquisition.

- **Easy injector program functionality**: The Injector Program dialog is added to support different pre-programmed functions on the Custom Injection tab. Users can select different workflows to streamline the process and decrease configuration time.

SCIEX OS 3.4.5 Firmware HotFix

The SCIEX OS software 4.0 includes the fixes that are included in this HotFix:

- SCIEX 6500+ systems, SCIEX 6500 systems, SCIEX 5500+ systems, SCIEX 5500 systems, and SCIEX 4500 systems with ICB5: If a method with the Scheduled MRM (sMRM) algorithm was used with a diverter valve method to acquire data, then the diverter valve did not change positions as configured in the method. However, if a method without the sMRM algorithm was used with a diverter valve method, then the position of the diverter valve changed correctly.
- SCIEX 6500+ systems, SCIEX 6500 systems, SCIEX 5500+ systems, SCIEX 5500 systems, and SCIEX 4500 systems with ICB5 and an Acquity I-Class LC system: If the LC stop-flow cables were connected on the LC pump, then the system went to a fault status immediately after **Start** was pushed. If the LC stop-flow cables were disconnected, then the system operated correctly. Although this issue was not reported on other LC systems with stop-flow cables, those LC systems might have had the same issue.
- SCIEX 7500 systems, SCIEX 6500+ systems, SCIEX 6500 systems, SCIEX 5500+ systems, SCIEX 5500 systems, and SCIEX 4500 systems: To increase system reliability, the number of false errors that are created by the QPS exciter is decreased.
- SCIEX 7500+ systems and SCIEX 7500 systems: The number of redundant error messages shown for the OptiFlow Pro ion source is decreased.

SCIEX OS 3.4.5 Patch for Echo MS Driver

The SCIEX OS software 4.0 includes the corrections that are included in this patch:

- The patch corrects an issue that occurred when **Peak Type** is set to **Wide** and **Rep Rate (Hz)** has a value other than 10. (OPP-1030/BLT-6542)

SCIEX OS 3.4.5 Patch for Intabio icIEF-UV/MS Issue

The SCIEX OS software 4.0 includes the corrections that are included in this patch:

- The patch is required to meet performance requirements for mass accuracy and high sensitivity in ZenoTOF MS scans for icIEF-UV/MS analyses. (ONYX-52617)

SCIEX OS 3.4.5 Patch for ChemSpider URL Name

The SCIEX OS software 4.0 includes the corrections that are included in this patch:

- The patch updates the link to the ChemSpider web page to let users do a ChemSpider search in the SCIEX OS software. (BLT-6482)

Notes on Use

- For compatibility information, refer to the *Software Installation Guide*.
- Avoid processing a data file in the Analyst software during acquisition by the SCIEX OS software to that data file. Doing so might cause the software to become unstable and data to be lost. (ONYX-8514)
- To keep the Results Table and Peak Review pane consistent, users must use the same level of precision for the retention time for an analyte and the retention time for an internal standard.

LC Devices

- Multiple detectors cannot be used for data acquisition at the same time. (BLT-1146)

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.
- 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.

ExionLC AC, ExionLC AD, and Shimadzu Systems

- A column oven wait time of 0 means that the oven is READY when it is on. If the wait time is set to 0, then the column temperature set point does not control when injection starts.

Echo® MS and Echo® MS+ Systems

- Because the peaks are narrow, we recommend that the number of transitions be minimized. We recommend that each MRM method have a maximum of four transitions, for a scan time of 100 msec. If a large number of MRM transitionsa re required, then we recommend that **Wide** peak mode be selected in the configuration of the AE method.

Echo® MS+ Systems

The Echo® MS+ system has an OPI port wash feature. The following notes are applicable to this feature:

- The default flow rate and duration values for the OPI port wash are applicable for most use cases, wash solvents, and carrier solvents. The default values supply a good starting point for optimization.
- When the OPI port wash completes, the carrier solvent pump continues to supply carrier solvent at the flow rate specified in the last AE method, to prepare the system for acquisition. The pump stops automatically when the mass spectrometer goes to the Standby state.

  During the OPI wash phase, the user can stop the pump manually from the Device Control dialog. To stop the OPI port wash, click **Stop**. The carrier solvent recovery phase completes, and then the pump stops.

  If the OPI port wash stops incorrectly, for example, when the system goes to the Fault state, then the carrier solvent recovery step must be done manually. Do these steps:

  1. Select the **Run Only OPI Carrier Solvent Recovery** option.
  2. If the carrier solvent recovery does not complete, then click **Clear OPI Wash Fault/s**. On the confirmation dialog, click **Yes**.

     Note: To start AEMS acquisition again, clear the Fault status for the OPI wash manually. To make sure that the OPI wash continues to occur correctly, identify and correct the cause of the fault.

Intabio ZT Systems

- To make sure that the mass spectrometer and the Intabio ZT are synchronized, on the Devices page in the Configuration workspace, select the **Contact Closure** option for the mass spectrometer. If this option is not selected, the mass spectrometer will not wait for a sample to be injected, but will continue with batch acquisition.
- If a failure or error occurs in the mass spectrometer, then the Intabio ZT system gets out of synchronization, and continues to inject samples. If this issue occurs, then stop the batch.
- If a calibration failure occurs, then data acquisition continues. The setting of the **If calibration fails, then proceed to the next sample** option on the Queue page in the Configuration workspace does not have an effect on the behavior.
- If users create new ion reference tables, then to make these ion reference tables available in the **Ion Reference Table** column, they must close the Batch workspace and then open it again.

Agilent Systems

- If an autosampler with a thermostat is installed, then for temperature control to take effect, configure the Variable Temperature Control mode in the device configuration and direct device control.
- If Access Token Required is enabled in the InfinityLab Assist Hub, then click **Allow Access** to connect to the InfinityLab Assist Hub during device configuration.

- To use overlapped injection mode or the Load-Ahead feature, do this:

  1. In the LC method, set a stop time.
  2. Configure the overlapped injection in the LC method, and then in the batch acquisition, select **Enable Load-Ahead**.

  Note:

  - Overlapped injection mode does not support custom injection programs that use the inject function.
  - Batch Automation cannot be used with load-ahead features.
  - If the batch contains multiple LC methods, then the load-ahead feature cannot be configured for the batch.

- The steady-inject feature is only applicable for a multisampler with a multiwash hydraulic box and a 100 µL metered device installed. Before the steady-inject feature can be used on the SCIEX OS software 4.0, the calibration must be done with the Lab Advisor 2.2 software.

Known Issues

Issue	Notes
The Harvard syringe pump goes into Fault status when **Standby** is selected. (ACQ-2193)	To prevent this issue and clear the error, use the Direct Control feature to start the syringe.
SCIEX 7500 systems: Data with a long file path (129 or more characters) cannot be processed with the Analyst software 1.7.2 or the Analyst software 1.6.3 with HotFix 5. Also, the file information for such a data file cannot be fully shown in the Analyst software 1.7.2 or the Analyst software 1.6.3 with HotFix 5. (AN-2250)	To prevent this issue, use the Analytics workspace in the SCIEX OS software to process the data, or use a shorter file path.
If the Flexera Licensing Server is being used for other products, then the SCIEX vendor daemon cannot be run. (BLT-3318)	The Flexera Licensing Server does not allow the same vendor daemon to run simultaneously under different instances on the same server. If the Flexera Licensing Server is being used for other, non-SCIEX products, then add the SCIEX vendor daemon and concurrent license to the existing Flexera Licensing Server.

Issue	Notes
When the SCIEX OS software runs unattended, it shows an error dialog. (ONYX-40401)	Click **Yes** to close the dialog. The SCIEX OS software stays open, and no data is lost.
Acquisition stops intermittently because of a device fault with an Agilent device. (ONYX-58914)	N/A
In the Queue workspace, if the **If a sample is missing, then proceed to the next sample** option is selected, then acquisition does not stop when a sample is missing. (BLT-6746, ONYX-42717, ONYX-61930)	Agilent LC systems: To prevent this issue, in the settings for the controller, set **On missing vessel** to **Abort Current Sequence**. Waters LC systems: To prevent this issue, in the preferences for the sample manager, select **Injection fails on error**.
In the Explorer workspace, no progress indicator is shown for activities that require more than 3 seconds. (ONYX-57129)	N/A
ZenoTOF 8600 system: The valve model goes into Fault state on activation. (ONYX-63264)	If this issue occurs, then click  **(Direct device control)** adjacent to the valve model, and then, on the Device Control dialog, click **Standby** two times. If the issue continues, then push the valve control button on the front panel of the mass spectrometer to change the valve position. Then click **Standby** two more times.

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SCIEX Support

SCIEX and its representatives have a global staff of fully-trained service and technical specialists. They can supply answers to questions about the system or any technical issues that might occur. For more information, go to the SCIEX website at sciex.com or use one of the following links to contact us.

- sciex.com/contact-us
- sciex.com/request-support

Cybersecurity

For the latest guidance on cybersecurity for SCIEX products, visit sciex.com/productsecurity.

Documentation

This version of the document supersedes all of the previous versions of this document.

To see this document electronically, Adobe Acrobat Reader is required. To download the latest version, go to https://get.adobe.com/reader.

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 documentation that comes with the system or component.

The latest versions of the documentation are available on the SCIEX website, at sciex.com/customer-documents.

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