Analyst 1.7.3 Software

Release Notes

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Introduction 1

Thank you for choosing SCIEX to supply your LC-MS/MS system. We are pleased to give you the Analyst 1.7.3 software, which provides liquid chromatography-tandem mass spectrometry (LC-MS/MS) functions.

The *Release Notes* describe the features in the Analyst 1.7.3 software as well as troubleshooting guidelines. Use these release notes for reference as you become familiar with the software, and for future reference. For installation and software compatibility information, refer to the document: *Software Installation Guide*.

Note: The Analyst 1.7.3 software is only supported on the Windows 10 operating system.

How to Use These Release Notes

To help you understand what is new and what is fixed relative to your current Analyst software version, the *Release Notes* for the Analyst 1.7.3 software have been structured so that you only have to read the sections that are relevant to you.

Everyone should read Notes on Use, as this section applies specifically to issues that are known in the Analyst 1.7.3 software.

Note: To view the enhancements, fixed issues, and known issues for previous versions of the Analyst software, refer to the document: *Release Notes* for previous versions.

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

New in Version 1.7.3 $\qquad$ 2

This section describes the enhancements and fixes in the Analyst 1.7.3 software. To view the enhancements and fixes for the previous releases of the Analyst software, refer to the document: *Release Notes* that came with that version of the software.

New Features and Enhancements in Version 1.7.3

The following features and enhancements are available.

Storage of LC auxiliary traces with the datafiles for faster troubleshooting

The auxiliary traces, including the pressure trace, if enabled, are stored with the acquired data files for the ExionLC, ExionLC 2.0, Shimadzu LC-20, and Shimadzu LC-30 system controlled in either of the Integrated System Shimadzu LC Controller or the Integrated System Shimadzu LC-20/30 Controller, and the Shimadzu LC-40 system. Refer to the document: *Laboratory Director's Guide* that comes installed with the software.

A new injection counter feature

The injection counter feature was implemented for proactive column maintenance to prevent a batch stop. Refer to the document: *Laboratory Director's Guide* that comes installed with the software.

Note: This feature is not supported when samples are submitted from the MPX software. Do not enable the injection counter if the MPX software is used.

Support for software installation with a deployment tool, such as MECM, using a non-administrator account

Support for software installation with a deployment tool, such as Microsoft Endpoint Configuration Manager (MECM), using a non-administrator SYSTEM account to push software installation remotely and securely.

Support for saving the ExionLC and Shimadzu LC configuration with each individual hardware profile

For a hardware profile created in version 1.7.3 or later, the LC configuration is saved within each hardware profile for all of the devices controlled by the MIMIC2 driver so that each hardware profile can have a different LC configuration. This includes the ExionLC, Shimadzu LC-20, and Shimadzu LC-30 systems configured with the Integrated System Shimadzu LC-20/30 Controller, and Shimadzu LC-40 systems. The user does not need to reconfigure the LC when switching

between hardware profiles that include different LC configurations using one of these LC systems.

Support for quantitation of UV and DAD/PDA data in the same Results Table

Support for individual valve control and additional valve configurations for ExionLC 2.0 systems

Support has been added for individual valve control and the use of any combination of the following two valves for ExionLC 2.0 systems, either two of the same valve or one of each:

•   2-position 6-port valve drive

•   8-position 9-port valve drive

Merging of the ADD and Analyst software autosampler databases during installation of the Analyst software

The Analyst Device Driver (ADD) autosampler database is merged with the Analyst software autosampler database during the Analyst 1.7.3 software installation. This avoids the need to reinstall the ADD 1.3 software after the Analyst software version upgrade.

Support for the Keystone software

The Analyst 1.7.3 software added support for wiff file conversion with the Keystone Converter software.

Note: This support was first added in the **Analyst 1.7.2 Patch for Keystone Software**. (AN-2198)

Support for a new plate layout for the Shimadzu SIL-30ACMP and Shimadzu SIL-30AC autosamplers configured through the Integrated System Shimadzu LC Controller

The 96 deep well plate layout with alphanumeric numbering starting from the bottom left of the plate, horizontally, is supported. Refer to the figure: Figure 2-1. The following are applicable when this new plate is selected for the Shimadzu SIL-30ACMP or Shimadzu SIL-30AC autosampler:

•   The locations in the Batch Editor are assigned numeric values, arranged horizontally.

•   The Batch Editor supports the fill down feature.

•   The Batch Editor can export to txt and csv files.

•   The Batch Editor can import from txt and csv files.

Figure 2-1 Batch Editor: Locations Tab
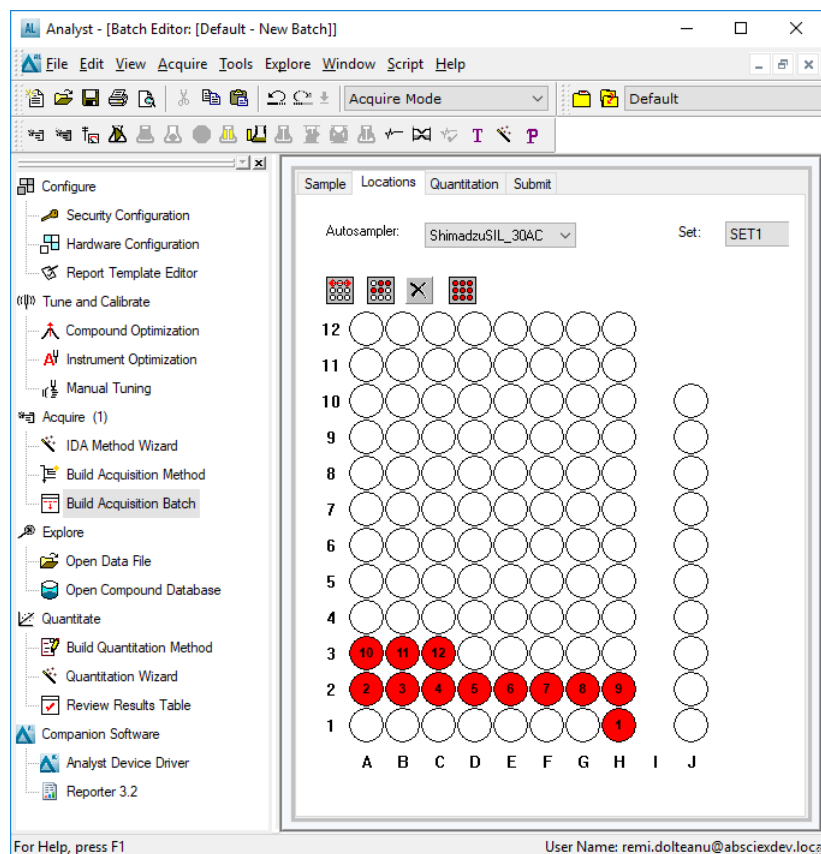
Note: This support was first added in the **Analyst 1.7.2 Patch for Shimadzu LC30 Plate Layout**. (AN-1571)

Fixed Issues in Version 1.7.3

The following issues have been fixed in this release:

A chromatogram might have been missing in the report when Microsoft 365 Apps instead of Office 365 was installed

After Office 365 was updated to MS 365 Apps by Windows, the chromatogram of the internal standard for one of the samples might have been missing in the generated Analyst report. (AN-2540)

When solvent level parameters were changed, the status was not updated immediately

After changing any parameter in the solvent levels panel, wait five seconds for the updated parameters to be shown in the status window or to change any parameter again. (AN-2038)

The Quantitation audit trail incorrectly added the word Samples to the change descriptions

In the Quantitation audit trail, the word "Samples" was incorrectly added before the text, "The concentration/calculated concentration units were changed to…" in the **Change Description** when the concentration or calculated concentration units were changed for either the analyte or internal standard. (AN-430, AN-2259)

Starting batch acquisition after equilibration but before an ExionLC or Shimadzu LC column oven temperature had reached the setpoint prevented the acquisition from starting

If an acquisition method containing an ExionLC or Shimadzu LC column oven was used to equilibrate the system, and the column oven temperature had not reached the setpoint, then selecting **Start Sample** in the toolbar prevented the batch acquisition from starting. (AN-1670)

Using special characters such as a period in file names could cause the file to be corrupted

Special characters such as a period could not be used in file names. For example, `tes.t` could not be used for a Results Table file name. Using a special character in a file name might corrupt the file. (AN-1697)

The time stamp for a quantitation method was updated when the method was opened

If a quantitation method was opened and then closed without saving any changes, the time stamp of the quantitation method was changed to the time when the method was opened. (AN-1715)

The Analyst software closed when an IDA data file was printed from the IDA Viewer with a mass selected

After an IDA data file was opened in IDA Viewer, selecting the checkbox for one of the masses under the Mass List and then printing this view caused the Analyst software to close. (AN-1716)

Deactivating a hardware profile containing a Shimadzu LC-40 system caused the autosampler and the platechanger to stop cooling

If the **Cooler temperature** option was selected for use before a hardware profile containing a Shimadzu LC-40 system was deactivated, then deactivating the hardware profile caused the Shimadzu autosampler and the platechanger, if included, to stop cooling. (AN-2092)

New in Version 1.7.3

The Analyst software might stop responding if too many samples were removed at the same time from a Results Table

After a Results Table was created, removing 35 or more samples at a time from the Results Table might cause the Analyst software to stop responding. (AN-1527)

Vial position 96 did not seem to be selected in the batch Locations tab for MTP96, MTP384, DWP96, or DWP384 wellplate for the Shimadzu LC-40 system

When vial position 96 was selected in the Locations tab in the batch editor by using a MTP96, MTP384, DWP96, or DWP384 wellplate for the Shimadzu LC-40 system, the position 96 did not turn red. This gave the user an impression that it was not selected, even though the vial position 96 was picked up by the software in the Sample tab for that sample. (AN-2169)

PDA in 2D/signal mode is now supported for ExionLC or Shimadzu LC systems

Because of a signal out-of-sync issue, PDA in 2D/signal mode was not supported for ExionLC or Shimadzu LC systems in the Analyst software version 1.7.2. As of Analyst software version 1.7.3, the PDA in 2D/signal mode is supported by using an updated version of the LC driver. (AN-1794)

The Full User Name field in the Audit Trail might be empty when there was a drop in network connection.

Intermittently, the **Full User Name** field in the Audit Trail was empty when there was a drop in the network connection. (AN-1643)

RT=0 was incorrectly included in sMRM method validation when Scheduled Ionization was turned ON

When a *Scheduled* MRM algorithm workflow method (sMRM method) contained transitions with a retention time of zero and scheduled ionization was used, an incorrect warning message indicating that RT=0 was smaller than the **Scheduled Ionization Start Time** was shown when the method was saved. This message could be ignored. When the user clicked **OK** to dismiss the message, the method was saved and could be used. (AN-1766)

For ExionLC system devices, the batch was suspended when a vial was missing even if the queue option Fail whole batch in case of missing vial was not selected

When a batch that contained a sample whose vial location was missing a vial was submitted and if the Queue option **Fail whole batch in case of missing vial** was not selected, then the sample experienced an acquisition error and the rest of the samples in the batch were suspended. (AN-965)

The issue fixed in the Analyst 1.7.2 Patch for Calculated Concentration Reporting is included in the Analyst 1.7.3 software:

If the value of the **Calculated Concentration** column in a Results Table was a non-numeric value, such as **no intercept**, then the calculated concentration shown in the generated report was always **N/A**. When this patch is installed, the calculated concentration shown in the generated report is the same as the content of the **Calculated Concentration** column in the Results Table. (AN-2154)

The issues fixed in the Analyst 1.7.2 Patch for Full User Name (Rev.2) are included in the Analyst 1.7.3 software:

*   Only the last name of the user was shown instead of the full name in the **Full User Name** field of the audit trail. Reports created with a report template also showed only the last name in the **Operator** field (if used). (AN-2221)

*   If the full name of the user in the Windows Server Active Directory was longer than 31 characters, then the **Full User Name** shown in the audit trail or in reports could be shown with invalid characters. This issue only occurred in the first release of the Analyst 1.7.2 Patch for Full User Name. (AN-2407)

*   In Mixed Mode, the dialog to unlock the screen allowed the user to select a domain from a list, and the list was not always complete. Now, the **User Name** field accepts the user name in both Security Account Manager (SAM) and User Principle Name (UPN) formats. (AN-2187)

*   In Mixed Mode, users were unable to unlock the screen if their passwords were more than 13 characters long. Passwords up to 20 characters long are now supported. (AN-1194)

The issue fixed in the Analyst 1.7.2 HotFix 3 is merged in the Analyst 1.7.3 software:

The acquisition method may have been overwritten when the LC method information was saved in ADD or any applicable AAO program even if the user did not have Delete or Modify permission

If the Analyst logon user did not have **Delete** or **Modify** rights to the network root directory, and if the user had a role with **Overwrite acquisition methods** disabled, then when LC method information was saved for the second time in Analyst Device Driver (ADD) or another AAO application, the software overwrote the acquisition method instead of creating a new acquisition method. The same issue could occur on a local root directory in a non-standard workflow, if the Analyst software was configured for Mixed Mode and the user logged on to the Analyst software was changed to a user with limited rights while ADD was left open. (AN-2577)

Notes on Use 3

The following is a list of known issues, limitations, and important notes on using the software. There might be other issues or limitations with the Analyst software in addition to those listed in this section. If you find additional issues, contact SCIEX at sciex.com/request-support.

In general, if the Analyst software is not responding, then restarting the software might help. If this does not work, then restart the computer to make sure that the AnalystService and device drivers restart.

Guidance for Antivirus and Backup Software

Many widely-used applications can be configured to either disable real-time protection or ignore certain file types (for example, rdb, wiff, and wiff.scan). Failure to configure them in this way might result in either failed acquisitions or acquisitions that take longer to complete than expected.

In general, the antivirus or backup software on the Analyst software acquisition workstations should be configured in a manner that disables real-time scanning and archiving of files in the `Analyst Data` folder. For more information, refer to the section: CyberSecurity.

Exclude the following list of programs from consideration by real-time scanning:

- `C:\Program Files(x86)\Analyst`

- `D:\Analyst Data`

If the Agilent Infinity II, CTC PAL3, and the associated Device Driver for the Analyst software is used:

- `C:\Program Files (x86)\AB SCIEX\AnalystDeviceDriver`

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

Guidance on File Encryption

When using software to encrypt the contents of your hard drive, make sure that the `Analyst Data` folder is not encrypted. Encrypting this folder might result in failed acquisitions or corrupted data files.

Notes on Use

It is recommended that the computer be restarted at least once a week.

- As of Analyst 1.7.3, the About Analyst dialog has been changed to include the software version information in the following format, without a build number:

  - Analyst Software

  - Published Version: 1.7

  - Full Version: 1.7.3 (1.7.3 HotFix 1, if there is a HotFix 1 installed)

- Do not add or delete the Analyst software files with File Explorer. Such an event is not audited by Analyst Audit Trail. (AN-967)

- If the Analyst Administrator Console (AAC) is used, then make sure that only one root directory is added for all the projects within the same workgroup. If more than one root directory is used for the projects within the same workgroup, then users who logged on to Analyst through the AAC can only access the root directory that was first added to the AAC. (AN-2565)

- When a user who has no rights to overwrite a method or a batch file tries to overwrite a file, then a new instance of the file is created using the same file name with a number added to the end of the file name. (AN-2688)

- To import a batch file into the Analyst batch editor, make sure that the number of columns is 255 or fewer. The number of characters per data line must also be no more than 2000 for the imported text file. (AN-1146)

- Do not create a project with the name `API Instrument` on a network root directory. Doing so causes instrument audit trail events to be recorded in the API Instrument project on the network instead of the local API Instrument project. (AN-2290)

- The special characters $ and % are not supported in the Analyst software for user names. Avoid using these special characters in user names. (AN-2369)

- The Analyst software only supports up to 5 channels, including the reference channel, if selected, for a 2D or Signal Data mode acquisition using a Shimadzu PDA or an Agilent DAD. (AN-1796)

- For acquisition using a Shimadzu or ExionLC PDA or an ExionLC 2.0 DAD, the Analyst software data stores either 2D data or 3D data depending on whether 3D is selected in the acquisition method. If 3D is selected, then only 3D data is stored in the data, even if 2D is also selected in the method. (AN-1148)

- The Q1 and Q3 masses for the MRM transitions in the quantitation method must be the same as those in the acquisition method. A wrong transition might be processed for an analyte if the data file is processed using a quantitation method that was created using a representative sample acquired with a slightly different acquisition method than the one used to acquire the data file being processed. For example, this would happen if a specific transition is slightly different in the quantitation method than in the acquisition method, and if another transition in the acquisition method is almost the same as this transition in the quantitation method. (AN-2131, AN-2314)

Notes on Use

- If a platechanger is configured with a Shimadzu LC-40 autosampler, then the 3-plate rack and the platechanger cannot be both selected in the **Rack Code** column for different samples in the same batch. When creating a batch, either use Plate Position 1, 2, or both in the 3-plate rack, or only the plates in the platechanger. (AN-2074)

- The root directory must follow the Universal Naming Convention (UNC) format: `\\<computer name>\<drive name>`. Mapped drives are converted automatically to full UNC paths. Full network path lengths must be limited to 128 characters.

- The default **CUR** setting has been changed to 35 for the SCIEX 3500, 4500, 5500, 5500+, 6500, and 6500+ systems, for all ion sources, to decrease the risk of instrument contamination.

- Starting from Analyst 1.7.3, the *Getting Started Guide* is now called the *Analyst Software User Guide*.

- Do not use the Analyst software to process SCIEX 7500 system data currently being acquired in the SCIEX OS software.

- If the Analyst software Quantitation Wizard is used to process data acquired by SCIEX OS with a version earlier than 2.1 using a PDA/DAD detector in 2D/Signal Mode, a UV detector, or a Fluorescence detector, then the first five channels can only be integrated as DAD data, and the rest can only be integrated as UV data, regardless of the detectors used for acquisition. However, if the signal mode data was acquired using SCIEX OS version 2.1 or later, then the data is processed as UV data in the Analyst software Quantitation Wizard, regardless of the detector type. This is because of a design change to the way signal mode data is written in SCIEX OS. SCIEX OS can acquire up to 8 channels of signal mode data to a .wiff file that the Analyst software can process.

- Do not start Analyst file names with "-" or any other special characters. This includes, but is not limited to, data files, method files, and Results Table files. It's highly recommended to start the file name with an alphanumeric character. (AN-2430)

- In the Analyst 1.7.1 HotFix 1 and in earlier versions, the audit trail **Full User Name** column showed the **Display Name** of the user account as stored in the Windows Server Active Directory. In the Analyst 1.7.1 Patch for RODC Network, Analyst 1.7.2, and later versions, the audit trail **Full User Name** column shows the **Full Name** of the user account, as stored in the Windows Server Active Directory. The **Display Name** and **Full Name** of the user account are typically the same, but they do not have to be. The network administrator can make them distinct. (AN-2447)

- Each acqustion method is specific for each hardware profile.

  - If a user edits the hardware profile containing a Shimadzu LC-20 series autosampler and clears the **Rinse Pump Installed** check box, then the acquisition methods created with one of these rinse mode options (before aspiration, after aspiration, before and after aspiration) using the original hardware profile must be saved again after the hardware profile activated. (AN-1143)

- If a user edits the hardware profile for a specific LC configuration setting, for example, the Solvent Valve for an ExionLC pump, then the acquisition methods created with the original hardware profile must be saved again after the edited hardware profile is activated. In addition, the LC hardware setting must match what's selected in the hardware profile. If a method created with the original hardware profile LC setting was used for acquisition under the current modified hardware profile LC setting, then the original hardware profile LC setting might be used for data acquisition using this method, depending on the LC hardware setting. This is because the hardware profile LC setting is saved in the acquisition method even though that setting is not part of the method editor. (AN-2455)

- Internal rinsing in a Shimadzu LC system, controlled through the Integrated System Shimadzu LC Controller, didn't work properly in Analyst 1.6.3 and earlier versions. The defect was fixed in Analyst 1.7 and later versions. Expect retention time shifts if an internal rinsing mode is used for the acquisition methods when they are used in Analyst versions before and after the fix.

- If the stop time in the Analyst Device Driver (ADD) method is different than the MS stop time, then the time option for **StopTime** must be selected and the desired stop time entered. Do not use the default option, **As Injector/No Limit**, even if the gradient is defined in the **Timetable**. Otherwise, the LC controlled by ADD stops running the LC method at the MS stop time. (AN-2586)

- The Analyst software and the Analyst Administrator Console (AAC) do not support cross-domain login. The Analyst software computer, the AAC computer, and the network users should be on the same network domain.

- The following notes are applicable to ExionLC 2.0 systems:

  - If a cool oven temperature is used, setpoint of 5.5 °C is recommended as the lowest temperature. Do not use the lower safety limit, 5.0 °C, for a set point, because fluctuation to anything below 5.0 °C will cause a column oven error. The same applies to the upper limit. Use a set point lower than the upper safety limit, such as 84.5 °C or lower, to prevent a column oven error.

  - Make sure that the detector lamps are on and ready before starting acquisition.

  - If solvent level monitoring is used in the LC Integrated System Detailed Status window, then make sure that the current volume is correct before each batch acquisition.

  - When loading the sample trays, make sure to follow the plate layout in the software, or refer to the document: *ExionLC 2.0 Hardware User Guide*.

  - If samples are acquired to the same data file using a method containing a ExionLC 2.0 system diode array detector (DAD) in a 3D data mode with a high sampling rate, then delays in completing the sample acquisition might be observed while the data file size increases. This is because the Analyst software tries to collect all of the data points from the LC driver. As a result, the sample acquisition might seem to take much longer than the method run time. However, the data is for the correct run duration. To avoid delays

between samples caused by the transfer of a large number of data points, acquire each sample to a separate data file.

- When creating an LC method for a system with a DAD, make sure that the wavelength defined for each channel and each row in the Wavelength program for the 2D data mode is within the Wavelength range defined for the 3D data mode, even if the 3D data mode is not selected. For an example error message that is shown when an invalid method is saved, refer to the figure: Figure 3-1. The Row number refers to the row in the Wavelength program.

Figure 3-1 Invalid ExionLC 2.0 DAD Method Error Message
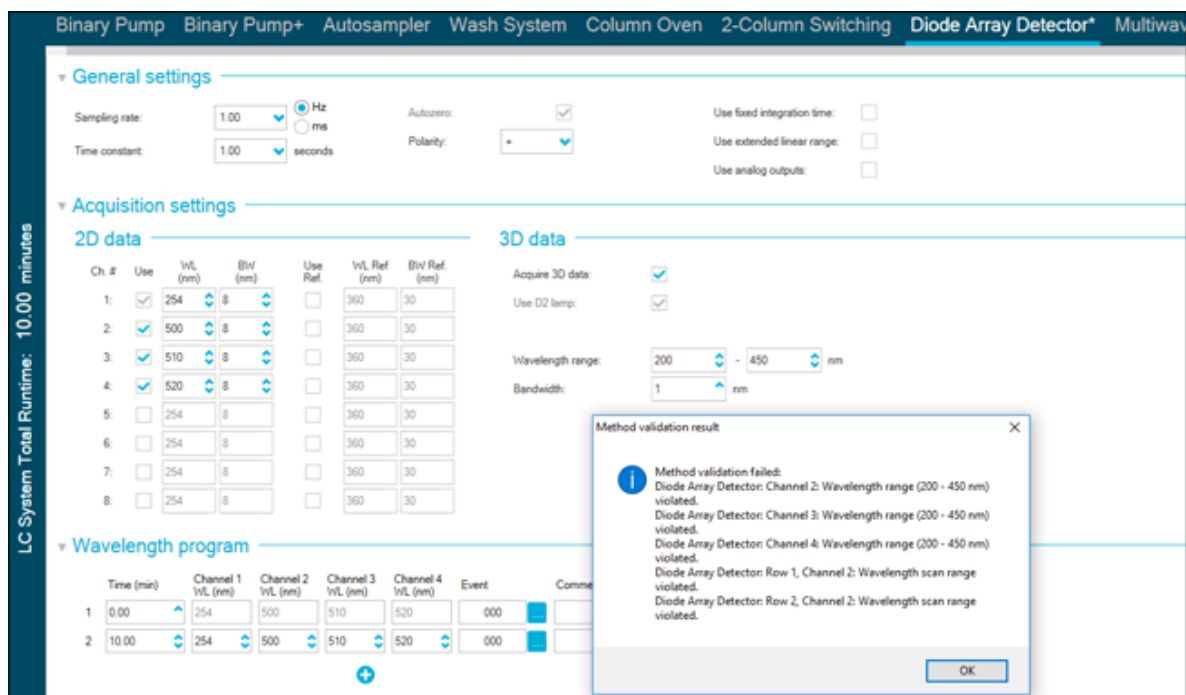
- In cases where the computer is shut down or restarted unexpectedly while the hardware profile is active, the ExionLC 2.0 system might lose communication with the computer. Turn all of the ExionLC 2.0 system modules off and on to detect them again. (AN-1988)

- If any of the ExionLC 2.0 system modules goes into an error state because of an issue requiring no physical fix, then the Standby button ( ) from the LC Integrated System Detailed Status window can be used to clear the error. Use this button to turn the LC modules off and then on again. However, a hardware profile deactivation and activation are still required. In rare cases, if this recovery approach does not work, then deactivate the hardware profile, turn off the computer, turn all of the LC modules off and then on, and then turn on the computer again.

- If a batch contains an LC method with the pretreatment option set to **Use first destination vial**, then before the batch is run again or the same LC method is used in another batch, the first destination vial position must be reset. It is automatically reset when the system state changes to Standby and when the hardware profile is deactivated and activated. The user can also reset the first destination vial position in the following ways:

1. Click **Reset vials** (⚙) in the Autosampler pane of the LC Integrated System Detailed Status window. Then select **Reset destination vials**.

2. Submit a batch containing a single sample that uses a different first destination vial position.

   If **Use first destination vial** (FDV) is selected for pretreatment, then make sure that the last destination vial position (LDV) is valid for the rack type selected and the number of samples (n) to be included in the batch. Otherwise, batch acquisition will stop on the sample with an invalid destination vial number. The destination vial position is always equal to the destination vial position of the preceding sample, plus 1.

   For samples 1, 2, 3, and 4, respectively, the destination vial positions will be FDV, FDV+1, FDV+2, and FDV+3. If the number of samples to be included in the batch is 30, with vial positions 11 to 40, and FDV is 51 on a 2 × 48 vial rack, then the LDV = FDV + n − 1 = 51 + 30 − 1 = 80.

   Note: Make sure that a vial is present in every projected destination vial position.

- The detector lamp in an ExionLC 2.0 DAD or multiwavelength detector stays on if the system is left in **Idle** state after the hardware profile is activated and the system is not equilibrated or a batch is not acquired. To extend the detector lamp life time, do not leave the system idle for a long time immediately after activating the hardware profile. Either equilibrate the system or put the system in **Ready** state, and then let the system go to **Standby** state manually or automatically. (AN-2202)

- For network acquisition, use a Special Acquisition Administrator Account to avoid network-related acquisition issues. For information about a Special Acquisition Administrator Account, refer to *Select an Acquisition Account Mode* in the document: *Help* or the document: *Laboratory Director Guide*

- If a plate changer is installed with a Shimadzu LC-40 autosampler, then make sure that **Plate # 3** is not selected on the **3-Plate Rack** when saving and submitting a batch in one of the following ways:

  - Through the Analyst software

  - Through a vertical application

  - When scripting through the Analyst Access Object (AAO)

Notes on Use

This plate position is reserved for moving a sample tray from a plate changer to the autosampler for sample injection and cannot be used for this configuration. (AN-1780)

- If a different LC stack than the one that was previously configured is going to be used with the mass spectrometer, then the user must complete LC auto-configuration again to activate a hardware profile containing the different LC, even when a previously created hardware profile is used. This issue occurs when the user switches between LC devices that are controlled by the Shimadzu MIMIC 2 driver on the same mass spectrometer. The LC devices using the MIMIC 2 driver include the Shimadzu LC-20/30 systems, activated through the Integrated System Shimadzu LC-20/30 Controller, the Shimadzu LC-40 system, and the ExionLC systems. (AN-1826)

Changes to Instrument Optimization

- As of Analyst software version 1.7.1, the results file for the Instrument Optimization results summary is changed to PDF format.

- As of Analyst software version 1.7.1, Instrument Optimization requires Microsoft Word 2013 or 2016 or Office 365 to be installed.

- Do not create customized csv files in the `D:\Analyst Data\Projects\API Instrument\Instrument Optimization\Settings` folder. In this folder, only the files installed by the Analyst software are supported. (AN-1551)

Auditing

- In the Audit Map Settings for the Instrument Audit Trail, the following events, even if they are selected in the **Audited** column, are not used to audit the Resolution Table or Calibration Table related events in the Analyst software:

  - Resolution Table(s) replaced

  - Resolution Table added

  - Mass Calibration Table and Resolution Table changed

  Instead, the following four events are used for auditing the events of adding or changing the Resolution or Calibration Tables:

  - Resolution Tables replaced - No Prompt (This event is used to audit Resolution Table changes using any method and to audit the printing of the Resolution Table)

  - Mass Calibration Tables replaced (This event is used to audit Calibration Table changes made ONLY in the editor and to audit the printing of the Calibration Table)

  - Mass Calibration Table added (This event is used to audit when a new Calibration Table is created)

  - Mass Calibration Tables replaced - No Prompt (This event is used to audit the Calibration Table changes made through all the other methods other than those previously stated)

Therefore, the use of the Full Audit Map for the Instrument Audit Trail, whether or not the Full Audit Map triggers an E-signature for the Calibration Table change, depends on how the changes were made, that is, in the Instrument Data Editor, by Instrument Optimization, through the Analyst Access Object (AAO), or in the advanced calibration table. A change to the Resolution Table, however, does not trigger an E-signature.

- Make sure that there is sufficient empty space in the `C:\` drive for the Analyst software audit trail to function correctly. If the drive is full, then the audit trail might show 0 records, depending on the audit trail (atd) file size. If the `C:\` drive becomes full, free up some space, and then the audit trail will show all of the records. (AN-1722)

- The data file components, wiff and wiff.scan, must have the same name. If one of the component names is changed, then the Audit Trail cannot record the event correctly when the user attempts to open the data file. In addition, the data file cannot be viewed properly if the names do not match. (AN-1370)

- On a computer configured with the Windows 10 operating system, if the user who logs on to the Analyst software in Mixed Mode is a different user than the user who is logged on to the computer, then the Audit Trail record printing function is not available. The Windows 10 component that the Analyst software uses to print has a known limitation that prevents different users from doing so. In addition, opening the Analyst software as a different user in Integrated Mode or Single User Mode is not supported. (AN-1358)

- **The audit map for a Results Table has a different Modified date and time than the Modified date and time shown under the Projects node or in a Windows folder**

   In the Audit Trail Manager, the audit map associated with a Results Table (accessed under the Results Tables node) might have a different **Modified** date and time from its **Modified** date and time shown with the project node (accessed under the Projects node) or in a Windows folder. This can happen with Results Tables created with the factory-installed audit maps (cam files in the `Project Information` subfolder). To resolve this difference, in the Audit Trail Manager, select a project under the Projects node and then open the Settings tab. Select each factory installed audit map and then click **Save**. From this point on, the audit map dates and times for Results Tables created with the audit maps will match the dates and times shown with the project node.

   This issue will only occur if an existing `Analyst Data` folder was used to upgrade to Analyst 1.7 with HotFix 1, and then upgrade to a later version, or to directly upgrade to the Analyst 1.7.1 software or a later version from the Analyst 1.6.3 software.

Use the DT parameter to control the temperature

If a NanoSpray or OptiFlow Turbo V ion source with a Nano probe installed is used in conjunction with the SelexION/SelexION+ device, then leave the IHT at its default value. Do not change the IHT setting. The DT parameter should be used to control the temperature.

The Review option is not supported when the Results Table uses these certain layouts

Notes on Use

When an internal standard is re-integrated, the Review button in the History column for the audit record for that operation is not available. This feature has been disabled. The Review option is not supported when the Results Table uses these layouts: Summary, Analyst Group, Sample Type. A message is shown prompting the user to switch to either Full Layout or Analyte Layout for the analyte of interest. The Review option is also not supported if Peak Review is configured to review internal standards before all analytes. In this case, Peak Review shows the internal standard chromatogram and not the analyte chromatogram being reviewed. In the Peak Review Options, use either **Don't review internal standards** or **Review with each analyte**. (AN-1103)

Delay Time does not function correctly in a multi-period method

When using the Delay Time option for the first period in a multi-period method, the periods after the first one finish prematurely. Do not use the Delay Time option for an MRM method, especially for multi-period methods. To achieve the same goal, an MRM or *Scheduled* MRM algorithm method with Scheduled Ionization can be used. (AN-1394)

Domain field is not available in the Analyst - Logon Information dialog

The **Domain** field has been removed from the Analyst - Logon Information dialog if the software is configured to use Mixed mode security. The **Domain** field is only available if the Analyst Administrator Console (AAC) is used. The user name field can be in SAM (`domain\username`) or UPN (`username@domain.com`) format. (AN-1564)

The Settling Time field for *Scheduled* MRM algorithm experiments is disabled for all mass spectrometer models except for SCIEX 5500+ and 6500+ systems

As of Analyst 1.7 and Analyst 1.7.1, the Settling Time field for *Scheduled* MRM algorithm experiments has been disabled for all mass spectrometer models except for SCIEX 5500+ and 6500+ systems. For other mass spectrometer models, the values being used are defined in the software and not in the Method Editor user interface. (AN-1037)

Do not modify the computer date and time after the Analyst software is installed

For both node-locked and server-based licensing, make sure that the computer date and time are correct on both the client computer and the server before installing the Analyst software. After the Analyst software is installed, manually changing the date and time might invalidate the license and cause users to be unable to log into the Analyst software.

Delay Time behavior in an MRM scan is different than in a *Scheduled* MRM algorithm scan

For a period that contains dynamic scans such as a *Scheduled* MRM algorithm experiment, a scan using DFT, or IDA experiments, the delay time should be less than the period duration. The MS acquisition duration is the **Duration** minus the **Delay Time** in minutes, and the MS period duration is the **Duration**. For a period that contains only non-dynamic scans, such as one or more MRM experiments that are not looped with a *Scheduled* MRM algorithm or a scan using DFT or an IDA criteria, the MS acquisition duration is the **Duration**, and the MS period duration is the **Duration** plus the **Delay Time** in minutes.

LC Help and Analyst software *Help*

If an LC *Help* file is open is open, then opening the Analyst *Help* automatically closes the LC *Help* file. If both *Help* files must to be open, then open the LC *Help* file after opening the Analyst *Help* file.

Convert Methods Script

Converting methods from High Mass mode to Low Mass mode is not supported. Users also cannot convert a method with a mass above the mass range limit of the mass spectrometer in the active hardware profile.

The Analyst software starts acquiring without waiting for the column oven temperature to reach the set temperature

When an ExionLC column oven is used in the acquisition method, then the Analyst software will start acquiring without waiting for the column oven temperature to reach the set temperature if the **Wait for temperature equilibration before run** checkbox is selected and the **WAIT TIME** is set to 0 on for the column oven.

If the **WAIT TIME** for the column oven is manually set to 0, then make sure to equilibrate the system and wait for 10 minutes 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 the **Wait for temperature equilibration before run** checkbox for the acquisition method. In this case, the software will wait for the **WAIT TIME** after the column oven temperature has reached the set temperature before the injection.

For ExionLC system methods, the default pump stop time is longer than the default MS stop time

When the ExionLC pump is being used and an acquisition method is created in the Analyst software, the ExionLC pump has a default Stop Time of 10 minutes and the Analyst software MS method is 5 minutes. The ExionLC method stop time should be adjusted to be appropriate for the MS method. To avoid any issues, use a method with an LC run time equal to or slightly longer than the MS method.

ExionLC devices that are started manually must be manually stopped

If the user manually starts an ExionLC pump or an ExionLC column oven from the Sciex LC

Controller status dialog by double-clicking on the Status bar in the Analyst software, then these devices stay on even after the hardware profile containing these devices is deactivated. The user might think that the devices are turned off. This could lead to the mobile phase running out and the column being dried out. If the ExionLC devices are started manually, then they must be turned off manually.

The ExionLC 100 system is turned off when it is put in the standby mode

Notes on Use

The ExionLC 100 system turns off when the Analyst software puts the ExionLC devices in standby mode either when the user clicks the **Standby** button or after the batch finished and reached the idle time specified in the Queue Options. This happens only with ExionLC 100 system. The hardware profile might still be activated during this time. To start the ExionLC 100 system, manually turn on the system again either from the Sciex LC Controller status dialog or from the LC system front panel.

Known Issues   4

This section describes the known issues in the Analyst 1.7.3 software.

Audit Trail

The Administrator Console Audit Trail records the user log on event on the AAC server, but the corresponding log off event is missing

In an Analyst Administrator Console (AAC) environment, the Administrator Console Audit Trail creates an event record when a user logs on the AAC software on an AAC server, but might not create an event record when a user logs off or closes the AAC software, depending on which node was selected in the left pane before the user exits or closes the program. (AN-1674)

Instrument Audit Trail records NA in the User Name column for the Queue event when batches are moved

The Instrument Audit Trail records NA for the user who moved the batches in the queue. To identify who moved the batches, search for the user name for the latest Security event with the **Change Description** "User successfully logged in", before the Queue event when batches were moved in the Instrument Audit Trail. (AN-1347)

The audit trail time stamp for the Results Table changes when the computer time is changed

When the computer time is changed, the audit trail time stamp for a Results Table reflects the change. However, the Project audit trail stays the same. (AN-746)

Audit maps and QuantSettings.sdb might get overwritten during a fresh installation

Audit maps and QuantSettings.sdb are overwritten during a fresh installation of the Analyst 1.7 Software with HotFix 1, or a later version, using an existing Analyst Data folder. This happens if the time stamp of these files is before the time stamp of the factory shipped files. (AN-1101)

The audit trail wrongly records that the Analyst Classic algorithm parameters changed when in fact the MQ III algorithm parameters changed

When the MQ III algorithm is used for processing data, the audit trail wrongly records that Analyst Classic algorithm parameters, such as Area threshold and Noise threshold, were changed. This does not affect the data in any way. MQ III was used to process the data. (AN-403)

Known Issues

Analyst software use in an RDP (Remote Desktop Protocol) environment (that is Citrix)

Accessing the Analyst software using RDP is not recommended. Users who access the Analyst software using RDP are logged in the Analyst software audit trail. The logons of users at a workstation that is running RDP are recorded in the audit trail using the credentials of the first user.

Special characters fix

Although audit trail entries occurring after the installation of the Analyst 1.5 software appear properly, this release does not address those entries made by prior versions of the Analyst software. In some instances, records containing certain special characters not used in the English language (for example, é, ö) are not visible in the audit trail. However, they can still be retrieved by searching or filtering the audit trail by date. (ST 14394)

Some specific special characters might not be shown properly following the installation of the Analyst software. Audit trail records are shown correctly, but these special characters are shown differently in the record. (ST 14394)

For example:

Д is shown as a box

Ň is shown as a G

β is shown as a superscript z

Avoid using the preceding characters in the audit trail.

Wrong audit trail information with manual integration

The information in the audit trail is incorrect when the user chooses to revert to the manual integration results (that is, when **Reject Manual Integration** is configured). The audit trail record shows the **Change Reason** and **E-signature** even though they are not configured. (SCR 13761)

Audit events are cleared unexpectedly

In the Audit Map Editor dialog, if the user right-clicks the **Audited** column and then clicks **Fill Down**, the **Project Settings Have Been Changed** and **Instrument Settings Have Been Changed Events** check boxes might be cleared. Do not use **Fill Down** over these events. (SCR 14266)

Closing the IDA file is not logged as an event in the audit trail

If IDA data file is closed, then the event is not logged in the audit trail. (ST 9487)

The Analyst software stops responding when performing print preview

If the user selects to print preview an audit trail that has more than 100 records using the **All Pages** menu option (right-click), then the Analyst software might stop responding. The user can preview one page at a time using the **Current Page** menu option instead. (ST 4284)

Audit trail printout columns are truncated

When the user prints the audit trail in both Portrait and Landscape modes, some columns might be truncated. In some cases, this issue might be minimized by printing in Landscape mode. (ST 2261)

The wrong module is recorded in the audit trail

When the user changes a Quantitation algorithm to another algorithm, the audit trail incorrectly records the module name as "Build Acquisition Method". (ST 4922)

An error occurs during printing of a large audit trail

Printing the audit trail from the active Results Table (**Tools** > **Audit Trail** > **Show**) might cause an error if there are more entries in the audit trail than can be printed on a single page. Print audit trails only from within the Audit Trail Manager (Menu Bar: **View** > **Audit Trail Manager**). (ST 6374)

Network time is used for audit events on a network server

When writing audit events to a project residing on a network file server, the audit information uses the network server clock time instead of the local computer time. This is expected behavior. (SCR 12390)

Configure — Administration/Security

A user logging on to a computer or the Analyst software for the first time might encounter an error when submitting a batch

When User Account Control (UAC) Settings is set to **Notify me only when apps try to make changes to my computer** or a higher level, and a user who is in the Analyst security database but has never logged on to this computer before tries to log in to the Analyst software for the first time, then a UAC dialog opens to ask permission to enter data in the User registry for the new user. Click **Yes** to continue. However, the project drop-down menu might appear empty, and the user might encounter an error when trying to submit a batch. If this error occurs, close the Analyst software, and then start the Analyst software again. (AN-2671)

The software window might resize upon activating a hardware profile with an LC system

When using a high-resolution monitor, the software window might resize upon activating a hardware profile with an LC system. This might affect viewing the LC detailed status information and LC method content in the Method Editor. Should this issue occur, change the monitor resolution to a lower setting In most cases, dropping the resolution to 2048 x 1152 or 1920 x 1080 can resolve this issue. For SCIEX provided monitors, the recommended resolution is 1920 x 1080. (AN-2699)

The Analyst software toolbar might not refresh properly on the Windows 10 operating system

On the Windows 10 operating system, the Analyst software toolbar might not refresh correctly and some icons might turn black. After the Analyst software window is minimized and then maximized, the user interface is refreshed correctly. (AN-1204)

Error messages are generated when the screen is locked or unlocked and during Auto Logout in Mixed mode security

In Mixed mode security, when the screen is locked or unlocked during Auto Logout, the Analyst software generates an error message repeatedly. When the screen is unlocked by an Administrator or Supervisor user, the same error message is shown, but the screen is unlocked. The same error message is shown when the Analyst software logs out the current user after the time specified for the Auto Logout option has elapsed. (AN-427)

User names must not contain spaces

Although Windows supports the use of user names containing spaces, the Analyst software does not. If, in Mixed mode security, a user tries to log into the software with a user name containing a space, then the Analyst software shows an error and the login fails. (AN-50)

Managing Windows operating system file permissions

To use the Analyst software to manage Windows operating system file permissions, give the Analyst software Administrator software change permission rights for the project folders, including any network-based project folders.

Stopping the AnalystService

Only Windows Local Administrator group members are allowed to stop the AnalystService (the Acquisition part of the Analyst software). If other users need to stop the service, then refer to the Microsoft Management Console for configuration instructions. Alternatively, users can restart the computer.

Method Editor access

Users must have read and write permissions for the Project Information folder to access the Method Editor. If users who have read-only permission try to open the Method Editor, then the system might stop responding. (SCR 8037)

Mapped network drives might not be visible in Mixed Mode

When the user sets the root directory in the Analyst software Mixed Mode security environment, the Browse for Folder dialog does not always show the mapped network drives. Use the computer name in the (Universal Naming Convention (UNC) format (\\computer name\drive name) instead of the mapped letter. (SCR 11094)

The Analyst software does not start if the user has no file permissions

Users cannot start the Analyst software if the root directory is set to a network drive for which no file permissions were set for the user. If the user trying to log on is an Administrator, then the Analyst software prompts for an alternate root directory. (ST 9836)

The screen lock wait time is incorrect in the audit trail

In the audit trail data, the wait time recorded for the **Screen Lock** in the Security Configuration is incorrect. Also no audit record is created when the wait time for the **Screen Lock** and **Auto Logout** fields are modified. (SCR 12935)

Issue deleting user-defined role

Before deleting a user-defined role, first remove all users assigned to this role. If the users are not removed, then the results might not be shown properly.

Unlocking the Analyst software using the UPN name format causes an error

If a user who was not logged on to the software when it was locked attempts to unlock the Analyst software using the UPN format, then the Analyst software shows an error stating that the user is not recognized, even though the user has unlocking rights. This happens even if the new user is a legitimate user in the domain. To unlock the software, click **OK** in the error dialog and type the credentials a second time (in UPN format).

Disabling access to Select processing algorithm does not take effect

Although access to the **Select processing algorithm to retrieve peak list** function is disabled for Explore mode for a user role, the user with this role can still modify the integration algorithm for retrieving the peak list.

The Find tab cannot be activated in *Help*

Only the Windows Local Administrator or equivalent can activate the Find tab in the *Help* for the first time after installation. Otherwise, the software shows the message "Unable to display the Find tab (177)". (SCR 13792)

Screen lock settings are not retained on reinstall

After the Analyst software is installed, the Network Acquisition account screen lock settings are not kept. Configure these settings on the Security tab of the Security Configuration dialog.

Configure — Hardware Configuration

An incorrect profile is shown in the error message

An incorrect profile might be shown in the error message when a hardware profile fails to activate (SCR 13820)

An incorrect value is shown for the DuoSpray ion source Switching Valve Counter value

During IDA acquisition, the value in the **DuoSpray ion source Switching Valve Counter** field in the hardware profile is incorrect. (SCR 13635)

Temperature Reached might be shown intermittently while the Turbo V ion source is cooling

If the Turbo V ion source temperature is set to a value lower than the current setting, the ion source might intermittently report "Temperature Reached" while it is cooling. Users should allow the system to cool or stabilize for the recommended time while the source is cooling. (TT 35398)

Deactivate hardware profile error message is shown during uninstall

Occasionally, during removal of the Analyst software, a message asking the user to deactivate the hardware profile is shown, even if the hardware profile has been deactivated. To resolve this issue, restart the computer and then remove the Analyst software. (ST 16060)

Tune and Calibrate — Compound Optimization

On SCIEX 3200 systems, the Compound Optimization report incorrectly shows the CEP parameter

The report that is generated as a result of Compound Optimization incorrectly shows the CEP parameter under the CE parameter. The CE parameter should read as CE. (AN-219)

Total sample volume does not update when the total number of injections is changed in the FIA (Flow Injection Analysis) source parameters in Compound Optimization if the Shimadzu LC is connected

When one or more parameters are selected for optimization and the number of replicate injections for each parameter is changed, the **Total # of injections** is updated correctly. However, the total **Sample Volume** does not update and stays 0 µL. (AN-610)

Transitions with the same name might not optimize correctly during Compound Optimization

When using the automatic Compound Optimization option, use a different name for each transition to be optimized. If the same name is selected for more than one transition, then some parameters are not optimized correctly for the duplicate transition. (SCR 9450)

Use of Shimadzu and Tempo MDLC devices when performing infusion Compound Optimization prevents optimization

The software will not optimize if the Shimadzu and Tempo™ MDLC devices are included in the hardware profile. Remove them from the hardware profile before performing this operation, or create a second hardware profile that includes only the mass spectrometer to be used for infusion Compound Optimization.

The Compound Optimization report shows that DP is ramped between 0 V and 400 V

On SCIEX 5500 systems, the actual range for the DP ramp used during the optimization is 0 V and 300 V. (ST 9248)

Compound Optimization does not start the integrated syringe pump for a SCIEX Triple Quad 3200 system

Users can start the syringe pump using Manual Tuning or they can use an external syringe pump. (ST 11130)

Tune and Calibrate — Instrument Optimization

Instrument Optimization cannot be used if users do not have delete privileges for the `API Instrument\Instrument Optimization` folder

Users who do not have the Delete privilege for the `Analyst Data\Projects\API Instrument\Instrument Optimization` folder cannot use the Instrument Optimization module. Make sure that all users who need to use this module have Delete rights for this folder. (AN-593)

The software cannot change to Tune mode

After performing Instrument Optimization, the Analyst software might not be able to change to Tune mode. The Tune button on the toolbar might be disabled. If this occurs, deactivate the hardware profile and activate it again, and then change to Tune mode. (ST 7002)

Empty subfolders are created in the Instrument Optimization folder

Empty subfolders are created in `Analyst Data\Projects\API Instrument\Data\Instrument Optimization` if Instrument Optimization is cancelled on the final page of the wizard (instead of clicking **GO!**). (ST 3767)

Additional 1 Da on Results graph

When the user is viewing the results summary, the graph shows an additional 1 Da on either side of the X-axis. This does not affect the accuracy of the graph. (ST 3775)

Click More Options to see more tuning options

On the Select the scan mode screen, clicking **More Options** allows the user to set additional Instrument Optimization parameters. This does not pause the Instrument Optimization wizard and the wizard can continue while this screen is open. (ST 3763)

Instrument Optimization stops responding when the Start Over button is pressed

Occasionally the Analyst software stops responding if the **Start Over** button is pressed after Instrument Optimization is run several consecutive times. Restart Instrument Optimization from the Analyst software Navigation bar instead of using the **Start Over** button. (ST 8029)

On rare occasions, the Queue Manager is inaccessible after Instrument Optimization is run

To correct this issue, deactivate the hardware profile, close and then open the Analyst software, and then activate the hardware profile. (ST 9678)

Instrument Optimization fails to run after installation

Occasionally, after the Analyst software is removed and reinstalled, Instrument Optimization fails to run and returns the error, "The current hardware profile is not supported by Instrument Optimization." To run Instrument Optimization, remove the Analyst software again and then reinstall it.

Correct masses are occasionally not selected when the Alternate Tuning option is being used

If Instrument Optimization is used to tune a system, then it is recommended that the approved tuning solution be used. If an unapproved solution is used, then some masses might not be correctly calibrated.

Occasionally, calibration shifts are observed after optimization of the 12,000 Da/s scan speed on the SCIEX 5500 system using Instrument Optimization

If this occurs after Instrument Optimization, then either restart the optimization process or manually calibrate the masses that are out of calibration.

Occasionally, Instrument Optimization becomes unresponsive during tuning

If this happens, do not close or reopen the Analyst software. Use the Task Manager program to close Instrument Optimization and then start Instrument Optimization again. (ST 13044)

Typing a negative value for the IonSpray voltage (IS) in Negative mode causes the optimization to fail

When running Instrument Optimization in Negative mode, type IS as absolute (positive) values. (ST 3778)

Data quality is poor during Instrument Optimization tuning

Occasionally, the Analyst software scans fewer than the number of MCA scans selected in an acquisition method. For example, the software only returns 3 scans for a Q1 scan when 10 MCA scans are specified. This MCA issue might affect Instrument Optimization. If this occurs during Instrument Optimization, then start the optimization process again. (ST 13460)

Tune and Calibrate — Manual Tuning

Updating resolution on-the-fly during data acquisition using a *Scheduled* MRM algorithm acquisition method in Manual Tuning causes the Analyst software to stay in acquisition mode

When a *Scheduled* MRM algorithm acquisition method is being run in Manual Tuning without the Q1/Q3 Resolution option selected, the sample acquisition or the queue cannot be stopped if the user changes the resolution settings on-the-fly on the Resolution tab. The computer must be restarted to regain the communication. To avoid this issue, do not change the resolution settings while running a *Scheduled* MRM Algorithm acquisition method in Manual Tuning. (AN-1071)

Known Issues

The Analyst software closes unexpectedly and the `Tunedata.tun` file is truncated after the user enters an invalid search range in Edit Tune Peak Parameters

The Analyst software closes unexpectedly after the user enters an invalid search range in **Edit Tune Peak Parameters** and the `Tunedata.tun` file size gets truncated. The reference table is cleared. If this occurs, restore a previously backed up `Tunedata.tun` file. (AN-497)

Poor mass calibration can lead to inaccurate MRM cycle time in systems (Not applicable to the SCIEX 3200, 4000, and 5000 systems)

When the mass calibration of the mass spectrometer is significantly off, users might see effects such as a significant difference between the observed cycle time in the data file and the expected MRM method cycle time. (AN-411)

Application Event Log errors are generated while a QTRAP 4500 system is being operated in Manual Tuning

When the QTRAP 4500 system is operated in Manual Tuning, the Windows Application Event Log shows the following error: "DDMSMassSpec, Process.cpp, Line 2399, EF:0x20000016=Unknown word <DPF> read". This error can be ignored and it has no effect on system operation. (AN-265)

The user is unable to paste a mass table in Manual Tuning for all scan types

Without the Method Editor open, the user cannot paste copied cells or rows from an Excel spreadsheet to the mass table in Manual Tuning. The workaround is to keep the Method Editor open, and then paste the copied content in the mass table in Manual Tuning. (AN-980)

GS2 is available when the APCI probe is in use (SCIEX 3200 systems only)

When the APCI probe is installed, the GS2 parameter is available, but should not be. When using the APCI probe, set and leave the GS2 value at 0. (SCR 14506)

View of metrics for mass calibration

Metrics for mass calibration do not show all the masses used if the calibration peak list is not in numerical order. (SCR 8483)

Instability in Manual Tuning

If the Graph Information pane is open in Manual Tuning, then the system might stop responding if one run is terminated and a new one started. Closing the Graph Information pane might prevent this issue. (SCR 8879)

TIC data might be incorrect when parameters are ramped using a negative step size

Ramp parameters with a positive step size only. Negative step sizes might yield incorrect TIC data.

Offset drop from unit resolution for the SCIEX Triple Quad 3200 system

For the SCIEX Triple Quad 3200 system, when tuning, set the correct Offset Drop from Unit Resolution values in the Tuning Options Resolution tab.

- In the Low Resolution group, in the Offset Drop from Unit Resolution box, type 0.03.

- In the Open Resolution group, in the Offset Drop from Unit Resolution box, type 0.5.

The syringe diameter does not change during acquisition

On SCIEX 5500 systems, if both the syringe pump diameter and flow rate is changed while the syringe pump is running and then **Set Flow Rate** is clicked, then the flow rate changes but the diameter does not. Stop the pump and then restart it for the changes to be applied. (ST 8291)

Data is not being recorded for the same number of cycles as requested when MCA is selected

Occasionally, the Analyst software scans fewer than the number of MCA scans selected in an acquisition method. For example, the software only returns 3 scans for a Q1 scan when 10 MCA scans are specified. To correct this issue, restart the scan or toggle between scan speeds and then restart the scan. (ST 13460)

Windows are not refreshing in Manual Tuning

In Manual Tuning, the user interface is not refreshed when the Resolution Table Editor is moved. Click between the tabs to refresh the user interface. (SCR 9327)

A syringe pump error does not clear if it is ignored

On SCIEX 5500 systems, when the syringe pump reaches the stop, a syringe pump error is shown. If the error is ignored for an extended period of time, and the user continues clicking through the Analyst software, then the error will return but the user might not be able to clear it because the **Clear Error** button might be unavailable. To clear the error and regain communication with the syringe pump, deactivate and reactivate the hardware profile. If the error is not cleared, then restart the computer. In rare cases, the user must deactivate the hardware profile and then restart the computer and the mass spectrometer. (ST 9880)

Visible graphs might be slow to update when the 12,000 Da/s scan speed is being run in Manual Tuning

When the 12,000 Da/s scan speed is being run in Manual Tuning, the graphs that are shown can be slow to update and the Analyst software might seem to stop responding. This often occurs if the user changes applications and then changes back. However, the data is collected successfully and the program updates when the scan stops.

On QTRAP 5500 systems, masses greater than 1,000 Da can be entered in the Isolation and Excitation tables

Although the mass range for the linear ion trap is 50 Da to 1,000 Da, the software allows the user to enter values for masses greater than 1,000 Da in the Isolation and Excitation tables. The effect of entering additional rows for masses above 1,000 Da is unknown but will likely affect the quality of data for the entire mass range and users are encouraged to avoid doing this. (ST 11622)

On QTRAP 5500 systems, after a fresh installation of the Analyst software, reference tables might appear empty

To avoid this issue, activate a hardware profile before attempting to edit a reference table. (ST 8788)

Acquire — IDA and IDA Method Wizard

A manually created information dependent acquisition (IDA) method cannot be saved if a copied survey scan experiment is changed to a dependent scan

The user is unable to save an IDA method if an IDA dependent scan was created by copying an experiment from a survey scan and then changing it to a dependent scan. The workaround is to create an IDA dependent scan by adding an experiment. (AN-1038)

IDA selects ions that do not match the isotope ratio criteria

Ions selected by IDA for dependent scans might still get passed even if the ion does not meet the ion ratios specified. (AN-260)

If there are two EPI scan in an IDA method, only the second EPI scan passes to the MS3 scan

If an IDA method uses two Enhanced Product Ion (EPI) scans, then the most intense ion in the combined EPI scan should pass to the MS3 scan. Instead only the second EPI scan is passed to the MS3 scan. (AN-157)

Changing the EMS mass range by using the Back button in the IDA Method Wizard might result in overlapping mass ranges

If the **Back** button is used to modify the EMS mass range in the IDA Method Wizard, then the created method might have overlapping mass ranges for EMS survey scans. If the **Back** button is used to modify the EMS mass range, then manually correct the produced method for the EMS mass ranges. (AN-705)

MS3 isolation always uses the new LIT resolution table

In the IDA Method wizard, although the choices for the **Resolution Q3** field (**High**, **Unit**, **Low**, and **Open**) are available for the MS3 scan type, the MS3 scan type always uses the LIT resolution table for **Resolution Q3**. The choices available for **Resolution Q3** are ignored. (SCR 11378)

Set to never Exclude Former Target Ions from IDA

If a quadrupole mass spectrometer profile is activated in the IDA wizard, then select the **For 0 secs** option to set the **Exclude Former Target Ions** on the IDA Critera page to **Never**. (SCR 11762)

IDA is not triggering on specific charge state

In the second level IDA, MS3 can be triggered by an ion of an unknown charge state even though the charge states are specified as the criteria at this level. (SCR 11551)

DP and CE values are not stored in the final method

When IDA methods including MS3-dependent scans are generated using the IDA Method wizard, DP and CE values specified for the survey and other dependent scans are not applied to MS3 experiments. Type DP and CE values for MS3 experiments in the Acquisition Method Editor after creating the method. (SCR 12463)

Doubly-charged ions are sometimes incorrectly recognized as singly-charged ions

Doubly-charged ions are sometimes incorrectly recognized as singly-charged ions in an EMS survey scan of an IDA experiment. (ST 14677)

Singly-charged masses are occasionally misidentified

In IDA experiments, singly-charged ions are occasionally identified as undefined charges. (ST 17100)

Undefined charge states are sometimes incorrectly recognized as singly-charged charge states

Undefined charge states are sometimes incorrectly recognized as singly-charged charge states in an EMS survey scan of an IDA experiment. (ST 17100)

In an IDA method, if a dependent scan experiment is deleted, then an additional mass range might be added to the survey scan

Refreshing the user interface by clicking in a different field, switching between the experiments, or saving the method, deletes the added mass ranges. (ST 17047)

On the QTRAP 5500 system, ER scans in IDA methods must have a mass range less than 1,000 Da

When the user creates an IDA method with a quadrupole survey scan and a confirmation scan (Enhanced Resolution), the method cannot have a survey quadrupole mass range greater than 1,000 Da. The user will be prompted to decrease the mass range or remove the confirmation scan.

On the QTRAP 5500 system, occasionally this message is shown: "No dependent parameters are found in the IDA method the file will open using Explorer" when opening non IDA samples in data files collected at 12000 Da/s

The data file opens normally, so the message can be ignored. (ST 13169)

Survey scan mass ranges are duplicated when users create an IDA method using the IDA wizard

To prevent this issue from occurring, do not go back to previous pages in the wizard. Alternatively, delete any duplicate ranges in the final method. (ST 17059)

On the SCIEX Triple Quad 5500 system, the IDA Method Wizard does not allow the user to select RF/DC scan rates

The RF/DC scan rates are currently unavailable in the wizard. The final method that the wizard creates uses the preset scan speed of 200 Da/s. This method is editable and can be saved with the new scan speeds. (ST 9272)

On the SCIEX Triple Quad 5500 system, mass shifts of up to 1 Da might be observed for data generated using the IDA Wizard

When a method is created with the IDA Wizard, the scan speeds are not available for selection. However, the scan time is available and editable, and is populated in the final method. The final method defaults to 200 Da/s. However, the specified scan time might not correspond to this scan speed. As a result, data collected with these methods might result in an observed mass shift

in the data. To overcome this issue, select a different scan speed, or, to use the 200Da/s scan speed, select a different scan speed, change back to 200 Da/s if required, and then save the method before running it. (ST 19703)

Looping opposite polarity EMS experiments as survey scans in an IDA experiment sometimes causes dependent data to not be triggered

The following scenarios prevent dependent data from being acquired:

- EMS+ve > EMS–ve > ER > IDA Criteria > Dependent scans

- EMS+ve > EMS–ve > IDA Criteria where charge state confirmation is selected to NOT include unknowns > Dependent scans

Therefore, to allow dependent data to be acquired, either remove the ER scan type from the method or change the IDA criteria to allow acquisition of unknowns. The latter scenario, however, allows dependent scans to be performed only on undefined charge states. The peaks with the specified charged states are ignored even if they satisfy all of the other IDA criteria. (ST 17045)

No dependent scans are performed for an IDA method that includes a quadrupole (–ve) > EMS (+ve) > dependent scan (+ve)

No dependents scans are triggered for data acquired with this type of method with or without a confirmation (Enhanced Resolution) scan type and with or without "Unknowns" selected for charge state confirmation. (ST 18132)

Incorrect ions are selected for a confirmation scan

An IDA method with a *Scheduled* MRM algorithm scan type as a survey scan and a confirmation scan type does not work as expected if the intensity threshold in the IDA Criteria is set to 0. The IDA method selects the ions from a future retention time window for the confirmation scan during the acquisition instead of the ions that were satisfying all the IDA Criteria. To avoid this issue, set the Intensity threshold > 0. (ST 18941)

IDA acquisition fails if the hardware profile contains an ADC device

Restart all the peripheral devices and then restart the AnalystService. To avoid this issue, do not include an ADC device in the hardware profile if IDA acquisitions are performed. (ST 16102)

Acquire — Acquisition Method Editor

Deleting the last experiment might cause a change to a parameter value on the first experiment in an acquisition method

For a method with three or more experiments of the following scan types, whether the same kind or mixed, deleting the last experiment causes the precursor ions for the **product of**, **1st precursor**, **2nd precursor**, or **Loss of** field in the first experiment to be replaced with the precursor ions from the deleted experiment, regardless of whether the first and the deleted experiments have the same scan type. Other parameters and mass range are still for the original first experiment. The following scan types are the affected:

- EPI

- MS3

- Product (MS2)

- Precursor Ion (Prec)

- Neutral Loss (NL)

(AN-2276)

The Convert Method script might not open methods containing an LC method

If an acquisition method was saved from the File Info of a datafile that used an LC system, then this acquisition method containing the LC method might not open in the Convert Methods script when the script is used to convert the method for use with a different mass spectrometer. To avoid any issues, open and then save this method in the Analyst software after it was saved from the File Info. (AN-1609)

The IonDrive Turbo V ion source and the OptiFlow Turbo V ion source were not listed in the Experiment information

The ion source type for the IonDrive Turbo V ion source or the OptiFlow Turbo V ion source on SCIEX 5500, 5500+, 6500, or 6500+ systems is not listed in the printed Experiment information in printed acquisition methods. To avoid any issues, use File Info instead. (AN-1523)

An acquisition method with 0 duration or 0 cycles might be allowed to be saved

Under a rare workflow, an acquisition method with 0 duration or 0 cycles might be saved. Make sure to review the method for the duration or cycles before saving the method. (AN-1199)

Copying and pasting a few cells in a *Scheduled* MRM method does not work when the compound-dependent parameters are in the mass table

In a *Scheduled* MRM algorithm method that contains compound-dependent parameters, when a few cells are copied from the mass table and an attempt is made to paste the copied content by clicking the first cell in an empty row and then pressing **Ctrl + V**, two error messages about invalid compound-dependent parameter are shown and the copied content is not pasted. To avoid this issue, either copy and paste by selecting whole rows instead of individual cells or copy by selecting whole rows and then paste by selecting the last empty row.

In rare cases, switching from the **Advanced** option to the **Basic** option in a *Scheduled* MRM algorithm method, then copying one row in the mass table and pasting it shows the following message: "To copy and paste data from one Mass Ranges table into another Mass Ranges table, the number of columns as well as the column headings in the source and destination tables must be the same. Add or remove columns from the destination table as required." Clicking **OK** on this message removes all of the existing rows in the mass table. Try to use one mode for copying and pasting in the mass table, and then switch mode. (AN-1061)

The Auto Equilibration option is not working

The **Auto Equilibration** option in the Acquisition Method Editor is not working. When this option is selected, the auto equilibration duration should be added to normal step 0 equilibration time, which lengthens the equilibration time between samples. The auto equilibration duration is not being considered and the sample acquisition starts as soon as **Run** is selected. (AN-784)

The user cannot add or delete the last transition for MRM or *Scheduled* MRM algorithm acquisition methods

In an MRM or *Scheduled* MRM algorithm acquisition method with 500 or more transitions that were added to the method either by copying from a text file or importing from a csv file, the last row in the mass ranges table might not be blank. In such a case, the last transition cannot be deleted and new transitions cannot be added after the last transition. Deleting or inserting at other rows is okay. To avoid this issue, edit one of the cells in the last row and click elsewhere in the table, which will create a blank last row in the mass ranges table. After this, the last filled row can be deleted or a new transition can be added. (AN-725)

The Analyst software stops responding when the Edit Parameters button is clicked after a switch to a different hardware profile

When an acquisition method is open, then switching to a different hardware profile and clicking the Edit parameters button causes the Analyst software to stop responding. To avoid this issue, close the acquisition method before switching to a different hardware profile. (AN-117)

The settling time does not update when the scan type is changed from an experiment with a higher default value to one with a lower value

If within a method the user changes the scan type from one with a high default settling time to one with a lower default settling time, that field is not updated in the method. Review the settling time before saving the method. (AN-691)

A Method Editor user interface (UI) issue occurs when scan type and polarity of a saved method is modified

If the user opens a previously saved MRM method and then changes both the scan type and polarity without switching tabs between changes, an error is shown and the method tabs (Source, Compound, Resolution) are empty. If users are working with saved methods, then they should change tabs when changing scan type or polarity, to refresh the method UI. (AN-48)

The filename is lost from the UI when an existing method that fails validation is saved again

If after the user opens (or creates and saves) a method, edits the method, and then tries to save it again, the method fails validation and an error is shown. The filename is no longer shown in the top of the Analyst software window, and the user is prompted to select a new file name after attempting to save the method again. (AN-78)

Different CEM values are not supported for multi-experiment methods with polarity switching

When creating multi-experiment methods, users can choose to switch polarities between experiments. If this option is selected, users should not choose different CEM values for the experiments. If they do, the CEM values are not applied correctly during acquisition. Users should set the same CEM value for all experiments when using polarity switching. (CBUFW-25)

IonSpray Voltage (IS) values should be the same for all experiments in the same polarity

When creating a multi-experiment method with a single polarity, users should use the same IS value for all experiments. If users select different IS values, then the voltages are not applied correctly during acquisition. (CBUFW-25)

Acquire — Method/Batch Editor/Queue Manager

The Internal Standards column in the Analytes table might auto-populate with internal standards from other data source

When a quantitation method is created in either Build Quantitation Method or Quantitation Wizard, the **Internal Standards** column in the Analytes table might auto-populate with internal standards from another data source if the Analytes table is filled out before the Internal

Standards table of that data source. The workaround is to deselect the auto-populated internal standards when there are no internal standards used for the current data source, or select the appropriate internal standards, if used, in the Internal Standards table before selecting the analytes in the Analytes table for the current data source. (AN-2601)

The Valco valve might not work properly if it is used with the Analyst Device Driver (ADD) software

The Valco valve might not work properly if it is used with the ADD software and Manual/AAO Sync is used for the **Synchronization Mode**. The issue might be resolved if **LC Sync** used the **Synchronization Mode**. The Sync Cable is required to connect between the autosampler and the mass spectrometer. (AN-1481)

Signal loss occurs on the negative EMC spectrum (Not applicable to the 3200 QTRAP and 4000 QTRAP systems)

On systems other than the 3200 QTRAP and 4000 QTRAP systems, signal cutoff might be observed for some mass ranges in the negative EMC spectrum. (AN-1198)

The user is unable to import batch files in xls, db, or xlsx formats in the Batch Editor

Importing a batch file in xls, db, or xlsx format might cause an error and the batch file would not be successfully imported. The xlsx format is only available in the **Files of type** list if the installed Microsoft Office is a 32-bit application. To successfully import a batch file, make sure to save it as a tab delimited txt file with the first line starting with `% header=SampleName`. Refer to the example file DABImport.txt in the `D:\Analyst Data\Projects\Example\Batch` folder. If a csv format is to be used, then edit the file in Notepad and make sure that the first line is `% delimiter=','`: and the second line starts with `% header=SampleName`. (AN-1282, AN-1234)

The Analyst software cannot write the checksum to a wiff file if the file stays open in the MultiQuant or other compatible software

If a data (wiff) file is being acquired to by the Analyst software, do not open that file in the MultiQuant software or any other application until acquisition has completed. Doing so might cause the Analyst software to not write the datafile checksum. (AN-305)

Queue: The Next Period button available on the toolbar in the Analyst software does not work when clicked

When the **Next Period** button is clicked, acquisition should move to the next period but the Analyst software remains in the same period even when the button is clicked. (AN-731)

Scheduled MRM Pro: File Info shows 0.0 if the Window field is left blank in the method

When creating a *Scheduled* MRM Pro method, users can type a value for **Window** to supersede the **MRM Detection Window** set in the method. If users choose to leave this field blank (the transition will use the MRM Detection Window), then the File Info shows 0.0 in the Window column for that particular transition. (AN-270)

Users should not turn on the SelexION device during an acquisition

If the user turns on the SelexION device during acquisition, then the currently acquiring sample is aborted and the system briefly goes to the Error state. When the system recovers to the Ready state, if users attempt to reacquire their sample, then there is no indication that the system has changed. Because of this, there might be a mismatch between the status of the system as shown in File Info and the actual status of the system. Users should refrain from turning the SelexION device on or off during acquisition. If it is turned on or off, then users should submit new acquisition batches, rather than using the reacquire function in the software. (AN-115)

The status of the integrated diverter valve is not updated when the diverter valve position switches

The status of integrated diverter valve is not updated when the diverter valve position switches, but the position does switch. There is no impact to the data. (AN-662)

Sample Details in the Analyst software Queue shows Manual Sync instead of Manual/AAO Sync

In the queue for a batch submitted with a method using **Manual/AAO Sync**, when the sample status is viewed by double-clicking the hour-glass icon, the Sample Details dialog shows **Manual Sync** instead of **Manual/AAO Sync** in the **Sync Mode** field. It is only a display issue. There is no impact to the data. (AN-1011)

An error is shown when invalid characters are used in sample names

If the user enters a forward slash in a sample name within a batch, then when the user attempts to submit the batch, the software shows the error: "Invalid character found in path (/)". If the user enters other invalid characters (:, ", <, >,?, |), then the software shows the error "Invalid character found in path (: "< >? |)". (AN-94)

Show all columns before pasting data in the Batch Editor

Although the Batch Editor supports copying and pasting from and to applications such as Microsoft Excel, users should be aware that the Batch Editor contains columns that are hidden by default, for example, **Sample ID**, **Dilution Factor**, and so on. When text is pasted from a spreadsheet into the Batch Editor, all columns are populated in sequence, whether visible or not. Therefore, it is possible for data to be pasted in an unintended column.

If users want to paste data in to the Batch Editor, then they should manually expose all columns first, to make sure that data is pasted as intended. Alternatively, users must make sure that the data they are pasting in the Batch Editor contains information for all columns, visible and hidden. (AN-216)

The last transition row cannot be deleted in an MRM method with 300 or more transitions

In an MRM acquisition method with 300 or more transitions, the last row of transitions cannot be deleted. (AN-198)

A filename containing a period and not the file extension is saved with an unknown file extension and cannot be opened

Do not include a period (.) in the file name because the software considers the information after the period to be the file type.

This issue occurs during batch creation, when using the Convert Methods script, when saving the optimization report during Compound Optimization, and when saving the report generated using the Reporter software. (AN-220)

The Pause Time in a saved method reverts to its default value when the access type for the CAD gas parameter is changed from Simplified to Operator

The Pause Time in a saved acquisition method changes to the default value of 5.007 ms when the Access Type for the CAD gas parameter is changed from **Simplified** to **Operator**. (AN-266)

Method duration might change when the user changes between tabs

When users change tabs in the Acquisition Method Editor, fields are recalculated. As a result, if the user sets a method duration and then changes between the Advanced MS and MS tabs, the duration might change slightly as the number of cycles is recalculated. This results in a method duration that best fits the number of actual cycles. (TT 34574)

The Analyst software might stop responding if an external valve is configured in the hardware profile but it is not used in the method

When configuring an external valve in the Hardware Profile, users must make sure that the valve is assigned a correct switching method in the acquisition method. If users submit a method that does not contain a valid valve switching method, then the Analyst software might stop responding during acquisition. If the valve will not be used during acquisition, then it should be removed from the hardware profile. (TT 34645)

Number of Scans to Sum might be reset to 1

When using the MCA data collection, if the user sets the **Number of Scans to Sum** field and then changes to the Advanced MS tab and back, the field might reset to 1. When using the MCA

data collection, users should set the **Number of Scans to Sum** field as their last step before saving the method. (TT 34787)

DFT scans might fail to maintain targets

In some cases, users might see Dynamic Fill Time (DFT) scans overshooting the target intensity. In these cases, users should switch to fixed fill times. (TT 34872)

Method Editor: Calculated Cycles are not immediately updated

When changing the parameters that affect the method duration, the **Calculated Cycles** field is not immediately updated. If users switch to the Advanced MS tab and back, they see that the field was updated. (TT 34884)

Simulation mode: Some methods might not end at expected times

When running acquisitions in the simulation mode (for example, to test new methods), some methods might not end at the expected time. The mass spectrometer should never be simulated for real LC data acquisition. (TT 34893)

Dynamic Fill Time might not work in Manual Tuning

When users run Manual Tuning with DFT enabled, changes to compound parameters might not trigger DFT to recalculate fill times. Therefore, when running Manual Tuning, users should use Fixed LIT fill times. (TT 34905)

DBS is not applied when a single MRM is acquired

When an experiment containing a single MRM transition is run, the Dynamic Background Subtraction (DBS) algorithm is not applied, whether or not the feature is turned on. (TT 35242)

Queue: Waiting samples are treated as Acquired when the Queue stops

When the queue stops (acquisition completed, acquisition error, and so on), any samples that are in the Waiting state are treated as acquired. If the Queue Options are set to show only a limited number of completed samples, then these waiting samples might be deleted from the queue. To avoid this issue, increase the number of completed samples shown in the queue. (TT 35286)

Queue: The Pause Sample Now icon is not available

The **Pause Sample Now** icon on the Queue toolbar is inactive and does not affect the acquisition of samples. (TT 35287)

Sample Details from the right-click menu shows incorrect information

Selecting **Sample Details** from the right-click menu shows incorrect information (**Sample Name**, **Status**) for samples with the status of Terminated or Partial. Sample details are available for waiting and acquired samples. To see the correct information for terminated or partially acquired samples, double-click the row. (ST 31086)

Columns cleared in the Queue Manager cannot be selected again

If users right-click in the Queue Manager, select **Column Settings**, and then clear the check boxes, the columns are removed from the Queue Manager. However, the right-click menu is subsequently not available and the columns cannot be restored to the Queue Manager. To avoid this issue, do not remove columns from the Queue Manager. (ST 31088)

Moving and then deleting a batch causes the Analyst software to stop responding

In the Queue Manager, if a batch is moved and then deleted, the Analyst software stops responding. To avoid this issue, delete the batch without moving it. (ST 31098)

Users are unable to delete the last row when the acquisition method contains more than the maximum limit of MRM transitions

When pasting more than the maximum limit of MRM transitions in the acquisition method, users cannot delete the last row. Users can delete row n–1 and then edit the last row to include the information that was just deleted. (ST 6968)

Note: For SCIEX 3200, 4000 and 5000 systems, 300 MRM transitions are the maximum during acquisition of MRM data and 1000 MRM transitions are the maximum during acquisition of *Scheduled* MRM algorithm data. For all the other systems, 1,250 transitions are the maximum during acquisition of MRM data and 4,000 per method is the maximum during acquisition of *Scheduled* MRM algorithm data. (ST 6968)

Copying and pasting acquisition methods

Copying compound-dependent cells that are partially exposed in a mass ranges table might cause the pasting action to result in an error. Highlight all cells completely (drag the mouse all of the way to the right) before copying them. Also make sure to copy into the same column for which the selection has been made, otherwise incorrect data and errors might result.

Copying and pasting to mass table

For instructions for copying and pasting to the mass ranges table from one acquisition method to another or from an external file to an acquisition method, refer to the document: *Help*.

Users are unable to change and save number of cycles

If users edit any previous version of method (dam) files, then they might not be able to change and save the number of cycles the first time. Repeat the process again to save this information.

Scans are unexpectedly set to sum to 1

If users set the scans to sum to more than 1, clicking the Advanced MS tab and then clicking the MS tab resets the scans to sum to 1. To store the value properly, type the value and save without clicking the Advanced MS tab. (SCR 11446)

Column headers are missing in previous versions of batch files

If users open a batch file created from an earlier version of the Analyst software, column headers might disappear in the Batch Editor. (SCR 11578)

Source/gas information might not reflect values set as default in parameter settings

After creating an acquisition method manually or through the IDA Method wizard, review and then update the Source/Gas parameters as appropriate. (SCR 11662, SCR 11711)

Users are unable to save or submit batches with long file paths

Users cannot save or submit an acquisition batch if the project path is longer than 126 characters. When this type of file is submitted, the software shows the error message: "Failed to set Header data". When this file is saved, the software shows the error message: "Failed to save BatchName".

Pasting columns in mass ranges table

Pasting of individual column of values for compound-dependent parameters in MRM and *Scheduled* MRM algorithm methods from an external csv or txt file might not always work. Copy and paste the whole Excel spreadsheet with updated dependent parameter values.

Pasting rows in mass ranges table

Pasting more than 300 lines into an MRM mass table might take several minutes.

Issue with importing file with MRM transitions

Make sure that the imported file is either a txt (tab-delimited text) file or a csv (comma separated value) file. Make sure that the number of columns in the file is equal to the number of columns shown in the Analyst software Method Editor and that the column order matches. Also, make sure that there are no empty cells in the file that are imported. (ST 2717)

An error message is shown when a text file is imported into an MRM or *Scheduled* MRM acquisition method

When a text file is imported into an MRM or *Scheduled* MRM algorithm method, the software might show the message: "Invalid value entered into table. Make sure only numeric values are entered". However, the file is imported correctly. This issue is not observed when csv files are imported or when content is copied and pasted from an external file, regardless of its format. (ST 19141)

Pasting into a mass ranges table during acquisition can cause the system to stop responding

When content is pasted into a mass ranges table during acquisition, the Analyst software might stop responding. Users can only copy and paste into an MRM or *Scheduled* MRM Algorithm table before and after acquisition.

Switching valve tables must be populated before using method

When using a method containing a switching valve, make sure that the table is populated before saving and using the method. If this method is used for acquisition, the system stops responding and you must restart the instrument. (ST 9431)

Pause time doubles if a quadrupole experiment is created after a change between LIT and quadrupole scan types in the Method Editor

When users create a method containing a quadrupole scan type with a mass range of, for example, 1,000 to 1,250 Da, and then change to an LIT scan type and then back to the original quadrupole scan type, the pause time nearly doubles. To prevent the pause time from doubling, do not change scan types during method creation. (ST 11465)

During batch creation, pressing Tab creates another row

When a batch is created, if the user goes to the last row in the Batch Editor and then click **Tab**, another row is created. After the row is created, the Auto-Increment or Fill-Down functionality does not work with this row. Also, any rows appended to the batch are shown before this one. When the batch is submitted, this phantom row is not submitted. If a user creates a batch with this extra row, the sample specified in this row is not collected. Avoid the use of the **Tab** key to add rows to the batch. Use the **Add Samples** button instead. (ST 14024)

Samples in a batch stay suspended after an instrument error is corrected

The batch must be resubmitted to the queue to continue. (ST 16247)

Ion energy is invalid in EMS scans

Although Ion Energy 1 is accessible in EMS scans, it is not applicable and should not be used. (SCR 11764)

Acquire — *Scheduled* MRM Algorithm

Scheduled MRM algorithm experiment limit

For SCIEX 3200, 4000, and 5000 systems, to maintain optimum system performance, a *Scheduled* MRM algorithm, non-IDA experiment should not exceed 1,000 transitions and three dependent parameters. A *Scheduled* MRM algorithm, IDA experiment should not exceed 1,000 transitions and two dependent parameters. If the experiment exceeds these limits, then the Analyst software might stop responding and the user must restart the instrument and reactivate the hardware profile. Reduce the number of transitions to increase the number of dependent parameters.

For all the other series systems, the limit is 4,000 transitions with three of the four dependent parameters (CE, DP, EP, CXP).

Multi-period *Scheduled* MRM algorithm experiments not supported

Multiple period *Scheduled* MRM algorithm experiments are not supported in the Analyst software. Users cannot create methods containing these experiments.

In certain cases, for the SCIEX Triple Quad 5000 system, sensitivity might be less for *Scheduled* MRM algorithm experiments than for MRM experiments

This issue might be observed for experiments covering a wide range of Q1 masses over several hundred Da. Keep this in mind when using the *Scheduled* MRM algorithm functionality on the SCIEX Triple Quad 5000 system. (ST 15149)

Batches containing the maximum number of *Scheduled* MRM algorithm transitions and three mass-dependent parameters where one of them is EP cause the system to stop responding

Batches containing the maximum number of *Scheduled* MRM algorithm transitions and three mass-dependent parameters, DP, CE, and EP, cause the system to stop responding. To avoid this issue, do not include EP as one of the mass-dependent parameters. (ST 16066)

Scheduled MRM algorithm parameters cannot be changed on-the-fly

Compound-dependent parameters for an acquisition method using the *Scheduled* MRM algorithm might not be applied when changed in real-time in Manual Tuning. When changing parameters for a *Scheduled* MRM algorithm method in Manual Tuning under Tune and Calibrate mode, stop the method between adjustments and then start it again. (ST 9436)

Modifying *Scheduled* MRM algorithm mass ranges table can take several minutes

Modifying a *Scheduled* MRM algorithm mass ranges table with 1,000 MRM transitions can take several minutes. (ST 5251)

Acquire — Network Data Acquisition

Submitting the same batch again for a network acquisition could cause data loss in case of network disconnection

If a batch has been acquired to a network location, submitting the same batch again using the same data file names to the same location could cause potential data loss on the samples or datafiles that were acquired twice. This issue occurs if the network is disconnected during the acquisition of the second batch. To avoid the issue, do not submit the same batch again, instead, change the data file names and save it as a different batch, and then submit the batch, just in case the network gets disconnected unexpectedly. (AN-1310)

Copy data to a network location before validating the checksum

If the user attempts to validate the checksum of a large file that is being acquired to a network location, then the Analyst software might stop responding or a failed checksum might occur. This is because network interruptions might cause a delay in writing the full file to the network. To resolve this issue, restart the AnalystService and client. Alternately, the file itself might become corrupted. Make sure that the file has been fully copied to the network location before attempting to validate the checksum. (AN-202)

Data might be lost during acquisition from multiple instruments to same data file

Do not acquire data concurrently from multiple acquisition workstations to the same network data file.

Network data security mode

For network data acquisition, use Mixed Mode or Integrated Mode. If Single User Mode is used, then make sure that the user is a network domain user with read and write access to the project folder. (SCR 11781)

Current data is not accessible

If network acquisition is used, then users cannot see the acquired data from a remote workstation until the sample is finished.

No audit trail records are created when the network is unavailable

When the network is unavailable, the data file creation and other non-processing activities performed during data acquisition only are not recorded in the audit trail database, which is not accessible. Add steps to the standard operation procedures (SOP) to contact the IT department regularly if there has been any network interruption during previous data acquisition processes and to avoid data acquisition during network maintenance work. Users can also review the Windows application event log for any network disconnection warning events. All relevant acquisition data is still logged in the data file even if the network is unavailable. (SCR 11648)

Reported Last Sample Finished time is slightly later than the time that acquisition completed

When data files are acquired to the network, the time reported in File Info in Explore mode for Last Sample Finished is the time the file was copied to the network, which might differ from the time of acquisition of the last sample. This is due to the delay when transferring files to the network. (SCR 9523)

Verify checksum after the file transfer is complete

When **Verify Checksum** is clicked on a file that has just finished acquisition, checksum verification might intermittently fail if the data file transfer to the network is in progress. Checksum verification works after the transfer is complete. (SCR 11419)

The wait period is long if the user does not have write access

If users do not have write access to a network project and try to open a data (wiff) file, they might experience a long wait period while the audit trail process tries unsuccessfully to update the information. (SCR 9906)

File transfers might fail due to limited space on the network

When acquiring data to a network server with user-specific space limitations, the Analyst software might not be able to detect the remaining space available. As a result, the data transfer process might fail, but acquisition is not affected. The data remains on the local acquisition workstation. To avoid this issue, always make sure that there is sufficient space. If the issue does occurs, make some space available, and then restart the Analyst software. (SCR 11420)

The spectral arithmetic output file is not saved

If the root directory is on the network, select **Open the New File Immediately** in the Analyst software in the **Output Filename** section in the Spectral Arithmetic Wizard–step 4. Otherwise, the output file might not be saved. (SCR 11746)

Explore

File Info pane saved to PDF file format appears empty when viewed in Adobe Acrobat

Select **Save to File** from the right-click menu in the file information pane of a data file, then save the file by choosing the PDF format. The saved PDF file seems to be empty when it is opened in Adobe Acrobat. To see the contents of the file, open the PDF in Chrome or Internet Explorer. Alternatively, the file information can be saved in RTF format, opened using Microsoft Word, and then converted to PDF. The converted file can then be opened properly with Adobe Acrobat. (AN-2670)

Auxiliary trace data not populated in Explore in real time after MS stops scanning

If a sample using a longer LC method duration than the MS method duration is being acquired with auxiliary trace enabled, and the sample auxiliary data is viewed in real time in Explore mode, then the auxiliary trace data is not populated after the mass spectrometer stops acquisition. (AN-2393)

LC method information might not be displayed properly if the Show Next Sample, Show Previous Sample, or Go To Sample buttons are used when the File Info pane is open.

If the File Info pane for a data file is open in Explore mode, then clicking the **Show Next Sample**, **Show Previous Sample**, or **Go To Sample** icon in the top tool bar might cause the LC method properties to show improperly. The LC method information might not be shown in full, and some of the period and experiment information might be repeated. If the issue occurs, then deactivate the hardware profile if it is active, close the Analyst software, and start the computer again. To avoid the issue, close the File Info pane before clicking these icons in the tool bar. (AN-1967)

The LC method file name and detailed information are not shown in the Analyst software File Info for the SCIEX 7500 system data files.

For SCIEX 7500 system data files acquired by SCIEX OS, the LC method file name and detailed LC information are not shown in the File Info in the Analyst software. To view the LC-related information, use SCIEX OS instead. (AN-1933)

Simplified CAD gas settings are shown incorrectly in File Info

If a data file was acquired using simplified CAD gas settings and opened in the Analyst software without the corresponding hardware profile active, then the CAD gas setting in the File Info is shown incorrectly. A CAD gas setting of Low is shown as –1, Medium as –2, and High as –3. (AN-299)

Centroid data is not shown correctly

Centroid data is not shown correctly when scan the user averages scans and steps the extracted ion chromatogram (XIC) to show the adjacent spectra. Instead of using Centroid, use Profile scan mode to show the data correctly. (AN-405)

High mass PPG values are shown for SCIEX OS 5500, 6500 (low mass mode), and 6500+ (low mass mode) systems in the calibration peak list

On SCIEX OS 5500, 6500 (low mass mode), and 6500+ (low mass mode) systems, additional ions 1,254, 1,545, and 1,952 are shown in the calibration peak list. This has no impact on the calibration of the mass spectrometers. (AN-500)

Processing large data files concurrently with long data acquisition

Avoid processing, such as generating a XIC, for a large data file that has more than 600 MRM transitions while performing a long data acquisition. Doing so might cause the software to become unstable and data to be lost. Use another computer to process such data. When data currently being acquired is opened, the display for currently acquiring *Scheduled* MRM algorithm data defaults to TIC to open the file faster. Processing these files should still be kept to a minimum during acquisition.

Processing Options truncates non-integer values

The Analyst software Integration tab on the Processing Options dialog (**Tools** > **Settings** > **Processing Options, Integration tab**), allows the user to type decimal values between 0 and 100. However, after the screen is closed and then reopened, these values truncate to their integer values.

The Subtract Range Locked option seems to be active and the menu item in the right-click menu does not update

When right-clicking on a chromatogram, the feature seems to be enabled whether or not it actually is. To see if the feature is enabled, use either the Menu bar (**Explore** > **Background Subtract** > **Subtract Range Locked**) or the Explore Toolbar. If the icon is shown as depressed, the feature is enabled.

Inability to sort Peak Lists correctly

Occasionally, the Peak List does not sort correctly. To restore functionality, close the Peak List (deleting the pane) and then open it.

The cursor location does not correspond to the time point of the spectral data

Occasionally, the cursor is incorrectly allowed to be placed between data points. The time in the header of the spectrum of the active chromatogram is always correct.

Data is missing after an export to the PDF format

When the Analyst software is active with several panes open, exporting the active window to a PDF file might not export all data from the window. Use **Export** when there are only a few panes in the window.

Time range discrepancy for Contour plot

When a processed data file (pdt) is saved with a Contour plot shown, the saved file shows a different time range than the original Contour Plot.

The X-axis is not extended

After a chromatogram is offset, the X-axis (time) range is not extended to include the shifted data.

The DAD margin for negative absorbance is not functioning

The diode array detector (DAD) margin for negative absorbance does not function.

Performance is impacted due to a large number of scans

Processing data can be slow when the data file contains a very large number of scans resulting from the use of short dwell times. Keep the number of scans below 30,000. (SCR 7964)

Viewing IDA data files

If an IDA experiment data file is opened during acquisition, it is shown in Explore mode even if the IDA Explorer is set as the default viewer in the Appearance Options dialog. If the data file is opened after acquisition, it is shown in the IDA Viewer. Samples that were opened in Explore mode during acquisition do so by default when the acquisition is complete as well. To open the file again, user the IDA Viewer. (SCR 9805)

The integrated Harvard syringe pump is not in File Info

In some cases the File Info in Explore mode indicates that the integrated Harvard syringe pump was not used even though it was used. (SCR 8643)

Smoothing does not consider 0 intensity points

The Smoothing function does not consider 0 intensity points. Holes might be visible in the spectrum after smoothing if there are intensities of 0 in the data file. (SCR 13204)

Show File Info

Opening the File Info pane using the **Show File Info** command might cause the software to stop responding or to omit information from the view. This is an intermittent issue and no data is lost. If this issue occurs, then configure the Audit Trail Manager settings to No Audit Map or alternatively clear the Closed Module event in the Audit Map Editor to view or save the File Info to a file. The original audit trail settings should be restored. Only an Analyst software Administrator can configure the audit trail settings.

Overlay on plot for isotopic distribution in calculator

Occasionally, this feature does not function as expected. However, the text is still accurate.

Incorrect status is shown in File Info

On SCIEX 5500 systems, the File Info incorrectly shows the status as "Bad" for the flow of gas for the Curtain Gas interface and interface pump. There is no interface pump on SCIEX 5500 systems. Also, although the file information will show "Bad" for the flow of gas for the Curtain Gas interface, this does not necessarily reflect the status at the time of acquisition. If during acquisition, the flow status for the gas for the Curtain Gas interface develops a true "Bad" state, then acquisition for that sample will stop with an error. (ST 8853)

Delays occur in showing the sample list

On SCIEX 5500 systems, it takes more than 90 seconds to populate the sample list for a data file acquired with more than 1,000 samples. Allow at least 90 seconds to populate the entire sample list. If more than 1,000 samples are acquired to a wiff file, then it will take at least 90 seconds to populate the sample list. The Analyst software will be able to open the file. However, we recommend that the samples be acquired into different data files, if possible.

Syringe pump method is information missing from the File Info

On SCIEX 5500 systems, details about the syringe pump used to collect the data are not shown in the File Info pane for data where a syringe pump was used. Note which flow rate and syringe diameter were used during acquisition. Alternatively, the user can obtain this information from the data file by recreating the acquisition method from the File Info by right-clicking on the **File Info** to select **Save Acquisition Method**. To recreate the method completely, make sure the hardware profile has the same devices. (ST 7861)

The Explore History file is not shown correctly

The description of all the changes is sometimes merged into one cell but it is often still legible. In some instances, some information might be missing. (ST 9481)

Changes to the offset in the History pane are not being shown

Open the History pane again to show changes to the offset. (ST 9486)

Reviewing MRM data changes the active XIC

When the user opens a saved Explore History File (eph) from a total wave chromatogram (TWC) where the data from the mass spectrometer is MRM data, the data is the overlaid XICs but reviewing the changes switches the active XIC. The listed history, however, is correct and can be used to manually apply those settings to the original data.

Occasionally, samples in data files collected at 12,000 Da/s cannot be opened

If samples cannot be opened, then open the previous or any subsequent sample and use the forward and back arrows to navigate to the sample that does not open. (ST 13169)

If data is expanded in the IDA Viewer during sample acquisition to the same data file, data from an acquired sample is not shown

No data is shown in Explore mode for an acquired sample if the data is expanded from the IDA Viewer during the acquisition of a second sample to the same wiff file. (ST 18228)

Undocking the Graph Information Window can cause the software to stop responding

Occasionally when the Graph Information Window is opened and undocked the software stops responding. This often happens when the window is left open and undocked for several hours while acquisition and processing take place. To avoid this issue, keep the Graph Information Window docked. (ST 16700)

The Q1 resolution offset table at 10 Da/s is missing in the File Information

The Q1 resolution offset table at 10 Da/s is missing in the File Information for a negative ER scan type. This does not affect the data or any future acquisition. To retrieve this information, look into a data file acquired in Q1 negative mode. (ST 13331)

Sections of ions appear to be missing in EPI scans

On SCIEX 5500 systems, when Q0 trapping is used, a fill time of at least 20 ms is required. EPI spectra acquired with a fill time less than 2 ms will result in a missing range of ions in the second mass range when Q0 trapping is On. In general, expect to see an overall decrease in sensitivity even with one mass range under these conditions. (ST 8200)

Compound Library databases with over 20,000 entries fail to show full information

When the user opens Compound Library databases that have over 20,000 entries, the individual fields do not show the full information used to populate the original database. The fields are

populated with **NA** instead. To overcome this issue, it is recommended that the user save the original database into two separate databases to be able to view all entries and then populate future entries in a new database. For example, delete the last 10,000 entries and save this database as "Part 1" and then reopen the original database, delete the first 10,000 entries and save this database as "Part 2".

Note: Deleting entries and then adding new ones is not recommended. (ST 19297)

The Analyst software stopped responding during real-time XIC data extraction

When large numbers of ions were extracted in real-time during acquisition using an MRM or *Scheduled* MRM algorithm method, the Analyst software might have become unresponsive. This issue has been corrected. However, users should be aware that there might be cases where extracting large numbers of chromatograms will still cause the software to slow or become unresponsive. For example, having multiple XIC panes open simultaneously, or acquiring data from multiple methods to the same wiff file. In these cases, users should refrain from extracting chromatograms in real-time. (AN-292)

Explore — Library Search

Blank results in new field

When performing a Library Search from an open spectrum, if the user clicks **View Manager** from the Search Results window and add a new field, then the results for this new field might seem to be blank. Clicking the field a few times causes the results to be shown. This is a graphical issue and does not affect functionality.

Hidden column in Compound Library view

When viewing the Compound Library, increasing the width of the last column might uncover a column named **Hidden**, with populated values. This is a graphical issue and does not affect functionality. Do not modify the data in this column. (ST 3165)

Editing the compound name twice might cause the Analyst software to stop responding

If the user edits the name of a compound in the library, clicks **OK**, and then attempts to edit the compound again, the Analyst software stops responding. To avoid this, after clicking **OK** to change the compound name, close and then open the library before attempting to change the same compound. (ST 2283)

Opening a library record in the default library might show a blank spectrum

If this occurs, then reconnect the library database (**Tools** > **Settings** > **Optimization Options** > **Library Manager**) to correct the issue. (ST 1860)

Explore — wiff Data File

Analyst software file compatibility

The Analyst software is fully backward compatible. However, it is not forward compatible. That is, the data files acquired in an older version of the Analyst software can be opened in the newer version of the software, but not vice versa. If the acquisition computers are upgraded to the newer Analyst software, also upgrade the processing computers to the same version.

Flat file size limit

The software can show data in the flat file (wiff.scan) for files up to 2 GB in size. Any data stored beyond this limit might not be shown correctly. In addition, larger file sizes might degrade overall performance. Begin acquiring data to a new data file if the file size nears this limit (for example at 1.5 GB).

Quantitate

With a Results Table containing more than one analyte in Full Layout, changing the Sample Type column drop down selection and then immediately, without clicking anywhere else, changing to another table layout, can cause the Analyst software to either stop working or alter the sample type of the wrong row

When the user clicks on an item from the **Sample Type** list while the Results Table is in Full Layout, and then immediately selects a different table layout that reduces the total number of rows to be shown, the current row is not updated. As a result, the software uses the same current row to update the sample type text but that row number either is no longer shown, which causes an exception or corresponds to a different row in the new table layout. To avoid the issue, click on another cell in the Full Layout Results Table after changing the **Sample Type** for any sample, then change the table layout if required. (AN-2654)

"Acquisition Methods" is shown as the acquisition method file name in the Results Table and reports for SCIEX 7500 System data files

In the Analyst software Results Table and the reports generated by the Analyst software Reporter, "Acquisition Methods" is shown as the acquisition method file name regardless of the MS method used by SCIEX OS to acquire the SCIEX 7500 system data files. To show the correct MS method and LC method file names in the Results Table and reports, use the Analytics workspace in SCIEX OS to process the data. (AN-1931)

Detector data containing channels labeled with duplicated wavelengths cannot be integrated in the Analyst software quantitation module

If detector data (PDA/DAD in 2D/Signal Mode, UV, Fluorescence, or any combination) containing channels labeled with duplicated wavelengths is processed in the Analyst software using the Quantitation Wizard, then only one of those channels is processed in the Results Table. (AN-1940)

The Y-axis maximum might become extremely high in the peak review pane for some analytes when using the option to zoom Y-axis to xx % of largest peak for all samples

Y-axis maximum might become extremely high in the peak review pane for some analytes when the option to zoom Y-axis to **xx % of largest peak for all samples** is used in the Peak Review Default Options or Peak Review Options. Double-click the Y-axis of the chromatogram for each sample to return the peak view to normal, or use the option to zoom Y-axis to **xx % of largest peak** instead. (AN-1302)

Only values of 0 or greater were exported in Quantitate mode for DAD data

If a user exports data using **Save Active to Text File** from a Peak Review pane or window in Quantitate mode, then only positive data, 0 or greater, is exported to the text file for DAD data. Negative numbers are not exported. To export a data list with both positive and negative numbers, use **Save As Text** in the Data List pane in Explore mode. (AN-1566)

The unit in the titles for the Analyte Concentration and Calculated Concentration columns in a Results Table is only for the first analyte

If a quantitation method used in a Results Table uses different units for different analytes, then the unit in the titles for the Analyte Concentration and Calculated Concentration columns in the Results Table is only for the first analyte. To view which units are used for all of the analytes, edit the Table Settings to show the Analyte Units column. (AN-1357)

Disabling a quantitation security setting causes errors when Results Table column settings are changed

Under Quantitation in the **Access to Analyst** list on the Roles tab in the Security Configuration dialog, if the **Disable, enable and clear audit trail** permission is disabled, then the user cannot change the column settings in a Results Table without getting an error each time. To change or modify table settings, make sure that **Disable, enable and clear audit trail** is enabled for that role. (AN-1018)

The Sum Multiple Ions option might produce results that are slightly incorrect

When using the Sum Multiple Ions option in a quantitation method, users might notice that the summed intensities of multiple ions is slightly different from the expected value (ion 1 + ion 2

+ ion 3 and so on). This is due to a rounding issue within the Sum Multiple Ions algorithm. In practice, the difference will be very small and should not affect reported values. (AN-1)

The changed file name of the Results Table is not shown in the Regression window

If the user performs regression in the Analyst software (Quantitation module) and then saves the Results Table using a new file name, the printout of the calibration curve still shows the original file name. The calibration curve shows the new filename only after the file is closed and then opened. (AN-555)

Adding a new column to a Result Table shows an error message but the column is added

If a new role is created in the Analyst software and the **Disable, Enable or clear audit trail (Quantitation)** privilege is disabled, then adding a new column in a Results Table generates an error message but the column is still correctly added to the table. (AN-641)

Discrepancy in Results Table file size

Depending on the number of samples, the Results Table file size might be larger than in the previous version of the Analyst software. (ST 33496)

Printouts are incorrect if manual integrations are not accepted

If the user performs a manual integration and tries to print the window or workspace without first "accepting" the changes (or completing an e-Signature, if required), the resulting printout might be incorrect. The user sees two Results Tables printed showing the areas before and after the manual integration, instead of the selected Results Table and chromatogram. If after performing a manual integration, the user accepts the change (or completes an e-Signature) or navigates to a different selection, the **Print** > **Window** and **Print** > **Workspace** commands functions as intended.

Algorithm compatibility

Scheduled MRM algorithm data cannot be analyzed with Analyst Classic. The IntelliQuan integration algorithms, IQA II and MQ III, should be used. Refer to the section: Technical Information Regarding Integration. Several behaviors are observed in the software:

- When creating a quantitation method with Analyst Classic as the preset algorithm, the software warns about algorithm incompatibility and the method uses IntelliQuan-MQ III instead. The operation does not affect the preset algorithm. (ST 5388)

- IntelliQuan Results Tables from versions of the Analyst software earlier than version 1.5 will continue to use the previous versions of the algorithms in the Analyst 1.5 software so that the results presented are consistent. This is the only situation in which previous IntelliQuan algorithms are used in the Analyst 1.5 software.

Known Issues

- The Quantitation wizard cannot create a quantitation method for a data file that contains more than 94 transitions. Before using the Quantitation Wizard to generate a Results Table, create the quantitation method using the Build Quantitation Method feature. Select this quantitation method on the Create Quantitation Set - Select Method page of the Quantitation Wizard. (ST 5919)

- Previously generated quantitation methods with the Analyst Classic algorithm cannot be used to analyze *Scheduled* MRM algorithm data. To carry forward the information, export the method as text using the Create Text File from Quan Method script and then import it using the Create Quan Methods from Text Files script. Both scripts are provided on `C:\Program Files\Analyst\Scripts\All Mass Spectrometers` folder.

- Users cannot add *Scheduled* MRM aelgorithm data to Results Tables using the Analyst Classic algorithms.

IQA II Integration algorithm occasionally does not find peaks on *Scheduled* MRM algorithm data

For *Scheduled* MRM algorithm data, it is recommended to use IntelliQuan - MQ III because the default integration algorithm, as the peak is sometimes not found in the retention time window when using the *Scheduled* MRM algorithm with IQA ll.

Default integration algorithms

Newly created projects always copy the default integration settings from the Default project. For fresh installations of the Analyst software versions 1.5 and later, the preset is IntelliQuan - MQ III. If the `Analyst Data` folder is used from a previous version, then the preset from that Default Project will carry forward to the later version of the Analyst software.

Large signal-to-noise values are sometimes reported in the Results Table

Occasionally, when very low or no noise is selected for a background, very large values to over 20 digits are reported. This might occur because there is no baseline noise for these cases. The signal-to-noise should be reported as **N/A** in these cases. Adjust the selection of the baseline to make sure that some baseline noise is applied to the signal-to-noise calculation.

Baseline Sub window

The IntelliQuan Baseline Sub window is actually a half window. The window used is twice the width that is entered. This applies both to the Integration tab of the Processing Options and IntelliQuan Parameters dialogs opened by right-clicking in a data list. (SCR 12984)

Exporting with Sum Multiple Ions produces a bad text file

Exporting a Results Table built with the **Sum Multiple Ions** option produces data in separate columns. The values are shown under incorrect headers and the text file might be incorrect. (SCR 10947)

Diode array detector results are not removed

In a DAD Results Table, even when all DAD data is removed and an ADC data sample is added, the DAD information stays in the Results Table. (SCR 7998)

The Analyte mass range column contains N/A

If an automatic quantitation method is used to build a new Results Table, then the **Analyte Mass Ranges** column contains **N/A** instead of the actual mass range for the corresponding sample and analyte, which might be all different. (SCR 8790)

Peak asymmetry error

If a Results Table is created and **Peak Asymmetry** is shown, then the column shows 0.00 if no peak is found. (SCR 10688)

Last decimal digit is inconsistent

If a Statistics table is opened for two Results Tables (by selecting **Group By Concentration** from the **Conc. as Rows** box and selecting **Area** or **Height** from the Statistics Metric box), then the last digit for some of the statistical results (Mean) could be different depending on the order in which the data files are opened. The same issue is also seen in mean calculations. (SCR 13198)

Quantitation integration mass tolerance

The algorithm for selecting a particular MRM transition from the Q1 and Q3 masses stored in the quantitation method operates as follows:

The transition whose masses are closest to the values from the quantitation method, but still within a tolerance of 0.1 Da, is used. The software determines which transition is closest by summing the Q1 mass variation and the Q3 mass variation (between the quantitation method and the acquisition method) and then selecting the transition whose variation sum is the smallest.

The quantitation of a sample with a large number of transitions might seem slow

For example:

• Generating a Results Table on the recommended computer using one sample containing 2,500 transitions can take about three minutes. (ST 9944)

• Creating or saving a quantitation method using *Scheduled* MRM algorithm data that contains 2,500 transitions can take up to 15 minutes. (ST 9944)

Adding a Formula column causes the software to stop responding

If the user performs an operation using a **Formula** column in a Summary Page in a Results Table the software stops responding. To prevent this behavior, remove the 500s in the brackets in the column names in the **Formula** field. (ST 12940)

The Cancel button is unresponsive when an unsaved quantitation method is being closed

When a workspace with an open, unsaved quantitation method is being closed, the **Cancel** button is not responsive. To close the window without saving the method, click **No** instead of **Cancel**. (ST 15477)

The Analyst software stops responding when a Results Table is exported to a non-existent directory

This issue occurs when the user specifies the incorrect path in the **File name** list by typing in the path. Make sure that the path specified exists and is correct. (ST 15992)

The Save As dialog points to incorrect folder

When users save a quantitation method that required a data file to open, the Save As dialog points to the folder where the data file was located instead of the Quantitation Methods folder. Browse to the appropriate folder before saving the quantitation method. (ST 16129)

A peak is not integrated as expected when the RT window is increased beyond 40 seconds

When the IQA II algorithm is used, RT windows larger than 40 seconds are ignored. If the user sets a window larger than this, then a window of +/- 20 seconds is used. Either adjust the expected retention time for the shifted peak, or, for batches where this is happening for many samples, use the MQ III algorithm. (ST 17676)

An error occurs during quantitation using the TIC as the Q1/Q3 selection

If the Quantitation wizard is used and the TIC is specified as the Q1/Q3 selection, then the Analyst software shows an error when the user advances the wizard. Click **OK** to successfully continue with the wizard. (ST 3242)

Column sorting

Occasionally, sorting columns in tables does not produce repeatable results. Sort on the index column to make sure that sorting is always correct.

Quick Quant with full scan methods

In the Acquisition Batch Editor, creating a Quick Quant method causes inconsistent behavior if the acquisition method selected is a full scan method. After saving this method, users cannot open it. Quick Quant works as expected with all other scan types. It is recommended that users do not use Quick Quant with full scan methods. (SCR 9866)

New Quick Quant methods do not apply new quantitation default values

New Quick Quant methods generated through Build Acquisition Batch do not use the modified quantitation default values specified on the Quant Method Editor Settings dialog. (SCR 6997)

An intensity drop might be observed when a *Scheduled* MRM algorithm experiment is run with masses greater than 1,000 Da

Avoid using masses above 1,000 Da in *Scheduled* MRM algorithm experiments. In these instances, it is recommended that you use the MRM scan type. (ST 11772)

Some items unavailable under the Administrator role for the Quantitate module are available

Although the **Change default number of smooths (in Wizard)** and **Change concentration units (in Wizard)** are not available for the Administrator under role-based security, a user with the Administrator role still has access to these features in the wizard. (ST 19149)

The concentration units specified when a quantitation method is created do not propagate to the Results Table if different units are used per analyte

Although a user can enter different units for different analytes when creating a quantitation method, only the first set of units is used in the Results Table. (ST 19151)

Incorrect data is shown in the calibration window

The data in the calibration window might not be consistent with the Results Table if few peaks are found in the Results Table. To correct this issue, refresh the window by saving it. (SCR 11282)

Analyst Software Reporter

An incorrect operator might be shown in the Analyst software Reporter for samples appended to a data file

If samples were appended to an existing data file that was acquired by a different user from the current user who submitted the appended samples, then the Operator tag, if included in the report template, shows the name of the user that first created the data file for the appended samples, not the one who actually submitted those appended samples. (AN-1612)

Analyst software Reporter cannot create reports on computers with SCIEX OS installed first

On a computer with SCIEX OS already installed, installing the Analyst software causes the Reporter not to work. A report cannot be created due to an unhandled exception error. However, if the Analyst software is installed first, and then SCIEX OS is installed, then the Reporter works, even if the Analyst software is sequentially upgraded to a higher version from the current configuration where the Analyst software was installed first, and then SCIEX OS was installed. (AN-2032)

A report cannot be generated when the Library search template is used in the Reporter 3.2 software

When the user tries to create a report using the Library Search template in the Reporter 3.2 software, an error message is generated that the report cannot be created. To resolve this issue, contact SCIEX support at sciex.com/request-support. (AN-39)

The Reporter Template Editor might not show the Tags panel for the Blank Template

When the Blank Template in Reporter is edited, the tags panel might not be shown by default, depending on the version of Microsoft Office used. If the panel is not visible, then users can make it visible by selecting **View** > **Document Editor**, followed by **View** > **Document Actions**. (AN-250)

Chromatograms are not shown if the Label field contains information

When a Reporter template is created, if the user adds a chromatogram and then types anything in the label field for the tag, then the printed report does not show the chromatogram. To avoid this issue, make sure that the label field is empty. (AN-255)

The Reporter Template Converter is unable to convert four templates

The Reporter Template Converter is unable to convert the following templates: `Select Analyst 20 percent Report.xml`, `Sample Report with MRM ratios.xml`, `Sample Report with MRM ratios2.xml` and `Sample Report with MRM ratios EU.xml`. Users will receive an error message when attempting to convert any of these templates. (AN-258)

Chinese characters might be unreadable in Reports

When the Reporter 3.2 software is used to print reports using Chinese fonts, the spacing between characters might be too small to allow the report to be easily readable. This might happen when printing to Word or PDF formats. If this happens, select the option to print to HTML format, as this format spaces the characters appropriately. (AN-131)

Adobe Acrobat might stop responding after printing to PDF

If the user selects both of the **Print to PDF** and **Print Automatically** options, then after the report is generated, Adobe Acrobat opens but stops responding. If the user manually closes

Adobe Acrobat, the report opens automatically as a PDF. This is a workflow defect and does not affect the generation of the actual report. (ST 35621)

Report names containing periods might cause the Reporter to stop responding

When creating a report, if users specify a filename that contains periods ('dots'), they must also specify the file extension. Failing to do so causes an error to be generated: "Failed to process the report file. Unsupported format requested." For example, specifying a report as "report 1.2.3" causes Reporter to stop responding. Specifying "report 1.2.3.docx" generates the report as intended. The extension must match the format selected in the Reporter software. (ST 35636)

Installer

A message about `DCOMPerm.dll` might be shown during Analyst software installation

During the installation of the Analyst 1.7 Software with HotFix 1 or later versions of the Analyst software, the installation program might show the message: "Cannot move `DCOMPERM.dll` while installing DCOMPerm. Win32 errrorcode 262272. Please contact your software manufacturer.". Click **OK** in the message to continue with the software installation. This may be caused by CTC PAL scripts. If a CTC PAL autosampler will be used, then test whether the hardware profile with the CTC PAL autosampler can be activated after installation. If not, then contact SCIEX support at sciex.com/request-support. Otherwise, the software works as intended. (AN-767)

The Analyst software cannot be upgraded or reinstalled if the Waters Acquity LC Device Driver has been installed on the computer or was previously installed on the computer and then removed

If the Waters Acquity LC Device Driver has ever been installed on the acquisition computer, even if it was later removed, users might have difficulties upgrading the Analyst software on the computer or reinstalling it. This might result in users losing their instrument tuning files. The issue is caused by the Waters driver and Waters support has been advised.

To avoid this issue, before performing an upgrade installation or re-installation of the Analyst software, always make sure to restart the computer right before opening the Analyst software `setup.exe` file. (AN-692)

Smart Services runtime error

Occasionally, a Smart Services runtime error appears when the HotFixes are installed on uninstalled. Click through the error. The error does not affect the installation or removal of the HotFixes. This error occurs only when Smart Services Mass Spec Gateway v 4.1 is installed. (ST 11498)

Other

Printing a workspace in Analyst software might cause Analyst software to stop responding

Printing in the Analyst software from > **Print** > **Workspace** might cause the Analyst software to stop responding. As a workaround, print from > **Print** > **Windows**. (AN-2079)

The Nebulizer Current status is not shown correctly in the Detailed Status window

On SCIEX 5500 systems, the Analyst software does not display the **Nebulizer Current** correctly in the Detailed Status window while the instrument is in operation. A value of 0 is shown but this does not accurately reflect the actual applied current. Contact an FSE if no change in performance is observed when the nebulizer current is changed in the method or if an issue with the nebulizer current is suspected.

Compatible Software

Automaton software support is discontinued

The Analyst software does not support the Automaton software. The Automaton software package is replaced by the DiscoveryQuant software.

Some LightSight software versions cannot create GSH precursor ion IDA methods

The LightSight software for metabolite identification is unable to create GSH precursor ion IDA methods when the molecular weight of the molecule is greater than 550 Da. In version 2.0 and 2.1, the LightSight software cannot create GSH Prec IDA methods and in version 2.2, the software cannot create GSH Prec IDA and GSH Prec/NL IDA methods. The LightSight software can create GSH Prec methods for molecules with a molecular weight greater than 550 Da only if an IDA method does not need to be created.

AAO Development Kit

Third party developers can find the AAO Development Kit on the Analyst software DVD or the web dowload package, whichever is available, in the `\Extras\AAO` folder. The kit contains a user guide, release notes, source files, sample code, and so forth.

When setting up a root directory for the AAC, make sure that the path name does not include the word "Projects"

When setting up a root directory for Analyst Administrator Console (AAC), make sure that the path name does not include the word "Projects". If the path name includes the word "Projects", then a series of messages are returned to the user that prevent the user from logging into the Analyst software through the AAC. The messages might indicate that the user does not have

access to the projects in the Workgroup to which they belong or that the projects included in the Workgroup do not exist. Contact the administrator to rectify this issue. (ST 19394)

Connection from AAC to the AAC server

Connection from the AAC to the AAC server should be made using the IP address and not the AAC server name. (ST 31068)

Scripts

The sorting feature for a column in the sMRM Calculator script might not function correctly when the number of digits before the decimal is not the same for all MRM transitions

When a method is loaded in the sMRM Calculator script, sorting in an increasing or decreasing order for a column might not function correctly. If the number of digits before the decimal for all MRM transitions in a column is the same (example: all RTs are greater than 1 minute but less than 10 minutes), there is no issue with sorting. There might be an issue if some RTs are less than 10 minutes and some are greater than 10 minutes (example: RT=1.2, 2.5, 10.6). (AN-1353)

The Convert Methods script does not show an error message on method conversion failure

The Convert Methods script does not generate an error message when it is unable to convert an acquisition method with Q1/Q3 above 1,250 for a SCIEX 6500 High Mass or SCIEX 6500+ High Mass system into a method for a SCIEX 5500 system. The **Save** button is not available indicating that the method conversion cannot proceed. (AN-128)

The Purge Modifier script does not work if the Analyst Data folder is stored on a network drive

For the Purge script to work, the `Analyst Data` directory must be stored on the local computer. (AN-505)

The Convert Methods script causes converted method to lose precision

In the acquisition methods converted using the Convert Methods script, the Q1/Q3 masses are rounded to the nearest second decimal place, making these values different from the original method. (AN-702)

Users should not launch scripts from the Analyst software folder in File Explorer

Some Analyst software scripts are available as exe files within the Analyst software folders. However, these scripts should not be launched manually. They should only be launched from within the Analyst software. (AN-120).

Known Issues

The AutoQuant with Automatic Reports.dll script does not support *Scheduled* MRM algorithm data

When the BatchScriptDriver Script is run and if a *Scheduled* MRM algorithm data file is selected to be processed with the AutoQuant with Automatic Reports.dll script, then an error message is shown, indicating that samples are not compatible with the quantitation method. Users can process MRM data successfully. (ST 9052)

The LabelXICs script labels traces with zeroes

If the LabelXICs script is run using *Scheduled* MRM algorithm data, then the XIC trace is labeled with zeroes. The mass corresponding to each XIC can be found in the header of the data file. (ST 6109)

The Mascot script fails to run for single EPI spectra

The Mascot script fails to run for single EPI spectra or for summed EPI spectra acquired with **MCA** turned on. Click **Explore** > **Show TIC**, highlight the entire TIC or highlight a small region around the peak of interest and then run the Mascot script. By default, the search option **All MS/MS spectra from selected region(s) in TIC** is selected. This option will run correctly. (ST 8856)

The Exclusion List cannot be imported into an IDA Method

The **Exclusion List** created from the Make Exclusion List From Spectrum script cannot be imported in an IDA method. To avoid any issues, enter headers in the list in the format provided by the returned error message. (ST 2027)

The mass range for Q1 and Q3 scan data is not extracted

Occasionally, the XIC From Table script does not extract the entire mass range for Q1 and Q3 scan data. The error message that is shown, indicating the mass ranges that can be extracted, can provide further guidance. Reopening the data file and then restarting the script might also correct this issue. (ST 9646)

Subsequent integrated area are not showing

When the Manually Integrate Script is run to integrate consecutive peaks, the blue integrated area is visible only for the first run of the script for the first peak. Subsequent integrations using the script do not show the blue area and the caption from the last integration remains. Reopen the data file and then run the script again to see the integrated area. (ST 9650)

Incorrect ramp information is given for the AF2 parameter

On SCIEX 5500 systems, the MS3QuantOptimization Script reports the incorrect ramp information for the AF2 parameter. The report shows that the AF2 parameter is ramped from

0 to 100 mV with a step size of 2 mV. The actual ramp range is 0 to 0.3 V with a 0.025 V step size. (ST 9821)

The AF2 graph is not always legible

Occasionally, the AF2 graph produced by the MS3QuantOptimization script is illegible during acquisition in the script user interface. This occurs only for graphs for which there is no resulting spectral information. This does not affect the operation of the script. (ST 9822)

The starter method must have a syringe pump enabled for the MS3QuantOptimization script

Make sure that the starter method has a syringe pump enabled. Open the starter method. If the syringe pump has a cross, right-click to select **Use** to enable it, and then save the method. If the syringe pump is not enabled, then the syringe pump will not run when the script is executed.

The Merge MRM Methods script causes the Analyst software to stop responding if the hardware profiles being merged do not match

The Merge MRM Methods script causes the Analyst software to stop responding if the hardware profile does not match the hardware profile used to create the methods being merged or if the matching hardware profile is not active. To prevent this issue, make sure that the hardware profile activated in the Analyst software matches the active hardware profile for the MRM methods being merged. (ST 17455)

The Merge MRM methods script does not merge the Compound ID

Enter the **Compound ID** manually. (ST 2474)

An error when Subtract Control Data from Sample Data is selected on the Scripts menu

Press **Shift** while selecting the script. An About dialog opens and the script runs. (ST 6208)

The XIC from BPC script causes the Analyst software to stop responding

Do not use this script. (ST 6209)

Inclusion and Exclusion lists are not copied when IDA methods are converted using the Convert Methods script

To prevent this issue, edit the masses in the **Inclusion** and **Exclusion** lists of the original method to fit within the accepted range of the destination method. (ST 18986)

Methods with LIT scan types that have mass ranges greater than 1,000 Da cannot be converted to QTRAP 5500 system methods using the Convert Methods script

To avoid this issue, change the mass range of the original method to fit within the acceptable range of the destination method. (ST 18670)

Convert Methods script

After a method is created using this script, review the new method to make sure that the method has been converted to correctly.

Peripheral Devices

ExionLC 2.0 Series Devices

The ExionLC 2.0 system status icon in the Analyst software is red but shows Ready

If an error occurs on the ExionLC 2.0 system, then the LC status icon in the Analyst software turns red but Ready might be shown as the LC status. To recover, deactivate the hardware profile and then activate it again. Make sure that the detector lamps are on and ready before starting acquisition, especially after the system has gone through Standby state. (AN-1966)

The Analyst software shows the ExionLC 2.0 system in Wait state when it is in Standby state if the LC system contains a detector

If the ExionLC 2.0 system contains a DAD or Multiwavelength detector, then after the LC system and mass spectrometer go to Standby state, the Analyst software status icon for the ExionLC 2.0 system turns yellow, but the LC system state is shown as Wait. This occurs because the detector lamps are turned off when the system is in Standby state. This is a status display issue and does not affect system operation. (AN-1968)

A method cannot be saved when valve wash is selected in the ExionLC 2.0 wash system settings

Intermittently, when valve wash is selected in the ExionLC 2.0 wash system settings, the method might not save successfully, instead showing an error message "Error writing acquisition method to the file! Copy method failed." If this issue occurs, then do the following:

1. Deactivate the hardware profile and then close the Analyst software.

2. Delete or rename the `Configuration_Default.xml` file (`C:\ProgramData\ExionLC2.0\Configurations`) and the `ExionLC2` folder (`C:\ProgramData\SCIEX`).

3. Restart the computer.

4. Turn off all of the ExionLC 2.0 system modules and then turn them back on.

5. Create a new hardware profile, reconfigure the ExionLC 2.0 system, and activate it. (AN-2246)

Every two data points are duplicated for the ExionLC 2.0 pressure trace

For the ExionLC 2.0 pressure trace, every two data points are duplicated. This is because the pressure values are collected at half of the frequency (0.5 Hz) of the publishing rate (1 Hz). In addition, the first data point at time 0.0 min for all of the auxiliary traces are artificial since the first actual point is usually collected at time greater than 0.0 min. (AN-2638)

ExionLC System or Shimadzu Devices

Acquisition using an ExionLC PDA might intermittently fail when all samples are acquired to a single data file

When all samples are acquired to a single data file, especially when the data file is large, using the ExionLC PDA, the acquisition might intermittently fail. To avoid this issue, acquire each sample to a different data file (multiple wiff files). (AN-1823)

The room temperature trace is written when the LC system does not have a room temperature sensor

For the ExionLC and Shimadzu LC system with auxiliary trace enabled, the room temperature trace is written and stored with the data file when no room temperature sensor is present with the LC system. The trace might incorrectly show temperatures such as 650 °C. (AN-2559)

The current list of auto-configured ExionLC system devices in the hardware profile is overridden by the list of devices from the last successfully activated hardware profile

When the ExionLC system devices are used, in rare cases, while auto-configuring the devices in the ExionLC system during hardware profile creation, the **Devices in use** list in the SCIEX LC Configuration window might show the ExionLC system devices from the last successfully activated hardware profile. In such a case, the hardware profile cannot be activated because of the mismatch between the devices listed in the hardware profile and the devices in the stack. The work around is to delete or rename the file `Configuration_Default.xml` in `C:\ProgramData\Shimadzu\LCMimic2\Configurations`, and then auto-configure the devices again. (AN-1023)

ExionLC autosampler internal rinsing-related issue

In the acquisition method with ExionLC system devices, if 1, 2, or 3 rinse solvents are selected in the Internal Rinse settings section, then the internal rinse does not take place. The workaround is to select 4 solvents to start the internal rinse. Users will need to decrease rinse volume to compensate for the added rinse time. Also, to start the rinse process, use the

following setting in the Rinse sequence: R0->None->None->R0. This issue might occur if the start or end of the rinse sequence is set to **None**. (AN-1086)

Configuration of a newly created or edited hardware profile for an ExionLC system is being applied to all existing hardware profiles that contain ExionLC system devices

If the configuration of a hardware profile containing an ExionLC system device is changed or if a new hardware profile containing any of these devices is created, then the configuration of existing hardware profiles containing any of these devices is also changed automatically. All configuration options such as Fast LC, psi units, relays, sync, system pressure max, and so on are saved to every other hardware profile containing an ExionLC system device, even if the edited or newly created hardware profile is not activated. For example, if there is an active hardware profile that includes a binary gradient ExionLC Pump and the user creates a hardware profile that includes an isocratic ExionLC Pump but does not activate the profile, then the active hardware profile becomes isocratic as well. (AN-943)

ExionLC devices: The Configuration UI dialog opens in the background behind all other open windows after a fresh Analyst software installation or after the computer is restarted

During hardware profile creation for ExionLC series devices, when the **Configure** button is clicked, the Configuration UI dialog opens in the background behind all of the other windows. This happens after installation or after the computer is restarted. To bring the ConfigUIDialog to the foreground (after clicking **Configure**), minimize all of the open applications until the ConfigUIdialog is visible. After this, every time **Configure** is clicked, the Configuration UI dialog will always open in the foreground. (AN-717)

If the Remote Instrument status feature is used in the Analyst, then the detailed status for a connected ExionLC devices stack is not shown

The detailed status of the connected LC devices stack is blank when viewed from the Remote Instrument Status. (AN-686)

Some methods with errors from LC can be saved but cannot be opened

When an acquisition method with an ExionLC method parameter outside of the allowed range is saved, the Analyst software generates an error about the wrong value but allows the user to save the method. However, this method cannot be loaded after being closed and cannot be used for acquisition. (AN-678)

In Manual Tune, all the parameters for pump, autosampler, and system controller are not shown when LC method is selected for ExionLC devices

When **LC Method** is selected in the Manual Tune mode for a hardware profile containing ExionLC devices, the timetable (located on the right side of the Pump, Autosampler, and System

Controller tabs) is not shown. As a workaround for this issue, create the acquisition method in the Acquisition Method Editor, save it and then open it in Manual Tune mode. (AN-644)

Users cannot configure a Shimadzu or ExionLC LC System in hardware profile setup

The Integrated System Shimadzu LC-40 Controller, Integrated System Shimadzu LC-20/30 Controller, and Integrated System SCIEX LC Controller use the MIMIC 2 driver. Occasionally, after this version of the software is installed, the user cannot configure a Shimadzu or ExionLC LC system device in the hardware profile through these controllers. To resolve this issue, delete the `Configuration_Default.xml` file from `C:\ProgramData\Shimadzu\LCMimic2\Configurations`, start the computer again, and then configure the device. If an existing hardware profile contains an LC device that uses the MIMIC 2 driver, then the user must complete auto-configuration again after the computer is started. (AN-1774)

Note: This issue can also occur if the Analyst 1.7.3 software is removed and then the Analyst 1.7.1 software is installed.

A hardware profile configured with a Shimadzu or ExionLC LC System might fail to activate

When the Analyst software or the AnalystService stops unexpectedly after a hardware profile configured with a Shimadzu or ExionLC LC system has been activated, a *device failed to initialize* error might be shown when the user tries to activate the hardware profile again. To resolve this issue, start the computer again, and then activate the hardware profile. (AN-1781)

A method with invalid LC parameters can be saved with an error but cannot be opened

When an acquisition method with an LC parameter outside of the allowed range is saved, the Analyst software shows an error about the wrong value but generates the method. However, this method cannot be opened after being closed and cannot be used for acquisition. This issue is applicable for most LC systems, including the Shimadzu LC-40 system. Agilent LC systems are not impacted. (AN-1813)

In Manual Tune, not all of the options for the modules are shown when an LC method is selected for Shimadzu LC-20/30 devices activated through the Integrated System Shimadzu LC-20/30 Controller, or for Shimadzu LC-40 devices

If an LC Method is selected in Manual Tune for a hardware profile containing Shimadzu LC-20/30 devices activated through the Integrated System Shimadzu LC-20/30 Controller, or for a hardware profile containing Shimadzu LC-40 devices, then the following options are missing from the right side of the module window:

- Time Program option, for all modules that have the Time Program option enabled in the Acquisition Method Editor

- Pretreatment option, for the Autosampler module

- Pump mode switching option (B. GE vs ISO), for the LC-40 Pump module

- Autopurge option, for the LC-40 Pump module

As a workaround for this issue, create the acquisition method in the Acquisition Method Editor, save it, and then open it in Manual Tune mode. (AN-1812)

The Shimadzu HPLC stack does not go into Standby state when Standby is selected during equilibration

The Shimadzu HPLC stack does not go to Standby state when Standby is selected during the equilibration period. The mass spectrometer goes to Standby state but the pump and oven continue to run. As a workaround, first press **Ready** and then press **Standby** during equilibration. (AN-663)

AutoConfig shows the same serial number for all pumps

The Shimadzu driver included in the Analyst software adds the ability to automatically scan and configure the hardware profile based on the devices attached to the CBM module. A defect in this driver causes all connected pumps to show the serial number of the first pump. However, if the devices are manually configured using the integrated device driver in the Analyst software, then the File Info for acquired data reflects the correct serial numbers. (TT 35101)

The layout of the 1.5 mL cooled rack has been changed

A new high capacity 1.5 mL cooled rack has been introduced for the Shimadzu LC-30 series autosampler. The layout of this rack has been changed to accommodate the 105 vials and therefore cannot be selected using the existing 1.5 mL Cooled rack option from the Location tab in the Batch Editor. To use this new rack, select the 1.5 mL Standard rack. The new rack will still be cooled. (ST 34061)

The IP address must be typed to establish an Ethernet connection

When establishing an Ethernet connection, the Shimadzu device search function cannot retrieve the IP address from the Shimadzu CBM. Users must type the IP address. (ST 29400)

If a different user logs on to the Analyst software, then the Shimadzu AAO might stop responding

In Mixed Mode, if a different user logs on to the Analyst software, then the Shimadzu AAO might stop responding. If this issue occurs, stop the AnalystService and the `ShimadzuAAO.exe` using Task Manager and then start the Analyst software. (ST 33331)

Batches can fail if the post treatment cycle does not complete before sample acquisition has completed

For the Shimadzu LC-30 series autosampler, when creating an acquisition method, do not select **After Acquisition** from the **Rinsing Start Time** list on the Internal Rinse dialog. Select **Specify**

Start Time or do not use this option in the acquisition method. The internal rinse must be completed before the sample acquisition has completed. (ST 33825)

Queue functionality is lost
Performing an abort when a Shimadzu device is in the Equilibrate mode (by manually putting the device in the Standby or Ready state before Equilibration has completed) results in a loss of queue functionality. To regain control of the queue, stop the AnalystService and power-cycle the Shimadzu stack. (SCR 9588)

Shimadzu SIL-10AF and SIL-10Axl autosamplers are not supported

The Shimadzu SIL-10AF and SIL-10Axl autosamplers are not supported even though the option exists in the Analyst software Hardware Configuration Editor. Do not select these autosamplers because the user might not be able to activate the hardware profile.

Enabling additional devices in the Shimadzu Prominence stack might require a reboot of the stack

When additional devices are enabled in the Shimadzu Prominence stack (such as the rack changer), a full reboot of the stack might be required to allow the hardware profile to be successfully activated in the Analyst software.

Loss of synchronization occurs when short acquisition times are specified for a Shimadzu Prominence stack

A loss of synchronization between the Analyst software and the Shimadzu Prominence stack might occur if the acquisition time specified is shorter than the time required for the autosampler to complete the rinse washes. Make sure that the MS acquisition method is at least one to two minutes long.

The pump pressure maximum limit might need to be increased during creation of a Shimadzu method

The default pump pressure maximum limit might be too low and might lead to pressure errors on the hardware and subsequent acquisition errors. Therefore, the default limit might need to be increased when Shimadzu methods are created.

No error message is shown when a Shimadzu deep-well plate is missing

If a deep-well plate is missing in the Shimadzu autosampler, then the autosampler fails to detect it and the run proceeds without the software being notified of any error.

Known Issues

Issues occur when AnalystService is restarted

If the user restarts the computer or the AnalystService.exe (with the Windows Services control panel), then the system might stop responding. Power-cycle the Shimadzu controller and then activate the hardware profile in the Analyst software to help restore the system. (SCR 13266)

The user needs Windows local Administrator rights to modify the hardware profile

To create or modify hardware profiles that include Shimadzu devices, the user must be a Windows Local Administrator or have equivalent permissions. (SR 11858, SCR 13261)

The wrong vial number is sent to the autosampler

When Shimadzu devices are used, the wrong vial number is sent to the autosampler if rack type 4 is in use. (SCR 12010)

Reset the device from the controller manually

Reset the Shimadzu autosampler from the controller after an abort or failure. Currently, there is no way for the Analyst software to do this automatically. (SCR 10532, SCR 12921)

Issues occur because of a mismatch of duration time

The default duration for Shimadzu methods is 90 minutes. When tuning with a mass spectrometer scan duration shorter than the Shimadzu time program duration (as in the default tune method), the user is not able to stop the tune run using the Analyst software after the mass spectrometer has finished scanning. Press **run** on the controller or change the default Shimadzu time program duration to match the MS duration in the Shimadzu method editor. (SCR 9515)

Clearing Fail whole batch in case of missing vial does not work

Clearing this feature found in **Tools** > **Settings** > **Queue Options** does not work. The batch fails regardless of whether the user has selected this check box.

Shimadzu Rack Changer racks are incorrectly labeled

Currently, the Shimadzu Rack Changer racks are labeled as follows: 1.5 mL Vial Cooled, MTP 96 Cooled, MTP 384 Cooled, Deep Well MTP 96 Cooled, and Deep Well MTP 384 Cooled. The Shimadzu Rack Changer racks are not offered in the cooled format but are incorrectly labeled with the "Cooled" suffix. Ignore the "Cooled" suffix. These trays do not provide the cooling capability. (ST 18032)

CTC PAL / Leap Devices

The batch fails to continue on a missing vial error for a CTC PAL autosampler with the dynamic load and wash (DLW) feature

If a CTC PAL autosampler is used with the DLW feature, then the batch fails to continue if it encounters a missing vial error, even though the **Fail whole batch in case of missing vial** option is not selected in the Analyst software Queue Options dialog. The workaround is to not use the DLW feature with a CTC PAL autosampler. (AN-1004)

The Locations tab does not show tray type or stacks correctly for a CTC autosampler with mixed stacks

When a CTC autosampler with mixed stacks is used, the Locations tab in the Analyst 1.7.3 software does not show trays or stacks correctly, and does not allow vials to be selected properly, which in turn prevents user from using the Locations tab to create batches. To avoid this issue, select **trays and sample locations** on the Sample tab in the Batch Editor. (AN-381)

CTC software update

If applications, such as the CTC Cycle Composer or CTC Cycle Editor, use the CTC SDK earlier than version 1.6.0.3, then the SDK might not work after the Analyst software is installed. Contact the manufacturer for the latest versions of the CTC software. (ST 32245, ST 33375)

Enabling and disabling barcode reading

The CTC PAL Autosampler Method Editor now contains an **Enable Barcode Reading** check box. Selecting this check box (flag **ON**) activates the barcode reading and storing feature. Clearing this check box disables barcode reading.

Figure 4-1 Enable Barcode Reading Check Box
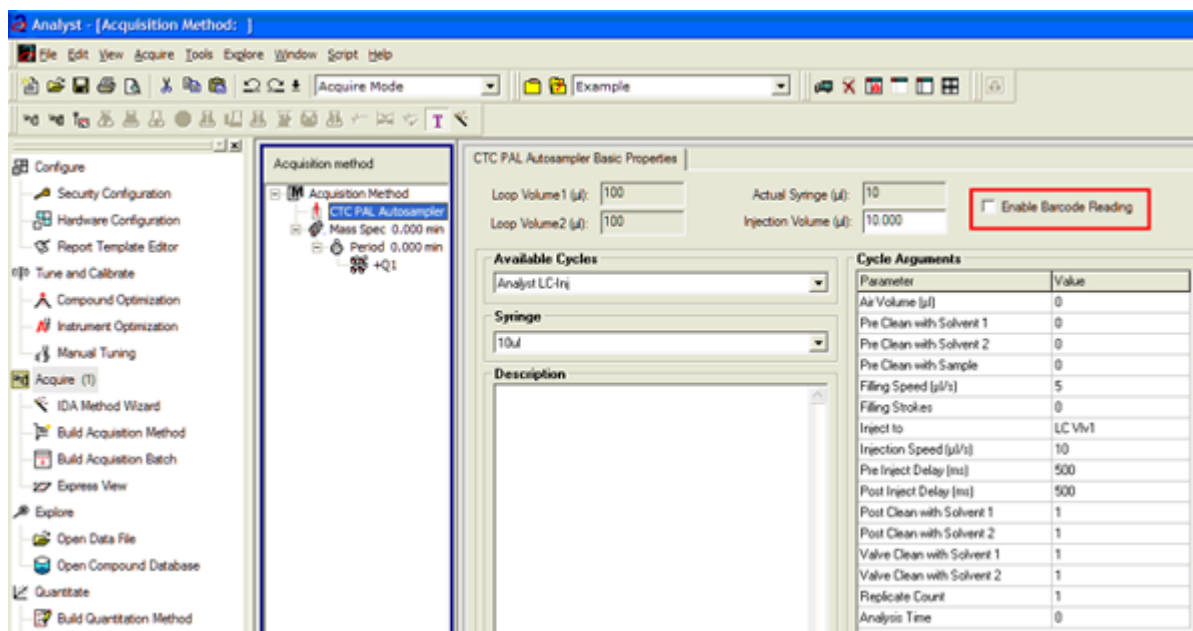
Barcode readings fail

If a barcode reading is attempted but fails (for example, because of torn, misplaced, or missing labels), then the barcode information for that particular sample is shown and stored as **N/A**.

Barcode reading is disabled

If the user disables the barcode reading feature, then no barcode information is added to the data file, and Results Tables created from these files do not show a **Scanned Barcode** column. If a mixed group of samples, some with barcode information and others without, are used to create a Results Table, then the samples lacking barcode information show **N/A** in the **Scanned Barcode** column.

Issue with multiple trays assignment

CTC Batch Editor Location tab sample assignments do not work correctly if a tray position has multiple trays assigned. Set the sample tray and vial positions on the Sample tab instead. (SCR 12921, SCR 12923)

A message is shown when removing the CTC cycle editor (version 2.0.7)

When the CTC Cycle Editor is removed, the message Remove Shared Files? is shown. Click **No**. If the user clicks **Yes**, then some required files installed by the Analyst software are

removed, and the Analyst software fails to activate the hardware profile that contains the CTC PAL autosampler.

The hardware profile must be reactivated to use the new custom cycles

Reactivate the hardware profile to view the new custom cycles created using the CTC Cycle Editor. (SCR 13501)

The Injection valve switches when the CTC method is stopped

The CTC injection valve switches after abort during injection. This can affect chromatography of the subsequent analyses.

The terminal unlocks when the CTC method is stopped

The CTC PAL terminal unlocks when the CTC method is stopped. To lock the CTC, reactivate the hardware.

Network data folder

The CTC PAL data folder must be on a local drive. If it is on a network drive, then the hardware profile does not activate. (SCR 11665)

DAD Devices

Use a single wiff file for large data

If a large amount of data is acquired using a Diode Array Detector (DAD) to a single wiff file, then the file might become corrupted. To prevent issues, always acquire DAD data to multiple wiff files if a large number of samples are acquired.

Agilent Devices

Integrated Agilent LCs stop running the LC method at the mass spectrometer stop time not the pump stop time

If the mass spectrometer method duration is shorter than the Agilent LC method duration, both sample acquisition and the LC run stop at the mass spectrometer stop time. To prevent the issue, set up the acquisition method with the same stop time for the mass spectrometer and the LC method. (AN-2657)

Acquiring DAD data at rates greater than 20 Hz is not recommended

For the Analyst software, the guidance is 20 Hz and less. Using higher acquisition rates causes the acquisition to take much longer than expected. (ST 25396, ST 35524)

The Agilent 1260 Pump G4220B is not supported (ST 33318)

Agilent Pumps	Compatibility
Agilent 1260 and 1290 pumps	The Agilent 1260 and 1290 pumps cannot be used in the same hardware profile. (ST 33313)
Agilent 1260 G1329B configuration	The Agilent 1260 G1329B autosampler must be configured as an Agilent 1200 G1329A autosampler to operate. (ST 34104)
Compatibility with Agilent 1200 Methods	Acquisition methods that were created for Agilent 1200-series devices can be opened and used if the current hardware profile includes Agilent 1260-series devices that are functionally equivalent to the 1200-series devices used in the method. The following devices are functionally equivalent: • 1200 G1312B Binary Pump SL and 1260 G1312B Binary Pump • 1200 G1316A Column Oven and 1260 G1316A Column Oven

Note: For methods to be compatible, all of the devices in the currently active hardware profile must be the same as, or functionally equivalent to, the devices used in the original method.

Note: If a previously created (1200) acquisition method is used to acquire data with a functionally equivalent 1260-series device, then the File Info shows that the acquisition method was created with a 1200-series device. To avoid this issue, open the acquisition method with the new 1260-series device active in the hardware profile and then save it (or save as a new method and then use the new method for acquisition).

Purging and priming issues using the Analyst software

The 4220A Binary Pump uses an integrated software-controlled purge valve.

The Analyst software supports this functionality in both the Acquisition Method Editor and Manual Tuning through the **Purge** option.

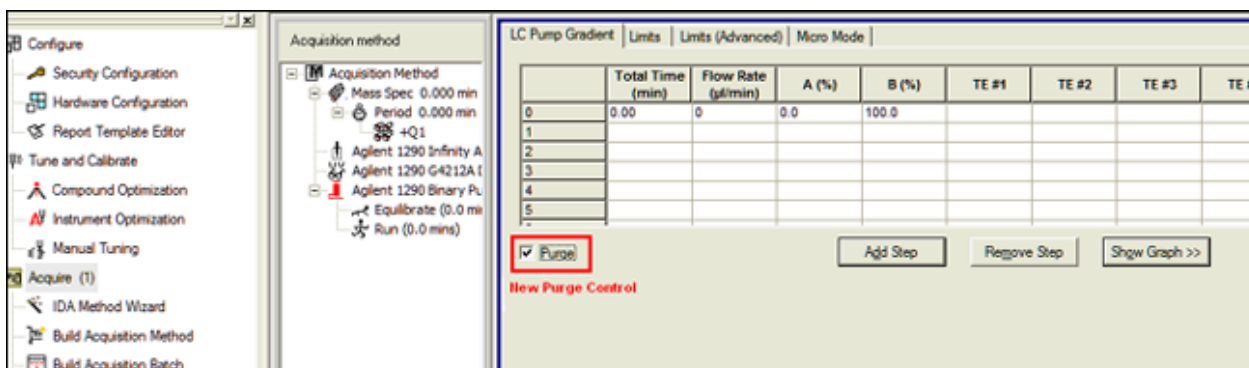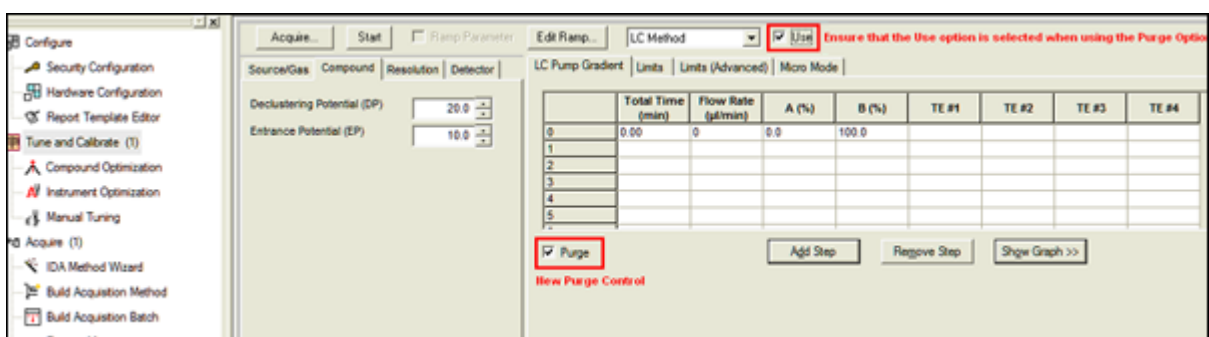**Figure 4-2 Purge Option in the Acquisition Method Editor**

Figure 4-3 Purge Option in Manual Tuning

When the **Purge** option is activated, the Agilent 1290 Binary Pump opens the purge valve, allowing system purging.

To create a purging method, use only the **Total Time**, **Flow Rate**, and **A/B(%)** fields. Values entered in the Limits, Limits (Advanced), and Micro Mode tabs are ignored.

Use Manual Tuning to purge or prime the system or create an acquisition method to be used exclusively for purging. This method can be submitted with the Acquisition Batch Editor in the same manner as acquisition methods. In this scenario, the mass spectrometer acquires data to the specified wiff file.

Figure 4-4 Example Acquisition Batch with a Purge Method Before Acquisition

Changes to DAD acquisition

The Agilent 4212A and 4212B DADs have a single lamp source. The usable wavelength range is 190 to 640 nm. Additionally, the 4212A DAD supports slit widths up to 8 nm, and the 4212B has a fixed slit width of 4 nm.

Baud Rate for Serial communication

If the Agilent 1290 or 1260 stack is configured for serial (RS232) communication, make sure that the baud rate is set in the Analyst software to 19,200.

Fractional injection volumes are not supported for Agilent autosamplers

When fractional injection volumes are requested, the decimal portion is truncated and only the integer value is injected. For example, if an injection of 2.5 µL is attempted, the actual injection is 2 µL. (ST 28340)

A hardware profile containing an Agilent DAD 1315D cannot be activated

When attempting to activate a hardware profile containing an Agilent DAD 1315D that has an incorrect IP address assigned to it, the Analyst software stops responding. Make sure that the IP address is the actual address of the DAD.

Agilent wellplate

Agilent well plate autosamplers generate a fault when a vial is missing. Reactivate the hardware profile and device to recover. (SCR 12060)

Agilent 1200 peripheral devices cannot use CAN connections over Ethernet

To use these peripheral devices, configure each peripheral independently using an Ethernet connection through an Ethernet hub or connect each using an RS-232 cable. (ST 16108)

LC Packings Devices

The device has issues locating reagent vial positions

The Famos Autosampler User Defined Program (UDP) does not properly locate Reagent Vial positions. (SCR 12204)

Users must define pressure in bar units

If the UltiMate Integrated System is used, then select the pressures in bar units. (SCR 9257, SCR 13863)

Missing vials cause acquisition issues

Acquisition issues might occur if there are missing vials in a large batch with LC Packings devices (both Famos and UltiMate). (SCR 9353)

PerkinElmer

The last decimal number is missing in the Status dialog

The flow rate of a PerkinElmer pump reported in the Status dialog during acquisition is missing the last decimal number. For example, if the pump flow rate is 0.075 mL/minute, then the report shows 70 µL/minute instead of 75 µL/minute. (SCR 11370)

Tempo MDLC System

Acquisition using the Tempo™ MDLC system occasionally stalls

Occasionally, a sample in a batch submitted to the Queue shows as Acquiring even after the acquisition time is complete and the remaining samples show a status of Waiting; the batch never advances to the next sample. This issue is intermittent. If it occurs, then resubmit the remaining samples.

21 CFR Part 11 Compliance 5

The Analyst software can be used to make sure that the site complies with the 21 CFR Part 11 Electronic Records and Electronic Signatures regulations. This compliance relies on the ability of the administrator ability to create a secure environment for generating, analyzing, and storing data. Compliance often involves the software of many different vendors for functions ranging from laboratory information management system (LIMS) to data acquisition and from processing to archiving. The Analyst software has the necessary features for creating and maintaining an electronic record system by providing valid electronic records of the acquisition and quantitative processing of data.

The Analyst software is designed to be used as part of a 21 CFR Part 11 compliant system and can be configured to support 21 CFR Part 11 compliance. Whether the use of the Analyst software is 21 CFR Part 11 compliant is dependent on the actual use and configuration of the Analyst software in the lab.

Validation services are available through AB SCIEX Global Services - Regulated and Clinical Markets . For more information, contact complianceservices@sciex.com.

Programs and Utilities

A

The following utility is installed with the Analyst software in the `C:\Program Files (x86)\Analyst\Bin` folder.

Table A-1 Utilities

Program	Description
`Translat.exe`	Utility to convert Agilent data files to the Analyst software data format and Macintosh Library files to the Analyst software library format. Enables creation of databases on SQL Server. Translat.exe does not work over a network for Agilent data.
`CFR_FileCheck.exe`	Utility to rerun the installation qualification test. It is accessible from the Windows Start menu.

Technical Information Regarding Integration   B

Integration Issue Addressed in the Analyst 1.4.2 Software

This issue is found using the manual-parameter portion of the IntelliQuan Algorithm (named MQII). In the MQII portion of the IntelliQuan algorithm, a "Specify Parameters – MQII" mode exists when the **Show /Hide Parameters** button is pressed twice. The issue has only been observed when the "Specify Parameters — MQII" mode has been selected when reviewing the Results Table and the associated Peak Review panes. The results were calculated independently for the two displays and as a result conflicting data is observed.

The noise threshold calculation affects integration. During the process, the chromatogram is first baseline-subtracted. The resulting chromatogram is then used to calculate the Noise Percent: a method of setting the noise threshold by sorting all points by intensity, taking a point at the Noise Percent percentile, and using its intensity level as a basis for the noise threshold.

Normally when the Noise Percent point falls on zero-signal sections of the baseline-subtracted chromatogram, the noise threshold is calculated as zero and the noise percentage (Noise Percent point) is automatically increased to more accurately reflect the noise in the baseline. This results in the noise threshold recalculated to a more appropriate value and a lower peak area. The issue occurs when the Noise Percent point falls on a point with a very small near zero value, a numeric residual left after various numerical conversions and subtraction, that is usually evaluated as zero. In this case, the noise percentage is calculated as a non zero number and is therefore considered valid. The original noise threshold of approximately zero is chosen, instead of increasing the Noise Percent point and recalculating the noise threshold. This results in a near zero baseline and a slightly greater area under the peak being integrated.

The noise threshold value is lower than when the issue does not occur, leading to a higher integration value.

Changes Introduced in the Analyst 1.5 Software

Scheduled MRM algorithm functionality has been added to the Analyst 1.5 software. As part of this functionality, the IntelliQuan integration mode has been adjusted for all integrations to support unequal spacing of data points collected during acquisition. In addition, some smoothing functionality has been updated in response to customer feedback. However, they do have a minor effect on the way in which the area under the curve and peak height are calculated, regardless as to whether the *Scheduled* MRM algorithm functionality is used.

These include:

- Updating the IQA II and MQ III algorithms to use the trapezoidal area-under-the-curve method already used in the software with manual integration.

- In the specific case of smoothing of data with a 5-point smooth or greater (7-point, 9-point, for example), the interaction between the Savitsky-Golay smoothing algorithm and the count values for the peak start and end has been adjusted to correctly account for negative values created by the Savitsky-Golay smooth.

Guidance

- For peaks with > 10 points across the peak, these updates will have minor effect, most likely less than 1%.

- For peaks with < 10 points across the peak, especially when put under a smooth of 5 points or more, the changes should result in a more accurate calculation of the peak area, but the change will most likely be greater than 5%.

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